FEASIBILITY INVESTIGATION OF APPLICATION OF MPACT TO CORE DESIGN STUDIES OF NBSR-2, A HEAVY WATER-REFLECTED, HETEROGENEOUS LEU FUEL RESEARCH REACTOR

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ABSTRACT

Engineers at NIST would like to use the VERA software suite developed by CASL to study a new 20 MW research reactor design called NBSR-2, which uses heterogeneous MTR-type LEU fuel plates, a light water coolant, and a heavy water reflector. These features are a significant departure from the PWR-type power reactors previously benchmarked in VERA. Comparable 2-D models of NBSR-2 were developed in both MPACT and MCNP6, and the MPACT model was benchmarked to within 120 pcm (1 pcm = 10^{-5} $\Delta k/k$) and 1.5 % mean error in fast and thermal flux distributions. This work is intended to facilitate additional design studies of NBSR-2 with VERA software in the future, and to assess the maturity of MPACT's ability to model non-PWR reactors.

Key Words: **MPACT Validation MCNP, NBSR-2, Cold Neutron Source.**

1. INTRODUCTION

The Michigan PArallel Characteristics Transport (MPACT) [1] is a core neutronics program currently under development at University of Michigan and Oak Ridge National Laboratory for the Virtual Environment for Reactor Applications (VERA) package [2], in support of the Consortium for Advanced Simulation of Light-water Reactors (CASL) initiative. MPACT is designed to provide core-wide, pin-resolved power distributions for use in other VERA physics packages such as thermal hydraulics modules and material performance. MPACT obtains the neutron flux distribution in the reactor using a method of characteristics (MOC) algorithm, a deterministic method that uses modular ray tracing to solve the Boltzmann transport equation. In addition to eliminating the need for a random number generator, this MOC makes the code scalable to large, sophisticated systems. MPACT has previously been successfully benchmarked against Watts Bar Nuclear 1 [2], and the BEAVRS benchmark [3]; however, MPACT currently is not as well validated for designs outside this working scope.

The National Bureau of Standards Reactor (NBSR) is an operational test reactor used for public research at the NIST Center for Neutron Research (NCNR), a division of the National Institute of Standards and Technology that hosts 2,000 guest researchers each year. The NBSR has been the primary neutron source for the NCNR since its commissioning in 1967, but due to relicensing limitations and non-proliferation concerns a new LEU reactor, NBSR-2, is being designed to replace it. The new design utilizes heterogeneous fuel plate geometry, a heavy water reflector, and a weakly coupled horizontal split core configuration. In the last two years the Monte-Carlo based MCNP6 code has been intensively employed as the sole reactor physics tool for core design [4], and the NBSR-2 design team has great interest in further studies of core performance using advanced deterministic methods, which are preferable for fuel cycle analysis.

This paper describes preliminary benchmarking work using MPACT to perform physics calculations for NBSR-2, in which basic core performance characteristics were generated and compared against the results from an MCNP model. The main purpose of this study is to assess the feasibility of applying MPACT to a heterogeneous compact research core in preparation for potential future depletion and thermal hydraulics calculations with VERA. The results presented in the paper can also be used to gauge the applicability of the MPACT to similar research reactors.

2. PROJECT SCOPE AND METHODOLOGY

2.1. Description of MPACT

In MOC, a series of angular sweeps is performed over discrete ordinates in several geometric modules provided by the user, and the cross sections are calculated with local conditions in a discrete sub-mesh and applied to solve the Boltzmann transport equation (BTE). The system k_{eff} is calculated iteratively from the BTE and a given scattering order by systematically incrementing the neutron flux and checking for convergence. However, the BTE is non-linear because the cross sections for the user-defined geometry vary with the neutron flux distribution. Furthermore, when thermal hydraulic feedback is present each material constituent has a different energy-dependent cross section, so after every iteration all materials must be re-weighted against a new flux energy distribution. To simplify the BTE calculations in MPACT, the coarse mesh finite difference (CMFD) algorithm is used. In CMFD the flux is averaged over a series of discretized regions “j” to compute cell-averaged parameters. For example:

$$\bar{\Sigma}_{s,j,g} = \frac{\sum_{i\in j} \Sigma_{s,j,g}\, \Phi_{i,g}\, V_i}{\sum_{i\in j} \Phi_{i,g}\, V_i}\ , \qquad \bar{\Phi}_{j,g} = \frac{\sum_{i\in j} \Phi_{i,g}\, V_i}{\sum_{i\in j} V_i}\ , \qquad \text{and} \qquad \bar{\chi} = \frac{\sum_{i\in j} \chi_{i,g}\, \Sigma_{f,j,g}\, \Phi_{i,g}\, V_i}{\sum_{i\in j} \Sigma_{f,j,g}\, \Phi_{i,g}\, V_i}\ .$$

The flux-weighting method described above uses a volumetric integration that conserves the cell-averaged reaction rates, but it neglects the spatial distributions within the cell, and so fails to preserve the leakage rates at the cell surfaces. CMFD corrects for this by using a radial coupling coefficient, $\widehat{D}_{j,g,s}$, on each cell’s surface to maintain equivalent leakage rates across their shared boundaries, such that:

$$\widetilde{D}_{j,g,s} = \frac{2\overline{D}_{j,g}\overline{D}_{j(s),g}}{h_{j,s}\overline{D}_{j,g} + h_{j(s),s}\overline{D}_{j(s),g}}$$

$$\widehat{D}_{j,g,s} = \frac{\bar{J}_{j,g,s}^{net} + \widetilde{D}_{j,g,s}\left(\bar{\Phi}_{j,g} - \bar{\Phi}_{j(s),g}\right)}{\left(\bar{\Phi}_{j,g} + \bar{\Phi}_{j(s),g}\right)}$$

$$J^{net}_{j,g,s} = -\widetilde{D}_{j,g,s}\left(\overline{\Phi}_{j,g} - \overline{\Phi}_{j(s),g}\right) + \widehat{D}_{j,g,s}\left(\overline{\Phi}_{j,g} + \overline{\Phi}_{j(s),g}\right)$$

Depending on the input geometry, in MPACT this form of synthetic acceleration can reduce the number of BTE iterations required for convergence by an order of magnitude or more.

2.2. Description of Benchmark: NBSR-2

In recent decades cold neutron research has dominated the use of the aging NBSR facility, so the cold neutron yield is one of the most important metrics of NBSR-2's performance. The new vessel will extend 2.5 m in diameter and 2.5 m in height, and contain 18 MTR-type, 17-plate fuel elements with LEU U_3Si_2-Al fuel in a horizontally split core arrangement and a three-cycle burnup configuration as shown in Figure 1. In this new configuration the fuel elements are cooled and moderated by a light water coolant, while the vessel is filled with a heavy water reflector; and the two liquids are separated by zircalloy fuel boxes that surround the assembly groupings. A more detailed description of the NBSR-2 design can be found in Ref. 4.

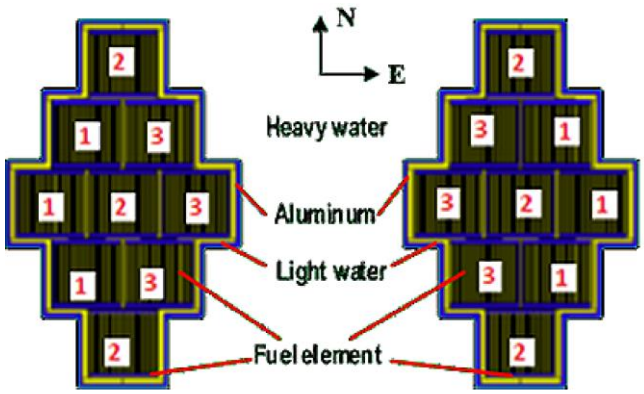

Figure 1. The current NBSR-2 core configuration.

Not pictured in Figure 1, two cold source cryostats filled with liquid deuterium will be positioned to the north and south along the vessel centerline, between the two horizontal core halves. The thermal efficiency of these cryostats is maximized when the kinetic energy of the incoming neutrons is minimized, and the horizontally split core configuration of NBSR-2 has been shown using MCNP6 to optimize the fast and thermal flux profiles at these sites, as seen in Figure 2 [4]. It is desirable to confirm these stochastic calculations with a deterministic method; however, the heterogeneous nature of the MTR assembly has historically proven challenging for traditional LWR tools like CASMO [5] and NEWT [6]. The confirmation method selected should be readily coupled to a thermal hydraulics package and capable of performing high resolution burnup calculations, and should represent the state of the art in neutronics simulation. MPACT is a modern neutronics code that currently meets these criteria – for PWRs.

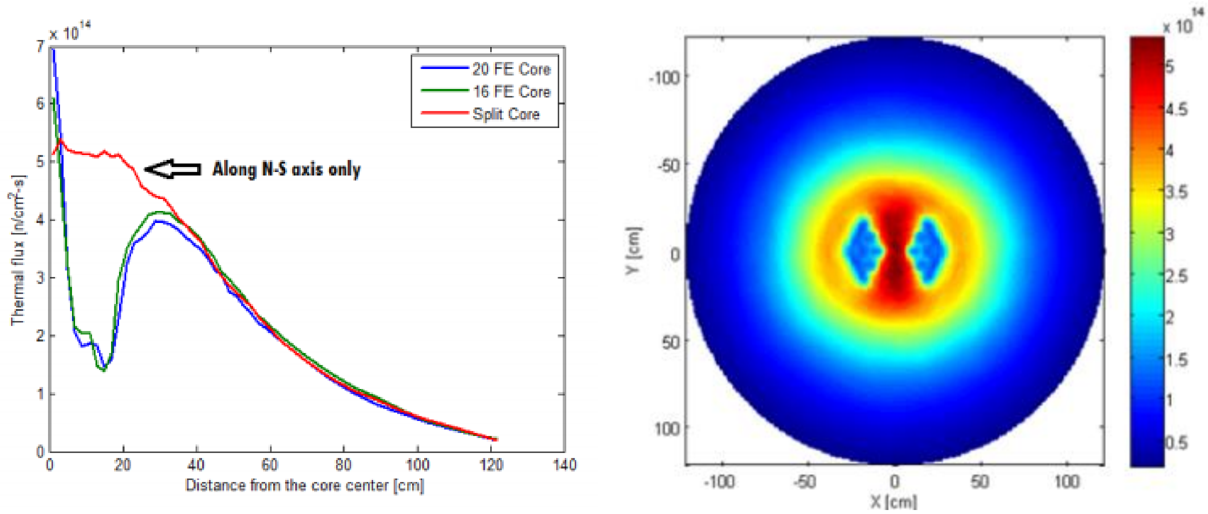

Figure 2. MCNP6 calculations for the thermal flux profile in NBSR-2 along the cryostat axis.

2.3. Modeling NBSR-2 in MPACT

MOC is conveniently implemented over equally sized geometry “modules” that comprise 2-D/1-D lattices in the core. To conserve time and especially memory, in MPACT ray tracing is performed only once for each unique geometric module regardless of how often it is repeated in the core. It is therefore prudent to design a model that utilizes as much repetitive geometry as possible. Additional performance increases are possible through the use of reflective boundary conditions along lines of core symmetry; in MOC, such conditions reduce the number of core calculations by powers of 2. However, in NBSR-2 the use of core symmetry requires halved or quartered modules, increasing the total number of ray tracing data to be stored in memory.

In this project each fuel element was modeled with four quarter-element modules, which allowed for placement in the horizontally staggered rectangular arrangement used in NBSR-2, and the use of symmetry along the south and east faces. Since NBSR-2 uses a 3-stage fuel cycle, a total of 12 unique modules were required to accurately represent the 18 fuel elements in the core. Additional modules were used to construct the zircaloy-2 walls and D_2O moderator. The submeshing used in the element modules averaged about 240 cells/cm^2. Figure 3 is a comparison of the final geometry inputs rendered from the MPACT and MCNP6 input files.

One significant limitation of geometry modeled in MPACT is that the split core gap was required to be a modulus of the module size. For the 4.1 cm × 4.0 cm modules used to maximize repeatability, this required an element gap of 16.4 cm, compared to the 20.5 cm gap used in the reference design. The MCNP model was adjusted accordingly for benchmarking, but this is an unnecessary constraint to the positioning of the cold source cryostat.

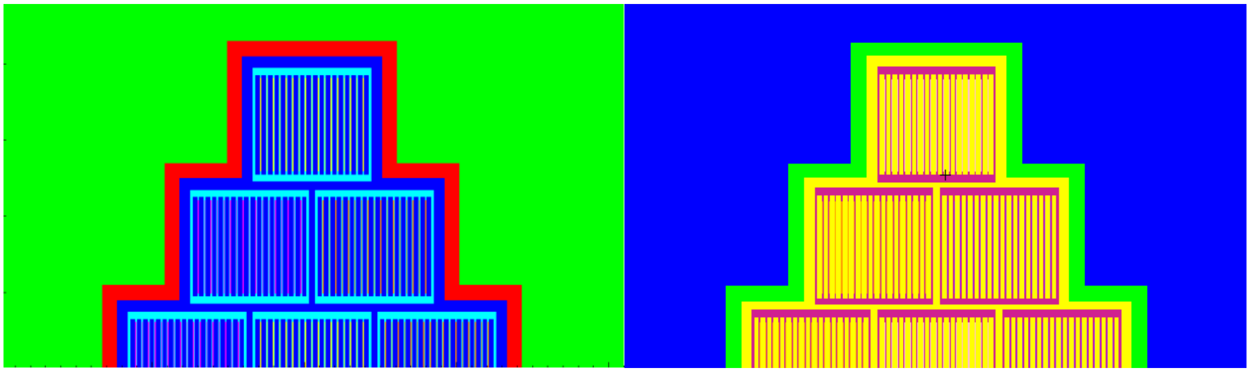

Figure 3. MPACT (left) and MCNP (right) models of NBSR-2 as rendered in VisIt and Xming, respectively. Reflective symmetry is observed along the right and bottom boundaries in each model.

A second limitation of MPACT is the processing time; thus for this feasibility study, the models were limited to 2-D cores with reflective top and bottom boundaries. In preparation for future 3-D analyses, a second model (hereafter referred to as the reduced model) was constructed with the reflector reduced from a total core volume of 11,480 cm^2 to just 984 cm^2. If the effect of this approximation is small and consistent, the pace of MPACT calculations can be reduced from hours to minutes.

3. RESULTS

3.1 Validating MPACT against MCNP6

Two important neutronics benchmarks for any research reactor are the core k_{eff} and the spatial scalar flux distribution in the core. The core k_{eff} is the eigenvalue of the Boltzman transport equation for a given core geometry, including boundary leakage. As shown in Table 1, the eigenvalues calculated by MPACT and MCNP6 corroborated within 120 pcm and 170 pcm (1 pcm = 10^{-5} $\Delta k/k$) for the full and reduced models respectively, indicating reasonably strong agreement between the two codes.

Table 1. Comparison of k_{eff} results from MPACT and MCNP.

	MPACT	MCNP	Disagreement (pcm)
Full model	1.2227606	1.22456 ± 0.00047 (1-σ)	-120
Reduced model	1.0048021	1.00312 ± 0.00060 (1-σ)	+170

To compare flux distributions, an FMESH spatial distribution tally of scalar flux was generated in MCNP6 in 0.1 cm^2 cells over a pre-determined region, and the cell-averaged flux results from MPACT were collected from the same area. To match the energy group structure of MPACT's cross section library, in MCNP6 the fast neutron spectrum was defined between 20 MeV and 0.625 eV, and the thermal neutron spectrum was less than 0.625 eV. All datasets were normalized to a peak total flux of 5×10^{14} cm^{-2}-s^{-1}, an anticipated value for this design.

Excellent qualitative visual agreement was observed between MPACT and MCNP for the fast and thermal flux distributions, as shown in Figure 4. In both figures the effect of the MTR fuel plates on flux distributions is clearly visible, indicating that the heterogeneous plate fuel geometry is being modeled correctly. As expected, the MPACT spectra appear smoother than their MCNP counterparts by nature of their deterministic computation, and thus present a higher degree of confidence when sampling individual points. This is naturally advantageous when performing design work.

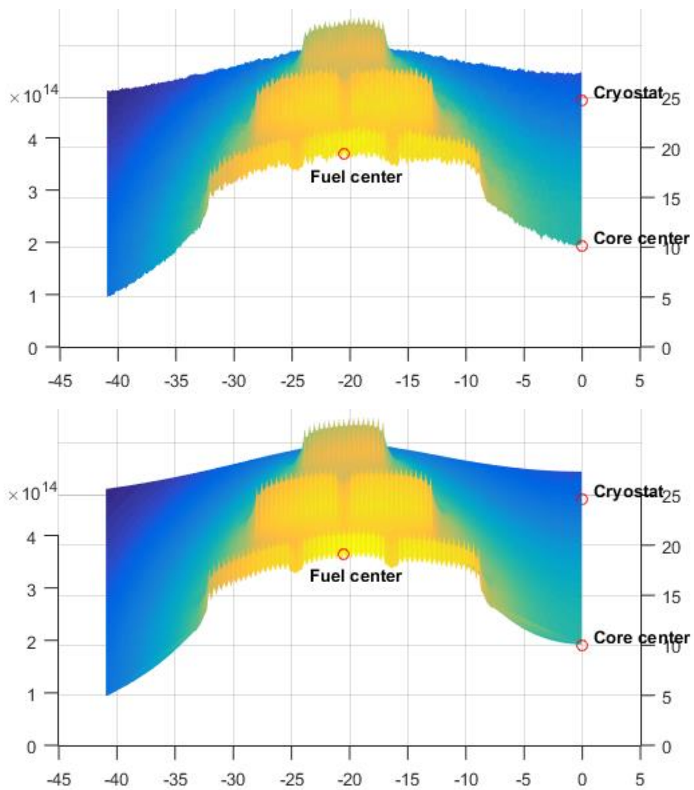

Figure 4. Fast flux in MCNP (top) and MPACT (bottom) with the full reflector model.

To evaluate the spectra quantitatively, each of the 98,400 MCNP6 FMESH nodes were compared to the nearest equivalent MPACT node (of 1,173,556 available). Using the full reflector model, the mean absolute difference of MPACT relative to MCNP6 was 2.1 % ± 1.7 % (1-σ) for the fast flux spectrum, and 0.9 % ± 1.7 % (1-σ) for the thermal flux spectrum. The differences in the reduced model averaged 2.5 % ± 2.1 % (1-σ) and just 0.2 % ± 2.6 % (1-σ), respectively. Three key points (indicated by red circles in Figure 4) were identified to represent the spectra; these data are summarized in Table 2.

3.2 Analysis of NBSR-2 Design Using MPACT

The single most important metric for NBSR-2 is the thermal-to-fast neutron ratio at the site of the cryostat, as this metric controls the ratio of beam brightness vs heat load. For the full reflector model, MPACT calculated a thermal-to-fast neutron ratio of 5.60 at this site – closely matching the MCNP6 prediction of 5.63. The thermal neutron flux at the center of the fuel cluster is also of considerable importance, as it drives the total fission density in the fuel and thus defines material and thermal hydraulic limits; MPACT predicted 7.20×10^{13} cm^{-2}-s^{-1}, compared to 7.33×10^{13} cm^{-2}-s^{-1} in MCNP6. Finally, the core center is of academic interest given the uncommon split-core configuration; MPACT returned a fast flux of 1.91×10^{13} cm^{-2}-s^{-1} against MCNP6's 1.94×10^{13} cm^{-2}-s^{-1}. The reduced model produced similar agreement, yielding strong proof of MPACT's merit in benchmarking test reactors like NBSR-2. The additional benchmarking and comparison calculations described in Table 3 likewise indicate excellent agreement between the two codes.

Table 2. Scalar flux at select points in the full and reduced NBSR-2 models.

Location	MPACT		MCNP		MPACT (Reduced)		MCNP (Reduced)	
	Fast Flux	Th Flux	Fast Flux	Th Flux	Fast Flux	Th Flux	Fast Flux	Th Flux
Core Center	1.91E+14	4.64E+14	1.94E+14	4.69E+14	3.61E+14	5.81E+14	3.63E+14	5.91E+14
Fuel Center	3.65E+14	7.20E+13	3.69E+14	7.33E+13	7.72E+14	1.41E+14	7.77E+14	1.41E+14
Cryostat	8.83E+13	4.94E+14	8.93E+13	5.02E+14	1.11E+14	2.14E+14	1.17E+14	2.18E+14

Table 3. Select scalar flux ratios averaged across the full and reduced models.

Location	Thermal-to-Fast ratio		MPACT-to-MCNP ratio	
	in MPACT	in MCNP	for fast n's	for thrml n's
In the reflector	2.8898	2.8858	0.9816	0.9851
In the fuel	0.1900	0.1903	0.9918	0.9909

It was desirable to review the optimization of the cryostat placement with the high fidelity data available from MPACT, in order to (1) assess the feasibility of design work with MPACT, and (2) verify the optimization itself. The peak thermal flux along the vertical centerline was determined to occur at 18.5 cm, and the thermal-to-fast flux ratio at that point was 5.07. However, Figure 5 shows that the thermal flux is nearly constant in this region, while the thermal-to-fast flux ratio increases markedly over the same space. This suggests that the cryostat could be placed several centimeters further from the core centerline than previously selected while maintaining a comparable brightness, which could be necessary when NBSR-2 undergoes its structural design phase.

3.2 Reduced Model

The reduced model was intended to minimize the computation time in MPACT in preparation for future 3-D calculations, and in this respect it succeeded, reducing the 2-D MPACT model computation time from 5 hours to 50 minutes. However, while the core eigenvalue (shown in Table 1) and the fast and thermal flux profiles (shown in Table 2) agreed closely with MCNP6, the shape of the reduced model output spectra were inadequate representations of the full reflector model – particularly near the all-important site of the cryostat. The disagreement of the thermal flux profiles along the cryostat axis can be clearly observed in Figure 6.

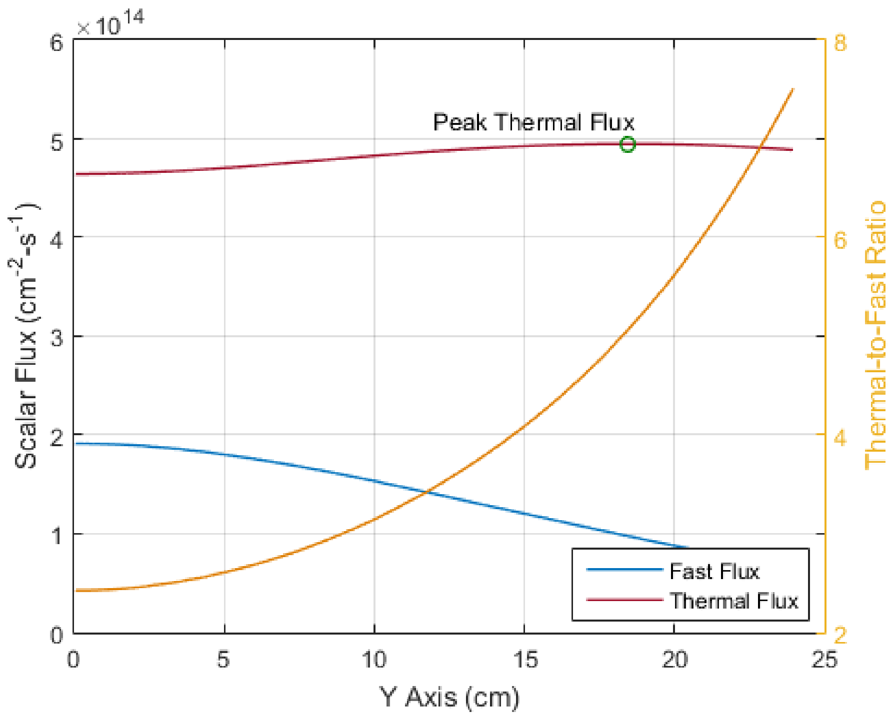

Figure 5. Flux and flux ratio profiles along the vertical centerline of the full reflector model, as calculated with MPACT using the full reflector model.

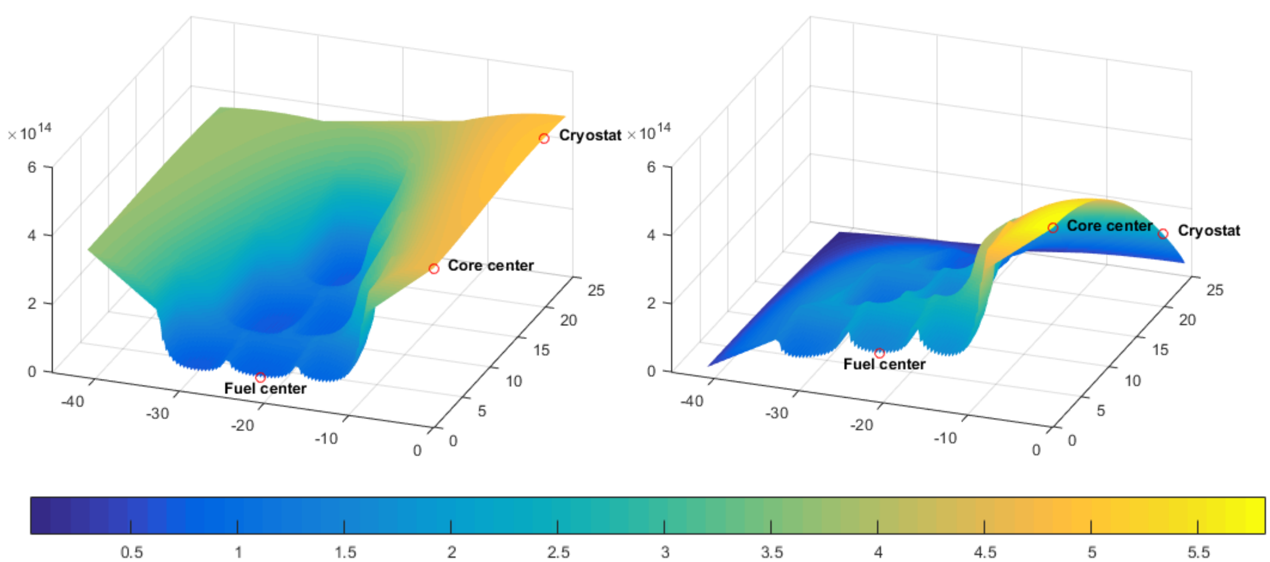

Figure 6. MPACT thermal flux from the full (left) and reduced (right) reflector models.

5. CONCLUSIONS

5.1 A Successful Validation

An accurate model of the NBSR-2 geometry was developed for MPACT using quarter symmetry and repetitive modules, with features including a large D_2O reflector, heterogeneous MTR-type fuel plate assemblies, and a weakly coupled core. A limitation that the fuel clusters be set to a modulus of the MPACT module size was overcome by adjusting the MCNP6 model by 2.05 cm. The resulting core k_{eff} and fast and thermal flux profiles were successfully validated against MCNP6, with k_{eff} results agreeing to within 120 pcm and flux distributions within 1.5 % ± 1.7 % (1-σ) on average for 98,400 points in the full reflector model. A neutronics study in the vicinity of the cryostat exhibited excellent agreement with previous calculations, yielding a thermal-to-fast neutron ratio of 5.07 at the point of maximum flux. This both (1) validated the cryostat placement, and (2) demonstrated the utility of MPACT as a design tool for test reactors like NBSR-2.

5.2 Computation Time: A Limiting Factor

A reduced model developed for MPACT successfully decreased the computation time by a factor of 6, and was benchmarked to within 170 pcm of MCNP6 with flux distributions in excellent agreement. However, the flux distributions themselves proved to be a poor approximation of the full reflector model, especially in the region of the cryostat placement. So, the lengthy computation time required for the full reflector model, which was 2-D, was disappointing because two limiting factors currently make 3-D calculations with it impractical. The first of these factors is the sheer size of the reflector geometry, which is atypical for PWR designs and was causing stability issues in the CMFD acceleration that will require further investigation. The workaround solution, using a simple source iteration in lieu of CMFD, increased the computation time by a factor of 5. The second limiting factor involved the material cross sections: transport-corrected P_0 (TCP_0) cross sections returned negative values in the reflector, so more accurate P_2 models were used instead; but this further increased the computation time by a factor of 4. Computation time is a limiting factor because MPACT is not publically available as of this paper, so these feasibility calculations were performed on limited private resources provided by the University of Michigan. However, the 5 hour wait for the 2-D model could be reduced to 15 minutes in the future, and this would make 3-D calculations much more accessible.

5.3 Future Work

The CMFD acceleration and TCP_0 limitations described above should be addressed before work continues, since moving to 3-D will multiply the computational cost by orders of magnitude. Subsequent efforts could include a 3-D depletion analysis of the fuel cycle, which MPACT is currently well suited for, and then thermal hydraulic benchmarking, which will require minor modifications to MPACT in order to model flow in rectangular channels. Consideration should be given as to whether the native MPACT input structure used in this analysis or the VERA common input system is more beneficial.

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REFERENCES

[1] Kochunas, B., B. Collins, D. Jabaay, T. Downar and W. Martin, "Overview of Development and Design of MPACT: Michigan Parallel Characteristics Transport Code," *Proceedings of the International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2013)*, **45**, pp. 42. (2013)

[2] B. Kochunas, et al., “VERA Core Simulator Methodology for PWR Cycle Depletion,” *Proc. M&C 2015*, Nashville, TN, USA, April 19-23. (2015)

[3] B. Collins and A. Godfrey, “Analysis of the BEAVRS Benchmark using VERA-CS,” *Proc. M&C 2015*, Nashville, TN, USA, April 19-23. (2015)

[4] Z. Wu, M. Carlson, R. E. Willams, S. O’Kelly, and J. M. Rowe, “A Novel Compact Core Design for Beam Tube Research Reactors,” *Transactions of the American Nuclear Society*, **112**, pp. 795-798. (2015)

[5] Studsvik Scandpower Inc., “CASMO-4 - A Fuel Assembly Burnup Program – User’s Manual,” Restricted Distribution – University Release, SSP-09/443-U Rev 0. (2009).

[6] SCALE: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design, ORNL/TM-2005/39, Version 6.1, June 2011. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-785.