Setting Up Validation Benchmarks for Deterministic Neutron Transport Methodologies on Fast Reactors

Alex R. Hagen – Purdue University
Micheal A. Smith – Argonne National Laboratory
7/28/2011

ABSTRACT

Setting up Validation Benchmarks for Deterministic Neutron Transport Methodologies on Fast Reactors. ALEX HAGEN (Purdue University, West Lafayette, IN 47906) MICHEAL SMITH (Argonne National Laboratory, Argonne, IL 60439)

The Zero Power Reactor and the Zero Power Plutonium Reactor were critical fast experiment facilities (split bed tube matrix reactors) at the Argonne and Argonne West sites. Because of the number of tests and amount of information gathered in ZPR and ZPPR experiments, data is almost ideal for benchmarking simulations. An integral fast reactor modeling tool has been developed at Argonne National Laboratory as part of the Nuclear Energy Advanced Modeling and Simulation (NEAMS) project. The work described here is to benchmark these tests by focusing on simplified, homogeneous X-Y-Z modeling of PROTEUS (the neutronics component). The first step is to identify the minimal number of unique compositions: each drawer (drawers filled with materials are inserted into each matrix tube). Axially, we find that each drawer is composed of a few unique regions. While each drawer could be treated as unique, a majority of the drawers have roughly the same amount of materials (exceptions can be treated as other bulk drawers). Determining the homogenization scheme accounts for the bulk of the work in creating a model (which must be properly documented). The outcome of building a homogenized model is input for the PROTEUS methodology, which is composed of MC^2-3 (Multigroup Cross section Code v. 3) for generating cross section data and SN2ND (2^{nd} order S_N) for solving the resulting multigroup transport problem. Input for several legacy codes, i.e., PARTISN (PARallel, TIme-Dependent S_N) and DIF3D (diffusion and transport theory codes) is also created. PARTISN is a conventional shielding code produced by Los Alamos National Laboratory. Loadings from various experiments have been set up and homogenized as described above. When running SN2ND using ZPR-6/7 Loading 104, a result of 1.00146 is obtained, which is 74 pcm from experiment and comparable to Monte Carlo results. Also, the results converged with increasing spatial, energy, and cubature resolution, providing good confidence in the result. In the future, the same analysis will be done on ZPR-6/7 Loadings 41 and 34 and ZPPR-21 Loadings B-F. Benchmarking this code would be a major step toward using PROTEUS for reactor design work and would further the multiphysics reactor simulations targeted by NEAMS.

INTRODUCTION

A thrust within Nuclear Engineering and Reactor Physics research is to replace unnecessary or improve experiments with simulations. Because of this thrust, the Department of Energy and Argonne National Laboratory have started development on an integral fast reactor modeling tool under the Nuclear Energy Advanced Modeling and Simulation (NEAMS) project. This modeling tool is intended to integrate neutronics, fluid dynamics, and structural mechanics in a multi-physics coupling framework [1].

Fast reactor technology is not new to Argonne. Argonne has been operating fast critical facilities since the 1950's, with a series of these facilities being designated as the ZPR (Zero Power Reactor) and ZPPR (Zero Power Plutonium Reactor) at the forefront of these studies. The ZPR and ZPPR programs had several different facilities, each with many different loadings (unique sets of materials within the core), and in turn each with numerous experiments. This enormous data bank of experimental data makes the ZPR and ZPPR projects ideal for use in benchmarking a model against experimental data .

ZPR and ZPPR are simply designed fast critical facilities. Two large tables hold the halves of the core (stationary and movable). Each of these halves is made of steel tubes stacked upon each other lengthwise. This creates a square matrix of empty steel tubes whose open faces match up to the other half's matrix when the tables are brought together. These tubes are loaded with drawers. A drawer (shown to the right) is a (generally 48 inch long) steel container that can hold plates of material. Differing plate combinations causes differing drawer compositions and therefore differing loadings. A diagram of the entire facility is shown below [2] [3].

FIGURE 1 PHOTOGRAPH OF DRAWER [12]

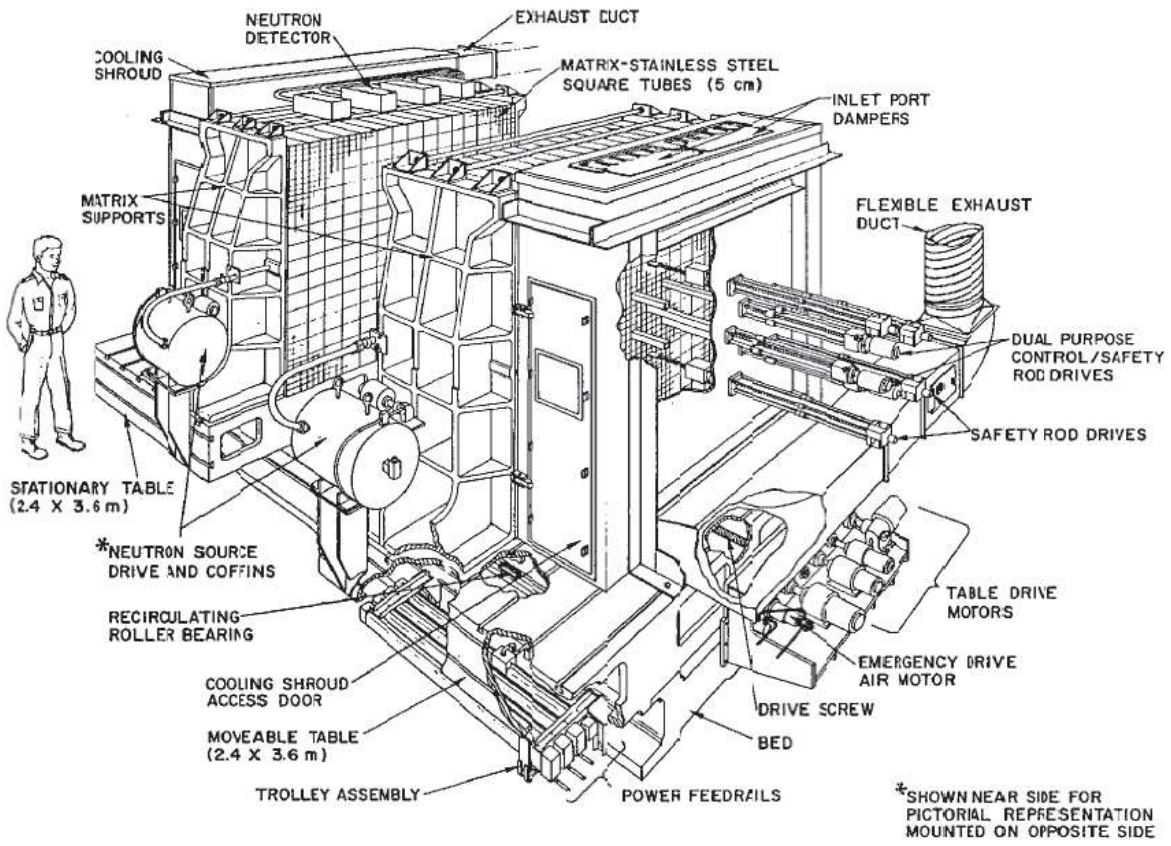

FIGURE 2 ZPR FACILITY DIAGRAM [4]

The NEAMS project has created several of the solver tools and this work is related to the quality assurance procedure of the neutron transport solver. The neutron transport solver of this code is currently being benchmarked by using the wealth of information provided by ZPR and ZPPR. The benchmarking includes comparison to the experiment and code-to-code comparisons with other solvers such as VIM (a Monte Carlo type neutronics code developed by Argonne [5]). Given that the neutron transport solver in NEAMS is deterministic, a detailed energy-angle-space convergence analysis is necessary, an example of which is discussed in this document. This paper describes research on ZPR-6/7 Loading 104 during which detailed radial reaction rate measurements were taken.

MATERIALS AND METHODS

The work described in this paper is focused only on benchmarking the PROTEUS methodology. The PROTEUS methodology includes the creation of cross section data using MC^2-3 (Multigroup Cross section Code version 3) [6] followed by the use of these cross sections and geometry in the SN2ND (2^{nd} Order S_n) neutron transport solver. In order to use this methodology, a geometric model of the experimental setup must be generated by hand. Currently three different simplifications of these models are being analyzed: a two dimensional r-z model (variations only radially and axially), a homogenous x-y-z model (variations in three dimensions, but simplified as specified later in this paper), and a heterogeneous x-y-z model (variations in three dimensions, with all plates included for calculations). This paper describes only results generated using an x-y-z homogenization.

The x-y-z homogenization must be carefully created to ensure a result commensurate with experimental values. The homogenization occurs in two steps: first axially and then throughout the Cartesian grid of drawers (along x and y). Note that in the model, the z axis is axial and runs orthogonal to the plane between the two halves of the facility.

The axial homogenization is reasonably straight forward. In each different drawer, there are generally only several unique compositions. One region, although complex and made of many different plates of Pu, U, etc., may be classified as a "core" region. Using this homogenization, each drawer may be broken into 5 or less axial regions. Generally core, axial blanket, matrix (empty) regions are used, among others.

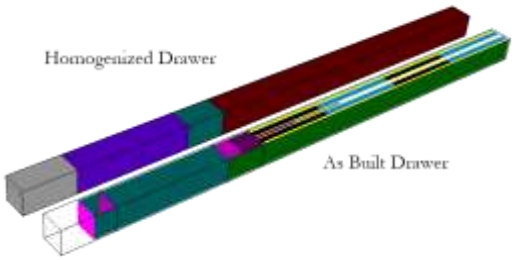

FIGURE 3 AS BUILT VS HOMOGENIZED DRAWER

The Cartesian homogenization is not as simple as the axial homogenization. Because of the size of the Cartesian grid (45 by 45 tubes in ZPR-6/7), many different types of drawers were used in each loading. There are many similarities between many drawers, and as such, each drawer is not treated as unique. As in the axial homogenization, only several regions are defined (such as central core, radial blanket, and matrix). This homogenization is more difficult than the axial homogenization because of certain types of drawers that are included in some loadings. For instance, in ZPR-6/7, thermocouples were included, and some drawers were split in half to accommodate control rods. These drawers would seem as though they should be considered a unique drawer, but to do so would invalidate the assumptions made in the cross section generation step. There are exceptions to this, such as in ZPPR-21, where some drawers include boron. Because boron is a neutron poison, the impact on the final result can be large if these drawers are not properly treated; thus ZPPR-21 has a separate mapping for the borated drawers. The majority of the work is to thoughtfully map drawers to correct regions so as not to force an incorrect result [7].

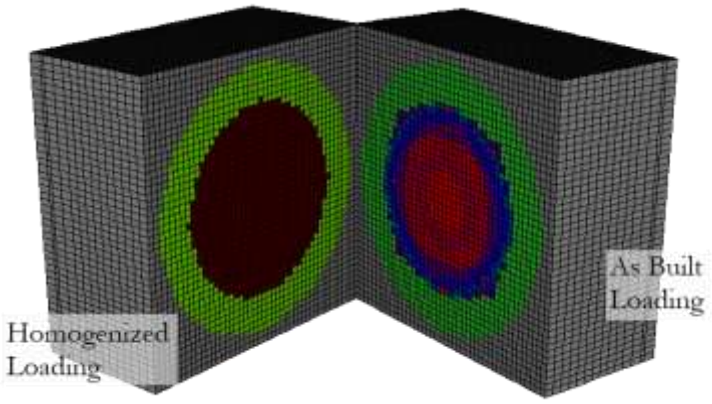

FIGURE 4 CARTESION HOMOGENIZATION OF LOADING 34

After a homogenization model is defined, a utility code is used to create input files for the various neutronics codes. The files of importance for this work are input decks for the $MC^2$3 code, through which a file (ISOTXS) including all the cross sections for all of the specified regions is made; the assignment materials file, which assigns names to the compositions of

regions specified in the model and also colors that will be shown in a visualization; and lastly a geometry or mesh file.

The ISOTXS file has several parameters which must be verified to correctly analyze a loading. First, the number of energy groups must be selected. Three resolutions were chosen for this analysis including 9 groups, 33 groups, and 70 groups. More energy groups will provide a more accurate answer of the problem, but will also require more computing power. The ISOTXS file generated includes all of the isotopes in the homogenized model and their principal cross sections (fission, absorption, etc.) as well as scattering data (group to group scatter probability). The utility code used also generates homogenized mixtures of isotopes with adjusted cross sections for these mixtures.

To simulate the geometry of the loading, SN2ND uses a finite mesh which is generated by the utility code using basic input criteria. A more refined mesh will create a more accurate answer, but can either take longer to calculate or require a more powerful computer. In this analysis, both a linear and quadratic (interpolation order of the finite elements) mesh was generated with a maximum mesh size of 8 cm in the x, y and z direction. The quadratic mesh has more than four times as many vertices as the linear mesh. To test spatial mesh convergence, two refined quadratic meshes were used, one with a maximum mesh size of 4 cm in the x and y directions and 6 cm in the z direction (Refined 1) and another with a maximum mesh size of 2.5 cm in the x and y directions and 4 cm in the z direction (Refined 2).

With these three files, a SN2ND calculation was executed on Fusion, a parallel computing machine hosted by the Leadership Computing Center at Argonne. SN2ND can decompose the problem in both space and angle. The number of processors that SN2ND uses was selected by allocating 4000-8000 vertices per processor and a minimum of 3 angles. To define the angles, cubature on the sphere are used which are designed to exactly integrate the spherical harmonics. As each cubature is refined, the maximum polynomial order of the spherical harmonics that can be integrated increases. A comparison showing the different between Legendre Chebychev cubatures and Carlson equal weight cubatures is shown in Figure 5. In homogeneous reactor problems like ZPR, the selection of the cubature is not that important and thus the Carlson equal weight cubature was used since it results in better asymptotic convergence with respect to angle. If all the above steps are correctly and diligently followed, flux results as well as k-effective eigenvalues can be obtained and analyzed for each loading of a ZPR.Results

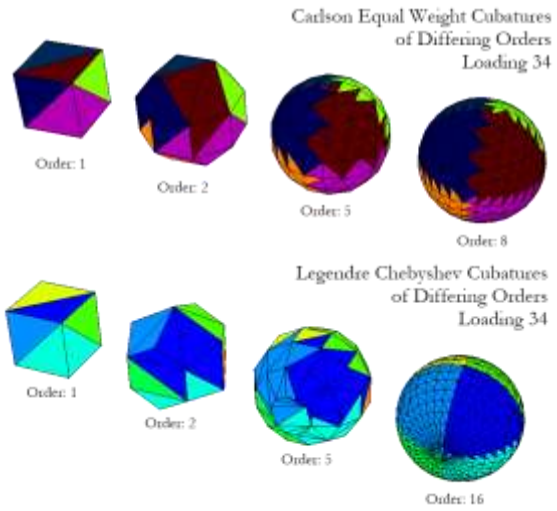

FIGURE 5 COMPARISON OF CUBATURES

Linear and Quadratic meshes were created for Loading 104 of ZPR-6/7. Three standard energy group structures were created including 9 groups, 33groups, and 70 groups. Finally, each of these tests was performed using different resolutions of the Carlson cubature (resolution of cubature, as described above).

Results for these tests all converged, and make physical sense. In general, the results obtained through SN2ND agreed well with the experiment measurement of 1.00072 and are

comparable to Monte Carlo result of 1.00490. A subset of the results obtained with SN2ND are shown in Table 1.

Mesh	9 Group		33 Group		70 Group	
Carlson Order	Linear	Quadratic	Linear	Quadratic	Linear	Quadratic
2	0.999333E-00	1.00085E+00	0.999405E-00	1.00095E+00	0.999912E-00	1.00147E+00
3	0.999330E-00	1.00085E+00	0.999401E-00	1.00094E+00	0.999908E-00	1.00147E+00
4	0.999328E-00	1.00084E+00	0.999399E-00	1.00095E+00	0.999907E-00	1.00146E+00
5	0.999329E-00	1.00084E+00	0.999399E-00	1.00094E+00	0.999907E-00	1.00146E+00

TABLE 1 LOADING 104 RESULTS (PROTEUS METHODOLOGY)

Several trends should be noticed. As the energy resolution is refined, the value calculated tends to get closer to the experimental value. The quadratic mesh with Carlson resolution 5 shows an increase of 10 pcm from 9 groups to 33 groups, and of 52 pcm from 33 groups to 70 groups, evidence of the effect of mesh refinement. This same trend can be noticed for cubature refinement, although only on the order of 1 or 2 pcm (the quadratic mesh with 70 groups decreases 1 pcm from Carlson resolution 2 to 5). Finally, the geometric mesh refinement shows the most defined increase in accuracy. In general, the linear results are over 1000 pcm away from the experimental value and their respective quadratic results. To further show mesh refinement, the 9 group, 5^{th} resolution of Carlson results are shown below with four different meshes (details for Refined Meshes can be found in the Methodology section).

Mesh	Linear	Quadratic	Quadratic Refined 1	Quadratic Refined 2
Carlson Order				
5	0.999329E-00	1.00084E+00	1.00093E+00	1.00094E+00

TABLE 2 LOADING 104 9 GROUP MESH REFINEMENT RESULTS

The power profile along a radius is shown below. This power profile clearly shows the maximum power at the centerline of the facility, with decreasing power towards the outside of

the reactor. Several key components, such as the "cliff" created by the edge of the inner core (a high Pu240 zone), and the "jump" created in the reflector are apparent in Figure 6.

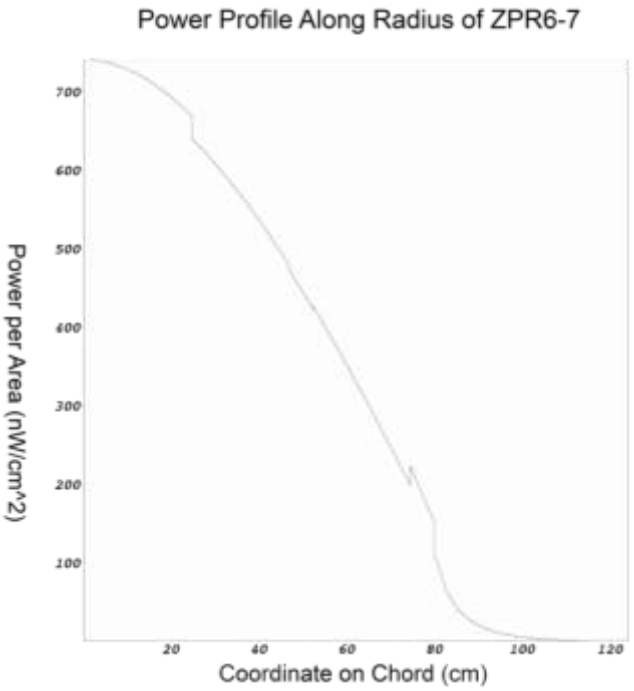

FIGURE 6 POWER PROFILE ALONG RADIUS OF ZPR-6/7

The following set of figures displays the convergence of the solution with respect to cubature resolution, spatial mesh, and energy groups. The central chord plots were created by sampling a line that stretched along a chord of the highest power region (not a radius to avoid the fission chamber in the middle of the reactor), and the reflector region plots were taken from a section of the radius from 39 cm to 54 cm on the Power Profile shown above (intersecting the reflector region). As is apparent in each figure, convergence does occur throughout each variable's trace. In energy convergence, it is obvious that the difference between the 70 group and 33 group results is smaller than that between 33 group and 9 group, even though the change in resolution is greater. The same is true of the most refined mesh: the refined 2 mesh is closer to refined 1 mesh than refined 1 mesh is to the unrefined quadratic mesh. In angle, the difference between each resolution decreases; e.g. the difference between the 5^{th} and 4^{th} resolution is much

smaller than the difference between the 3rd and 2nd resolution. These plots give another check (besides only eigenvalue convergence) to the convergence with increasing resolution in these three variables (cubature order, energy resolution, and spatial resolution).

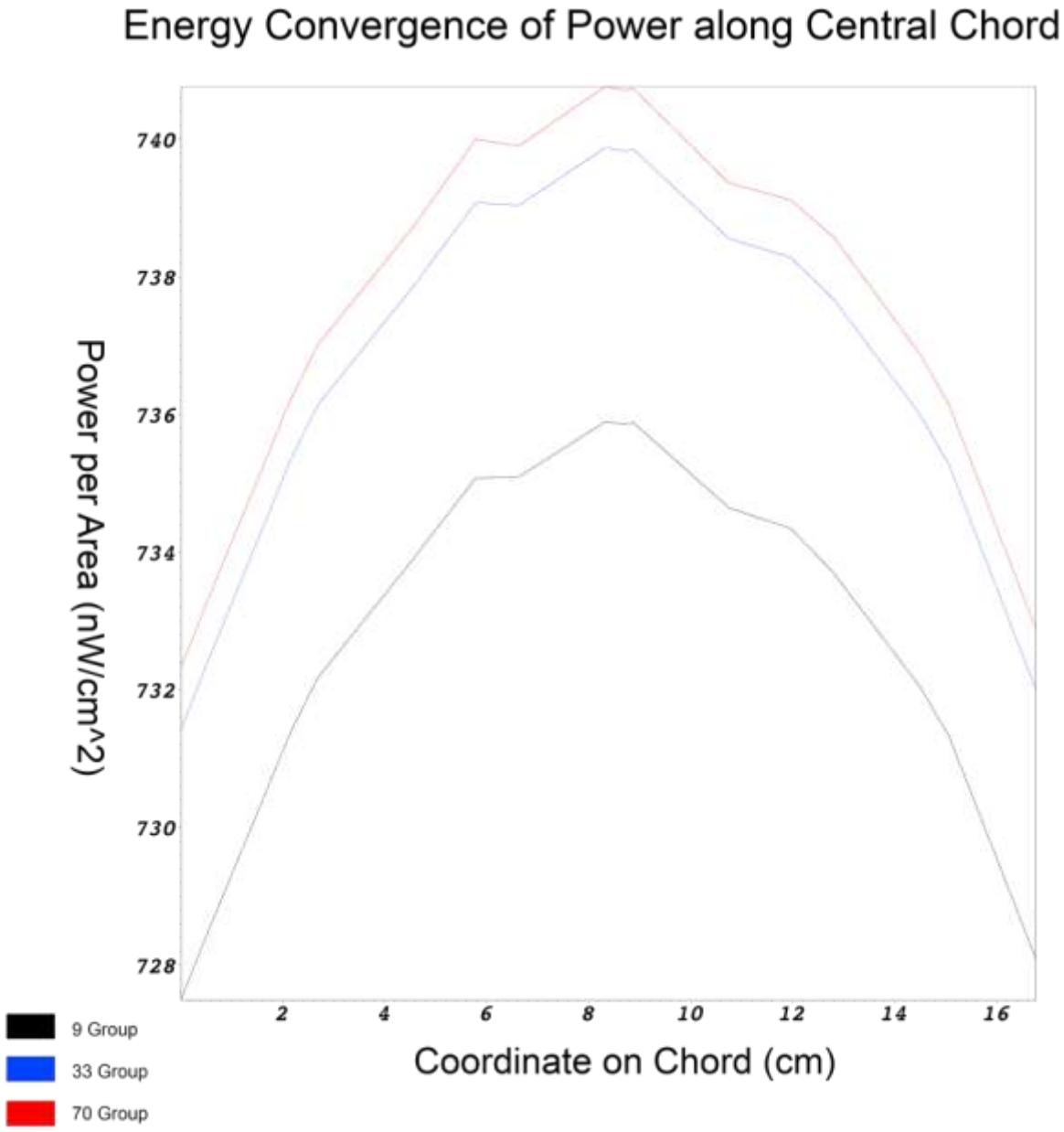

FIGURE 7 ENERGY CONVERGENCE OF POWER ALONG CENTRAL CHORD

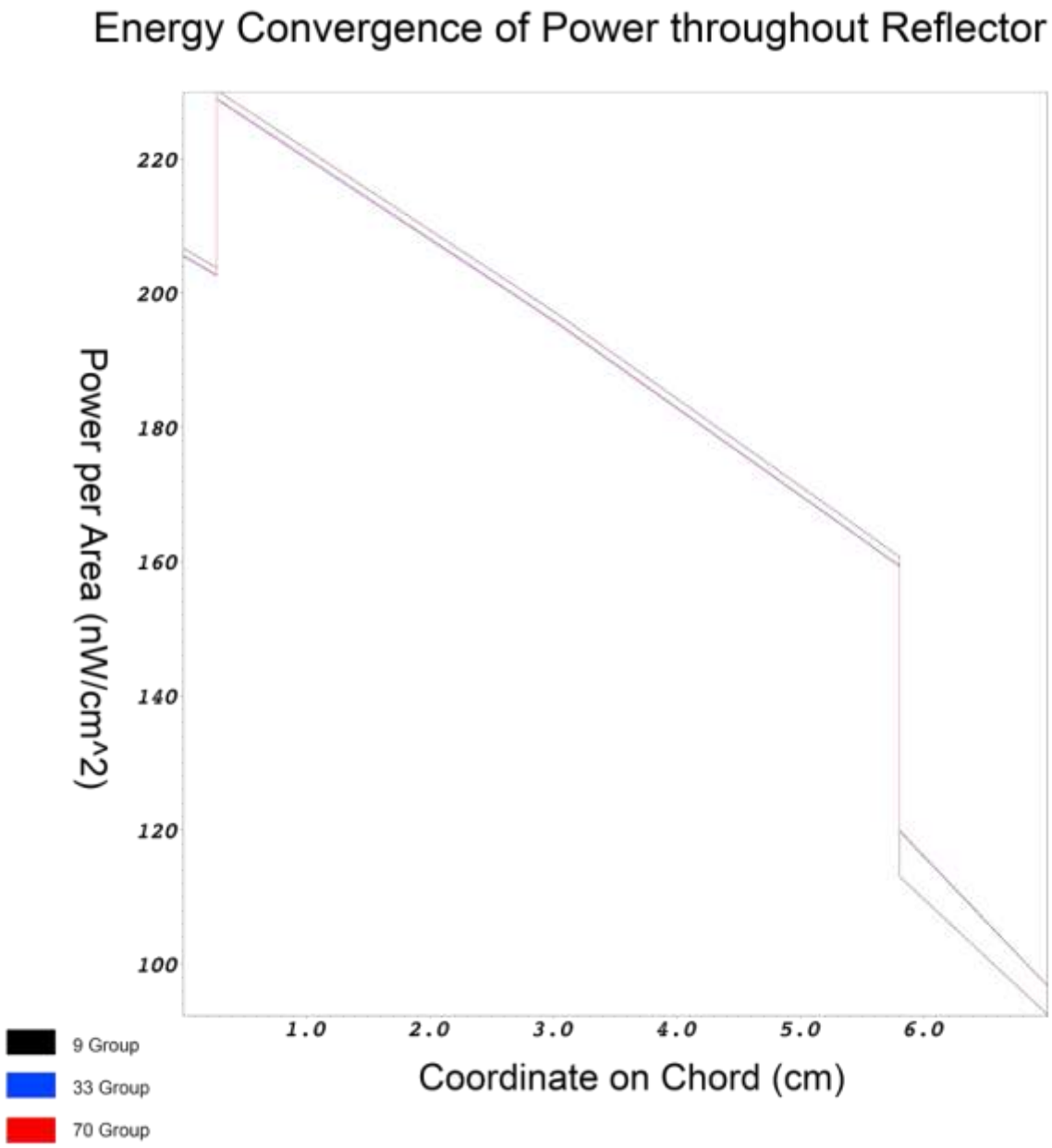

FIGURE 8 ENERGY CONVERGENCE OF POWER THROUGH REFLECTOR

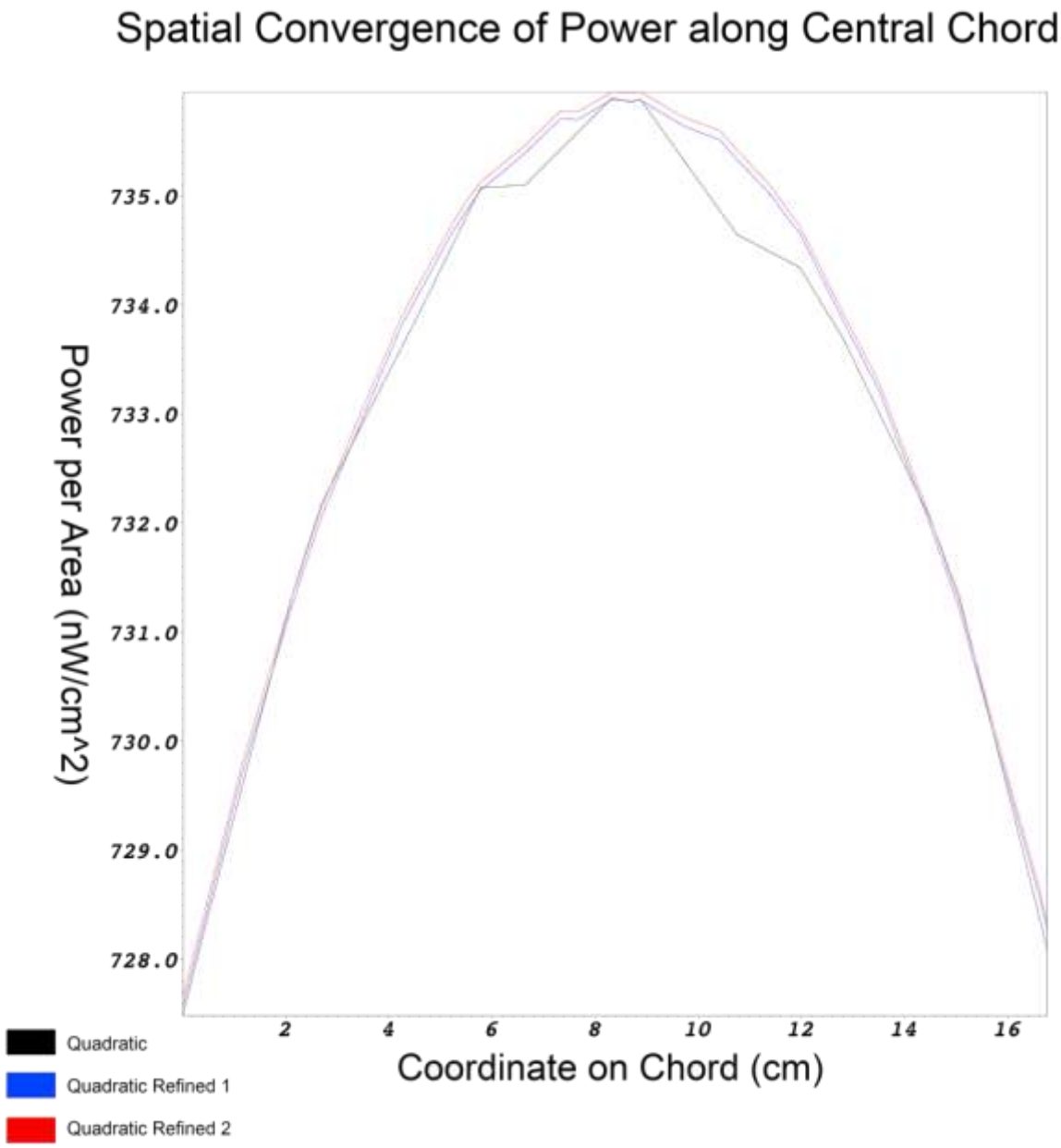

FIGURE 9 SPATIAL CONVERGENCE OF POWER ALONG CENTRAL CHORD

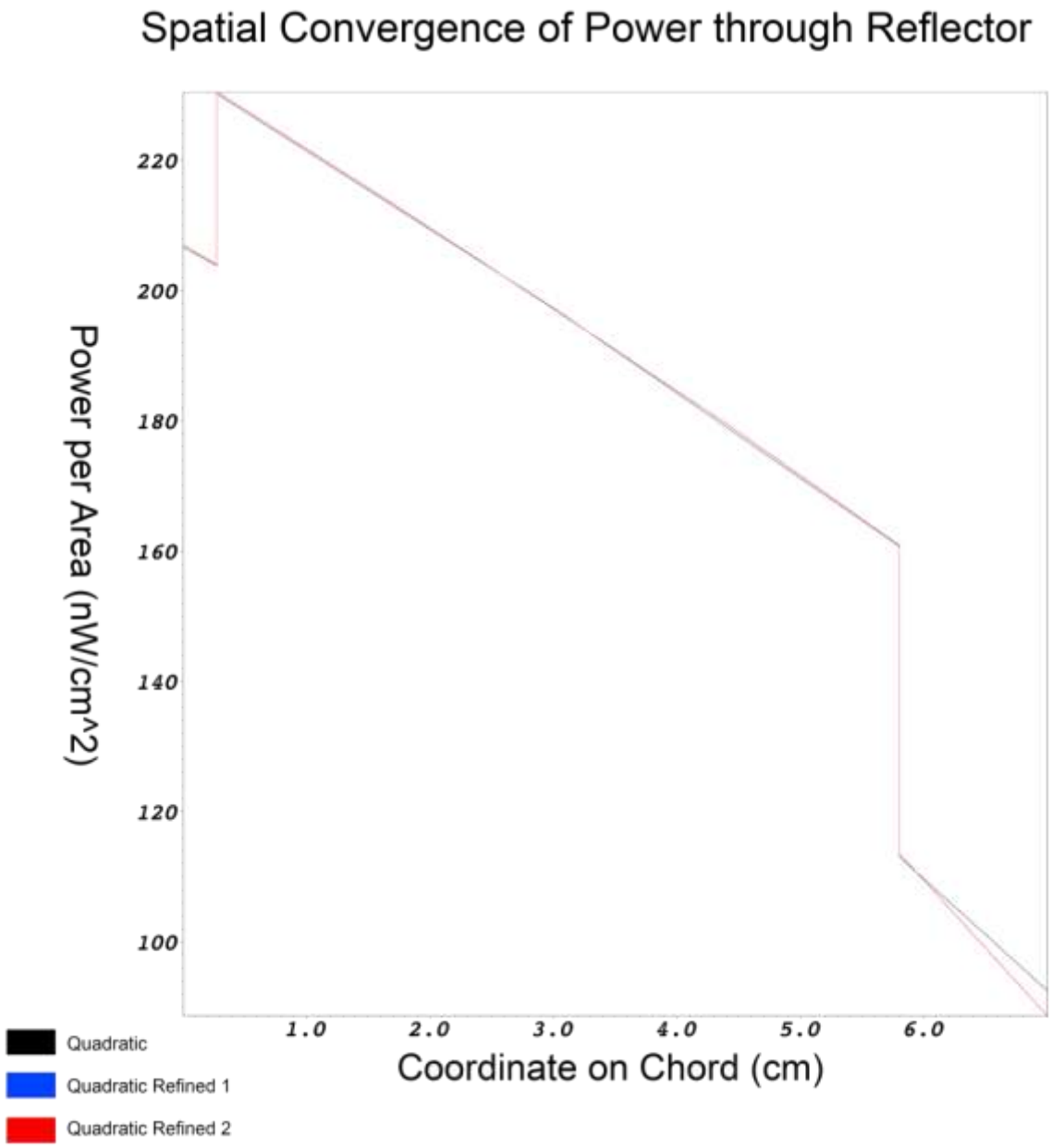

FIGURE 10 SPATIAL CONVERGENCE OF POWER THROUGH REFLECTOR

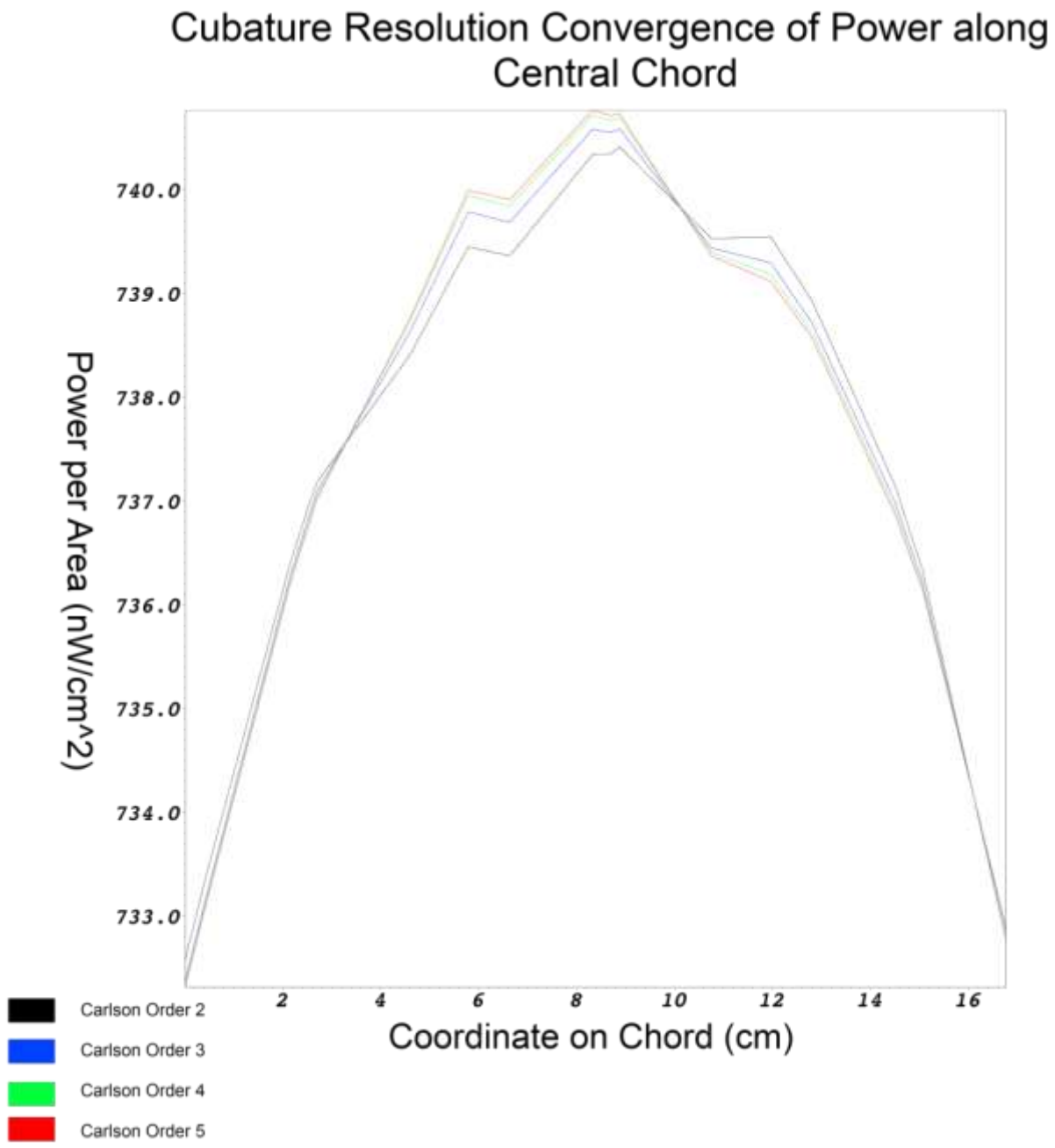

FIGURE 11 CUBATURE RESOLUTION CONVERGENCE OF POWER ALONG CENTRAL CHORD

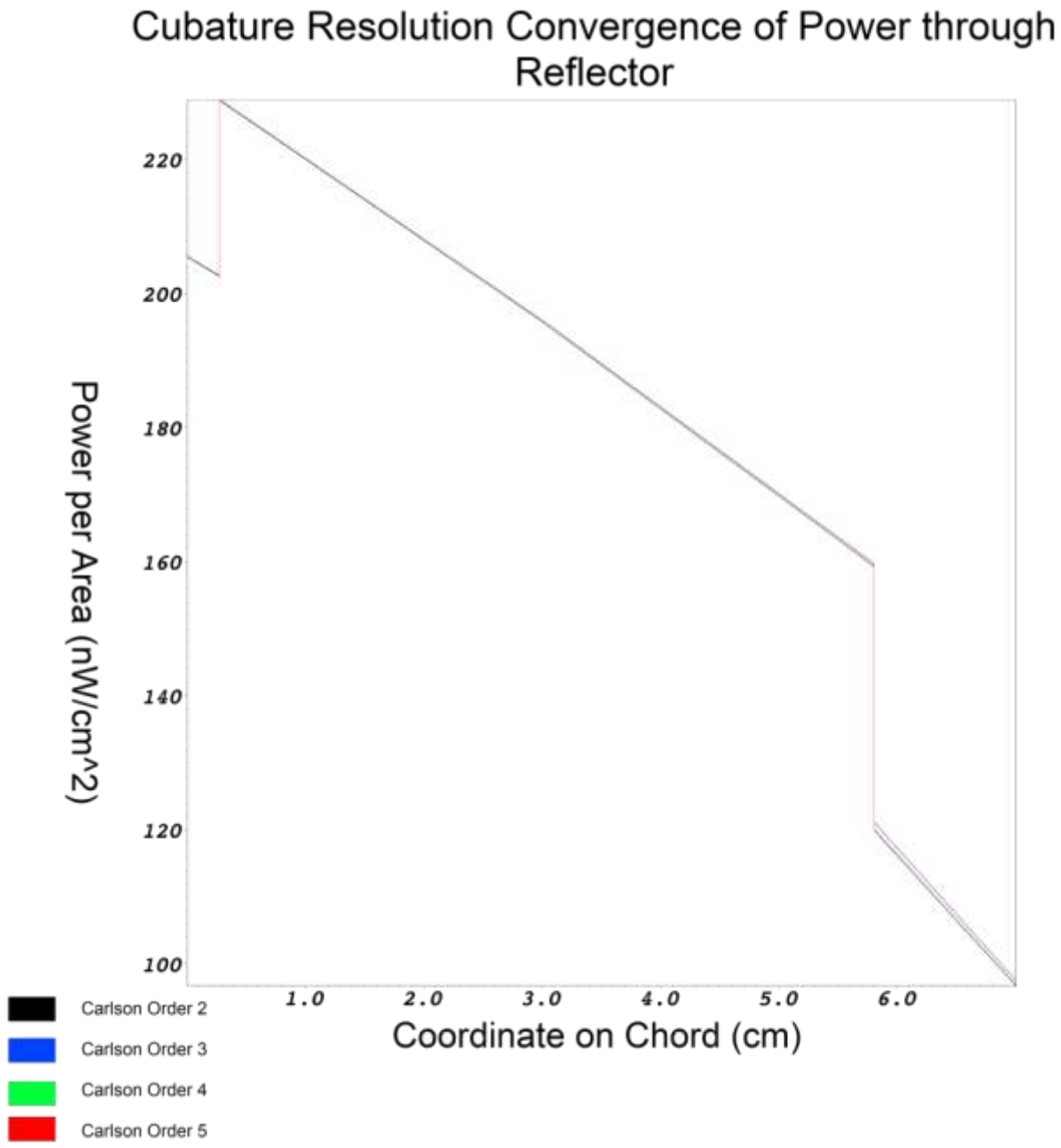

FIGURE 12 CUBATURE RESOLUTION CONVERGENCE OF POWER THROUGH REFLECTOR

CONCLUSION

Generally, the first step to benchmarking results obtained from the PROTEUS methodology is to compare the results to detailed experimental measurements. PROTEUS does well in this analysis, with the 70 group, quadratic, 5^{th} resolution of the Carlson cubature result (1.00146) only 74 pcm from the experimental value (1.00072) and comparable to VIM result (1.00490) [2].

The next step is to verify convergence along spatial refinement, energy refinement, and cubature refinement. As shown, the eigenvalues barely change with refinement of the angular cubature, which is indicative of convergence. Between linear and quadratic meshes, convergence in spatial refinement is not immediately obvious, however, when the mesh was refined further, convergence was clearly observable. Finally, energy group refinement shows a convergence trend, but more energy groups is known to be necessary to obtain full convergence. These quick analyses give added confidence in the result obtained by PROTEUS.

A more in depth analysis of convergence can be done by looking at specific power values and comparing these profiles to see convergence. This analysis was done in two different locations (a chord through the highest power region of the reactor, and a radius through the reflector region of the reactor) for each different variable (cubature resolution, spatial resolution, and energy resolution). In all three cases, the profiles began to converge at the highest resolution. This provides proof that the solution is converging towards an accurate and physical result.

Through the analyses described above, it is apparent that the model created does converge to an accurate result. Several things are of note: that homogenization did not cause a large departure from the experimental result, that resolution was important (cubature, spatial, and energy) even though the model had been homogenized. In follow on work, ZPPR-21, a set of loadings with varying ratios of Uranium and Plutonium, will be analyzed to benchmark the code through this range of compositions and reactor type. Also, with ZPPR-21, the effects of modeling the surrounding environment versus using an artificial boundary will be analyzed. Benchmarking PROTEUS with calculations like these is a continuous process of providing confidence to users for routine fast reactor design and analysis work in addition to achieving the multi-physics reactor simulation goal targeted by NEAMS [1].

ACKNOWLEDGEMENTS

Many entities contributed to the research done at Argonne National Laboratory throughout the summer of 2011 (June-August) that is described within this report. At the highest level, the Department of Energy and Argonne National Laboratory (Department of Educational Programs) have provided the opportunity and funding for the research done. Within the laboratory, the entire NE (Nuclear Engineering) division should be acknowledged, with special thanks to Amr Mohammed and Chang-ho Lee for their help and guidance with SN2ND analysis and MC^2-3, respectively. Finally and most importantly, Micheal Smith should be acknowledged for the daily help he provided, and the numerous debugging sessions he engaged in that made the research done possible and accurate.

BIBLIOGRAPHY

[1] Argonne Leadership Computing, "Scalable, Explicit Geometry, Whole-Core Nuclear Reactor Simulations," *Argonne Leadership Computing Facility: 2010 Science Highlights*, p. 26, November 2010.

[2] Richard M Lell, James A Morman, Robert W Schaefer, and Richard D McKnight, "ZPR-6 Assembly 7 Experiments: A Fast Reactor Core with Mixed (Pu,U)-Oxide Fuel and Sodium with a Thick Depleted Uranium Reflector," Argonne, IL, 2008.

[3] Richard D McKnight, Richard M Lell, Robert W Schaefer, and Amr Mohamed, "ZPPR-21 Phases B Through E: Cylindrical Assemblies of Mixed Fissile Pu and U Metal Reflected By Graphite," Argonne, IL, 2001.

[4] L. G. LeSage, "An Overview of the Argonne National Laboratory Fast Critical Experiments 1963-1990," Argonne, IL, 2001.

[5] Roger Blomquist. (2009, March) VIM Monte Carlo Neutron/Photon Transport Code. [Online]. www.vim.anl.gov/index.html

[6] C Lee and W S Yang, "Development of Multigroup Cross Section Generation Code MC^2-3 for Fast Reactor Analysis," in *International Conference on Fast Reactors and Related Fuel Cycles*, Kyoto, Japan, 2009.

[7] C B Carrico, E E Lewis, and G Palmiotti, "Three Dimensional Variational Nodal Transport Methods for Cartesian, Triangular and Hexagonal Criticality Calculations," *Nucl. Sci. Eng.*, no. 111, p. 168, 1992.

[8] Ray E Alcouffe, Randal S Baker, John A Dahl, Scott A Turner, and Robert C Ward,

"PARTISN: A Time-Dependent, Parallel Neutral Particle Transport Code System," Los Alamos, NM, 2008.

[9] Alex Hagen, "ZPR-6/7 Loading 41 Model Summary," Argonne, IL, 2011.

[10] Masood Iqbal, Hany Abdel-Khalik, and Paul Turinsky, "A comparative study of ZPR-6/7 with MCNP/5 and MC2-2/REBUS," *Annals of Nuclear Energy*, no. 36, pp. 995-997, 2009.

[11] Micheal A Smith et al., "Recent Research Progress on UNIC at Argonne National Laboratory," in *International Conference on Mathematics, Computational Methods & Reactor Physics*, Saratoga Springs, New York, 2009.

[12] Amr Mohammed, Won Sik Yang, Micheal Smith, and Chang-ho Lee, "Analysis of Reaction Rate Distribution Measurement in ZPR-6 Assembly 7 COres with MC2-3/UNIC Code System," in *International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering*, Rio De Janiero, 2011.

[13] Argonne National Laboratory. (1968, February) Photograph of ZPR Facility. Photograph. [Online]. Argonne Intranet