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BENCHMARKING THE U.S. NRC NEUTRONICS CODES NEWT AND PARCS WITH THE VENUS-2 MOX CRITICAL EXPERIMENTS

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ABSTRACT

The U.S. Nuclear Regulatory Commission (NRC) has supported the development of the neutron kinetics code PARCS at Purdue University for the best-estimate analysis of commercial nuclear reactor transients. At Oak Ridge National Laboratory (ORNL) the generalized-geometry discrete ordinates transport code NEWT has been developed as part of the SCALE 5 code suite. The U.S. NRC is currently supporting the enhancement of both PARCS and NEWT for the analysis of MOX-fueled light water reactors (LWRs). The focus of the work reported here is the benchmarking of NEWT and PARCS using the VENUS-2 MOX critical experiments. Results are first reported for VENUS pin-cell calculations with NEWT and compared to other participants. Results are then presented for the two-dimensional (2-D) version of the VENUS-II benchmark analyzed with PARCS using group constants generated with NEWT. The results agree well with experimental results as well as those of other participants.

Key Words: PARCS, NEWT, VENUS-2 MOX Benchmark

1. INTRODUCTION

During the past two years, the U.S. NRC supported the enhancement of the generalized geometry discrete-ordinates transport code NEWT [1, 2, 3] to provide lattice physics parameters for the PARCS core simulator. The NRC has also supported the implementation of a multigroup, pin-by-pin, transport capability in PARCS for the purpose of analyzing MOX fueled LWR cores [4, 5]. In order to assess the new methods, the OECD/NEA VENUS-2 MOX benchmark was performed with NEWT/PARCS.

VENUS-2 is an international benchmark with both 2- and three-dimensional (3-D) exercises [6]. The VENUS facility is a zero power critical reactor located at SCK CEN in Belgium. The core consists of 12 15×15 assemblies with the typical pitch of 17×17 assembly, 1.26 cm. The four central assemblies consist of the 3.3 w/o UO_2 fuel pins, with 10 Pyrex pins each. The 8 assemblies on the periphery of the core consist of UO_2 and MOX fuel: 7 internal rows contain 4.0 w/o UO_2 fuel pins, 8 external rows contain MOX fuel with 2.0/2.7 w/o high-grade plutonium. The core is 50 cm in height.

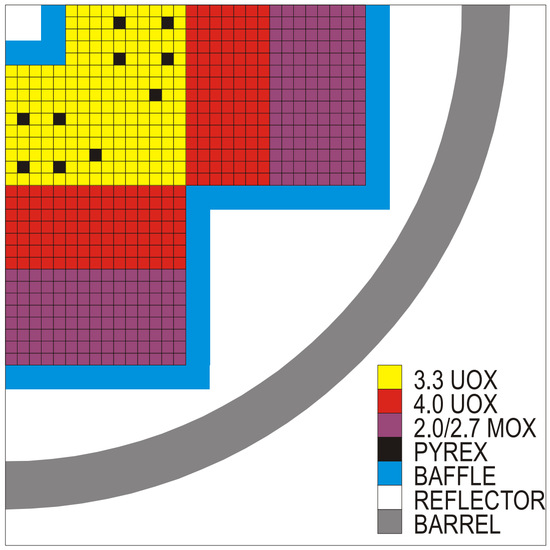


Figure 1. VENUS-2 Configuration (1/4 Core)

The 2-D VENUS-2 experimental data consists of pin power distribution measurements in 121 of the 325 fuel rods in 1/8th of the core: 41 with 3.3 w/o UO_2, 35 with 4.0 w/o and 45 with 2.0/2.7 w/o MOX. A complete description of the facility is given in the benchmark specifications, which includes all geometry and material composition data required to create a detailed computational model of the VENUS-2 core. The objective of the benchmark was to validate and compare the nuclear data sets and production codes used for MOX-fueled system calculations. The comparison of NEWT pin cell results and PARCS/NEWT core results assists in identifying the source of discrepancies and in identifying areas requiring continued code development.

2. NEWT AND PARCS BENCHMARK RESULTS FOR VENUS-2

2.1. NEWT Benchmark Results

The NEWT code employs discrete ordinates transport calculations using differencing based on the Extended Step Characteristic (ESC) method [1, 2, 3] and is capable of modeling generalized 2-D geometries. There are some fundamental differences between the ESC method in NEWT and the Method of Characteristics (MOC) as implemented in other codes. For example, in the HELIOS code, MOC is most often used to solve the characteristic form of the integral transport equation using collision probabilities within a cell, and the cells are then coupled using the interface current coupling method [6]. NEWT solves the differential transport equation using an

S_n method which differs slightly from the traditional S_n method in order to more easily treat complex geometries. The traditional S_n method uses a finite difference approach to approximate spatial derivatives, which is easy for rectangular mesh but difficult for irregular mesh. In the ESC method used in NEWT, the angular flux across a cell is replaced by direct solution of the characteristic form of the transport equation for each discrete direction in S_n quadrature. The ESC method has the advantage of permitting differencing within a polygon cell, whereas outside the cell, the transport solution is a discrete ordinates approach.

NEWT and the ESC method have some advantages over MOC, but there are also some disadvantages. Since it is based on the integrodifferential form of the transport equation, one advantage is that it can easily accommodate higher-order P_n scattering. One significant disadvantage of ESC is the considerable computational cost of the angular treatment, which as in any S_n code depends on the order of quadrature used. For most of the problems examined here, the execution time in NEWT was more than an order of magnitude greater than HELIOS.

A detailed NEWT model was constructed for VENUS-2 using polygonal cells conserving volumes in each region. A one-quarter core model was employed, taking advantage of symmetry. Pin cells were approximated using a 3×3 base grid inlaid with fuel and clad zones, resulting in 25 computational polygons per pin cell. This pin-cell model is illustrated in Fig. 2. A more coarse rectangular mesh (about the pin size) was applied in the moderator region outside the fuel assemblies. A 44-energy group neutron library from SCALE 5 was used for the analysis of VENUS-2.

Because one of the objectives here was to use NEWT for benchmarking PARCS, a modeling simplification was made to allow a consistent comparison between NEWT and PARCS solution. The core barrel and all other external structure material were neglected and replaced by the reflector. This was done in order to simplify the generation of homogenized cross sections for PARCS. (The difference in eigenvalue with and without core barrel was only about 20 pcm.) Limitations in the current version of NEWT prevented the direct application of the experimental buckling in the calculation. Instead, the buckling loss was approximated by assuming a 50-cm core height and allowing NEWT to determine its own buckling.

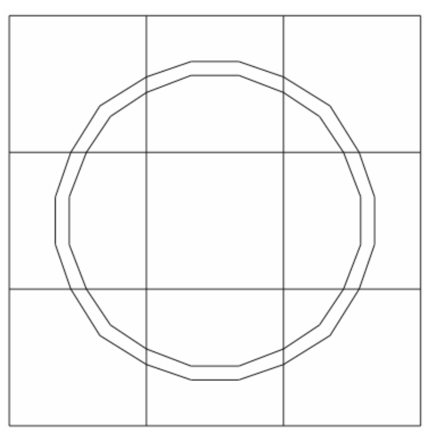


Figure 2. NEWT Pin-Cell Discretization

The 2-D version of the VENUS-2 benchmark consists of both pin cell and core calculations. Table I shows the pin cell k_{inf} results of NEWT compared to other benchmark participants. As indicated, there is reasonably good agreement between NEWT and other codes for the UO_2 3.3% pin, but for the UO_2 4.0% and MOX pins, there exists a relatively large k_{inf} difference (about 1%). A Monte Carlo calculation was performed with KENO using the same library, and as indicated, the k_{inf} results for all three pin types are in reasonably good agreement with NEWT. This suggests that the primary cause of the differences between NEWT and other codes is the neutron data library.

Table I. Results for VENUS-2 Pin Cells

Institution	**Code**	**UO_2 3.3%**		**UO_2 4.0%**		**MOX**	
		k_{inf}	**%Dev.***	**k_{inf}**	**%Dev.**	**k_{inf}**	**%Dev.**
Purdue/ORNL	NEWT (44 g)	1.40338	-0.18	1.33303	-0.32	1.25465	-0.13
ORNL	HELIOS 1.4 (190 g)	1.40847	0.18	1.34333	0.45	1.26254	0.46
KAERI	HELIOS 1.5 (35 g)	1.40904	0.22	1.34306	0.43	1.26339	0.53
Purdue	HELIOS 1.7 (190 g)	1.40850	0.18	1.34331	0.45	1.26339	0.53
ORNL	KENO (44 g)	1.40385	-0.15	1.33366	-0.27	1.25345	-0.26
Average**		1.40593		1.33726		1.25673	

*Deviation from the average k_{inf}.
**Average k_{inf} of all benchmark participants.

Because the modeling of the reflector/core interface is very important for the VENUS-2 core, a parametric study was performed to examine the effectiveness of NEWT for treatment of the water reflector region. Three different discretization schemes in the reflector region were used in NEWT and results were compared to HELIOS. The physical model was a 2×2 fuel pin array of 3.3 w/o enriched UO_2 pins with a similar sized reflector region as shown in Figure 3. Three different discretization schemes were used in the reflector region as shown in Figure 3: (1) the mesh size in the reflector is equal to one pin, (2) the mesh size in the reflector is 1/4 pin, and (3) the mesh size in the reflector is 1/16 pin. The same grid scheme is used in the fuel region for all three cases.

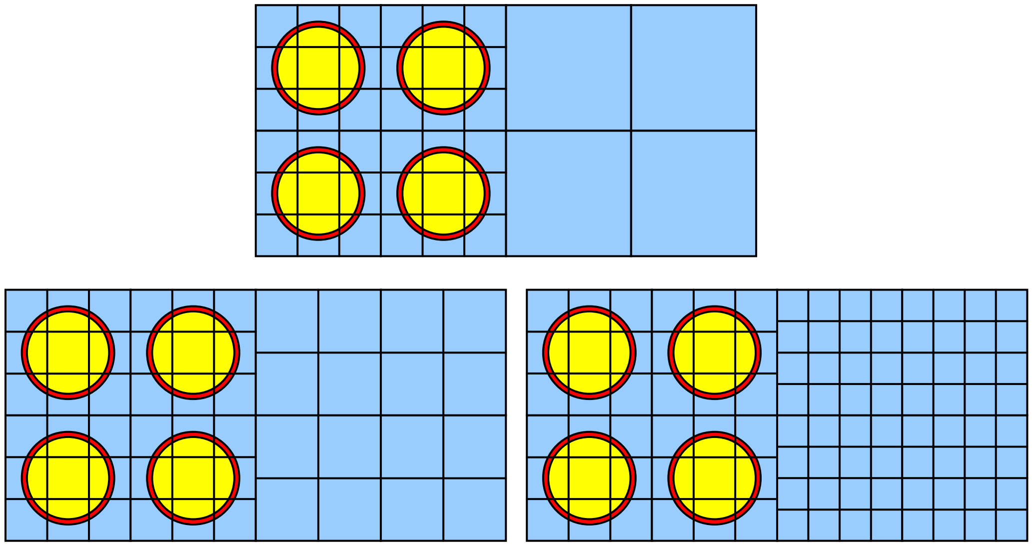


Figure 3. Grid Schemes for Reflector Model Study in NEWT

The NEWT and HELIOS results are summarized in Table III for the water/reflector discretization study. (Note: For the HELIOS model, the "windmill" discretization was used in the fuel region.)

Table II. Comparison of NEWT and HELIOS Results for Discretization Study

Discretization scheme	K_{inf} (HELIOS 45 g)	K_{inf} (NEWT 44 g)
(1) 1-pin pitch of a cell	1.23397	1.24132
(2) 1/4-pin pitch of a cell	1.20523	1.20475
(3) 1/16-pin pitch of a cell	1.18435	1.18431

As indicated in Table II, for both codes there is considerable variation in the k_{inf} for different discretization schemes in the reflector. However, there is reasonable consistency between the codes; the HELIOS k_{inf} dispersion between discretization schemes is about 5000 pcm, and the NEWT k_{inf} dispersion between discretization scheme is about 5700 pcm. A similar study was then performed for a MOX reflector model of VENUS-2 as shown in Figure 4 and the results are summarized in Table III.

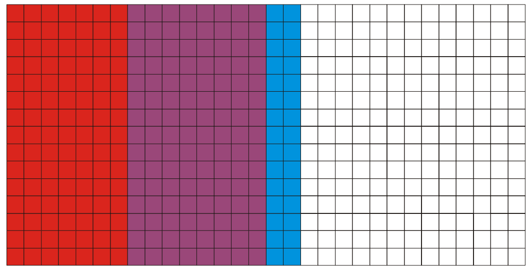


Figure 4. MOX-Reflector Model of VENUS-2.

Table III. Comparson of NEWT and HELIOS Results for VENUS-2 Reflector Model

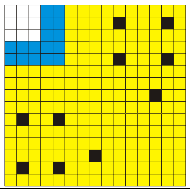
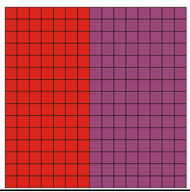
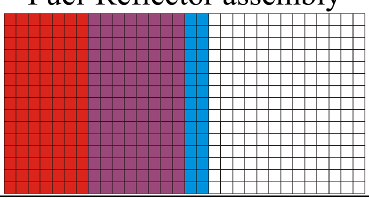
Discretization scheme	K_{inf} (HELIOS 45 g)	K_{inf} (NEWT 44 g)
1-pin pitch of a cell	1.15295	1.14284
1/9-pin pitch of a cell	1.15420	1.14458

For this problem, the discretization does not make a substantial difference; however, the differences between HELIOS and NEWT are considerably larger. The primary reason for this difference in the MOX case appears to be the increased importance of the prediction of the neutron spectrum in the reflector region when MOX fuel is on the boundary. The differences in the prediction of the spectrum at the interface of MOX/Reflector can be attributed to differences in methods used in HELIOS and NEWT methods, as well as in the neutron libraries of the two codes.

2.2. PARCS/NEWT Benchmark Results

A VENUS-2 model was constructed using the U.S. NRC core simulator PARCS v2.1.
A solution was performed using the recently developed pin-by-pin multigroup SP_3 capability. The homogenized cross sections were generated with NEWT using the models summarized in Table IV.

Table IV. Calculation Models Used in NEWT for Generating PARCS Cross Sections

Single Assembly Calculation	Nodal Parameters Generated	Fine Mesh Parameters Generated
3.3% UOX assembly 	1. 2G assembly XS 2. 2G pin power form functions 3. ADFs/CDFs	2 and 8G average cell XS: 1. 3.3% UOX 2. Pyrex 3. Inner baffle 4. Inner reflector
4.0% UOX/MOX assembly 	4. 2G assembly XS 5. 2G pin power form functions 6. ADFs/CDFs	2 and 8G average cell XS: 5. 4.0% UOX 6. 2.0/2.7% MOX
Fuel-Reflector assembly 	7. 2G reflector XS 8. ADFs	2 and 8G average cell XS: 7. Outer baffle 8. Outer reflector

Two sets of 2- and 8-group pin cell cross sections were generated using these NEWT VENUS-2 cross-section models. Assembly Discontinuity Factors (ADF) for reflector assemblies were calculated by solving analytically the 1-D diffusion equation in the homogeneous reflector region with the fuel-reflector boundary condition from NEWT. It was not practical to generate an additional cross-section set for the corner reflector having a baffle on two sides. Instead, the scattering cross section was modified using the following equation [7]:

$$r = \frac{FA\ Pitch - Baffle\ Thickness}{FA\ Pitch}. \tag{1}$$

The PARCS model for VENUS-2 is shown in Figure 5. As indicated, the problem is simplified by not explicitly treating the core barrel.

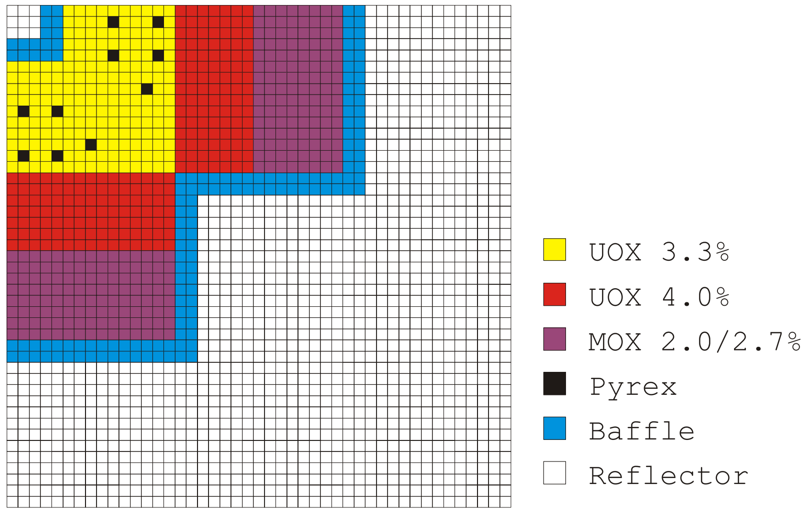


Figure 5. PARCS VENUS-2 Full-Core Fine Mesh Model

A summary of the PARCS results using NEWT cross sections is provided in Table V using both the diffusion and SP_3 kernel in PARCS [4]. For comparison, the PARCS results with HELIOS cross sections are shown in Table VI for the case with zero buckling. The HELIOS/PARCS results with the specified buckling were reported previously and compared favorably to a full core HELIOS result as well as to other benchmark participants [9]. As indicated in the Tables, there is good agreement between the NEWT/PARCS and HELIOS/PARCS calculations. The importance of using the SP_3 kernel in PARCS is indicated by more than a 1% difference in the diffusion and SP_3 transport PARCS calculations using either NEWT or HELIOS cross sections.

Table V. PARCS 2-D VENUS-2 Results with NEWT Cross Sections

Method	Group	Collapsing-spectrum	Angle	Core k_{inf}	Reference k_{inf} (from NEWT)
Fine Mesh*	8	Infinite	diffusion	1.06925	1.08829
			SP_3	1.08108	

*4×4 mesh per pin

Table VI. PARCS 2-D VENUS-2 Results with HELIOS Cross Sections

Method	Group	Collapsing-spectrum	Angle	Core k_{inf}	Reference k_{inf} (from HELIOS)
Fine Mesh*	8	Infinite	diffusion	1.07579	1.08902
			SP_3	1.08672	
		Critical	diffusion	1.07480	1.08849
			SP_3	1.08561	

*4×4 mesh per pin

Because of some temporary limitations in the current pin power edits available in NEWT, a direct comparison of the pin powers between NEWT and PARCS could not be performed. However, comparisons of the HELIOS and HELIOS/PARCS pin power distributions have been reported previously and showed good agreement. Therefore, it was useful to compare the pin power distributions of the SP_3 PARCS calculations in NEWT/PARCS and HELIOS/PARCS, as shown in Table VII. The agreement is generally good, with the most noticeable discrepancy being the 1.10% difference in the pin power prediction for a 3.3% enriched UO_2 pin.

Table VII. Comparison of Pin Power Distribution Calculated by NEWT/PARCS and HELIOS/PARCS

	UO_2 3.3	**UO_2 4.0**	**MOX**	**All**
RMS	0.29%	0.54%	0.50%	0.46%
Max error	-1.10%	0.85%	0.88%	-1.10%
Peak pin error	0.30%	-0.61%	0.87%	0.87%

It should be noted that the group constants generated by both NEWT and HELIOS for the results shown in Table VII used an infinite medium spectrum. This was because the current version of NEWT does not have the ability to compute a critical spectrum. Therefore a second set of group constants were generated with HELIOS to examine the impact of the critical versus infinite medium spectrum. As indicated by the results in Table VIII, the effect is not large.

Table VIII. Comparison of Pin Power Distribution Calculated by HELIOS/PARCS With Group Constants from Critical and Infinite Spectra

	UO_2 3.3	**UO_2 4.0**	**MOX**	**All**
RMS	0.30%	0.31%	0.19%	0.31%
Max error	1.11%	0.48%	0.50%	1.11%
Peak pin error	0.21%	-0.23%	-0.34%	-0.34%

3. CONCLUSIONS

The purpose of the work reported here was to perform preliminary benchmarking of the core simulation code PARCS and the lattice physics code NEWT using the VENUS-2 critical experiments. The 2-D versions of the benchmark were analyzed with PARCS using group constants generated with NEWT. Reasonably good agreement was observed between the NEWT/PARCS and HELIOS/PARCS 8 group, fine mesh SP_3 solutions.

Both NEWT and PARCS are under development for MOX analysis. Capabilities will continue to be developed in both codes as work progresses. Further evaluation of both codes is planned using the 3D VENUS-2 experiment, along with additional benchmark experiments to include depletion results for LWR MOX lattices.

ACKNOWLEDGEMENTS

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