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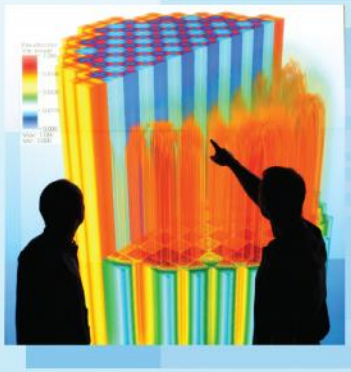

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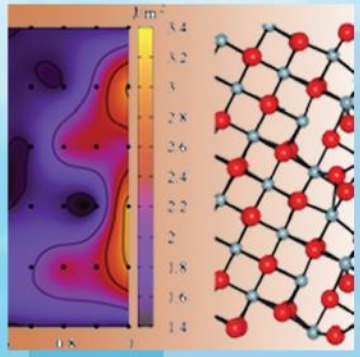

Fundamental science

Plant operational data

Consortium for Advanced Simulation of LWRs

Application of MPACT 2D/1D to AMA Benchmark Problem 5

Revision 0

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ACRONYMS

AMA	CASL Advanced Modeling Applications Focus Area
ORNL	Oak Ridge National Laboratory
RTM	CASL Reactor Transport Methods Focus Area
UM	University of Michigan
VERA	Virtual Environment for Reactor Applications
VRI	CASL Virtual Reactor Integration Focus Area
MPACT	Michigan Parallel Characteristics based Transport Code

INTRODUCTION

The pin resolved transport code MPACT is being developed at University of Michigan to provide CASL with 2D, 2-D/1-D, and 3-D MOC reactor analaysis capabilities. Previous reports have reported the development [#] and accuracy [#] of the 2D MOC solver in MPACT. This report focuses on the implementation and the initial testing of the baseline 2D/1D solver.

BASELINE 2D/1D SOLVER IN MPACT

In the baseline 2D/1D capability, the 3D domain is decomposed into 2D planes and the transport equation is solved for each 2D plane. The planes are coupled together through an isotropic leakage source and the axial variation in the flux is modeled using the diffusion approximation through either a nodal method or finite difference. The 3D solution is accelerated using a Coarse Mesh Finite Difference (CMFD) solver. The following section is separated into three parts; the first discusses the modifications made to the 2D MOC sweeper in MPACT, the second discusses the development of the nodal sweepers and the parallel algorithms, and the final subsection discusses the CMFD system and the global iteration algorithm.

The 2D MOC transport sweeper in MPACT that has been previously reported provides the foundation of the 2D/1D sweeper. Although, any 2D solver could potentially be used in the 2D/1D formulation, the basis of MPACT is the 2D MOC sweeper. The underlying 2D MOC data structures in MPACT remain the same regardless if the problem is 2D or 3D. A method has been implemented to the MOC data to change planes which alters the pointers in the data structure for the appropriate plane. In addition to allowing the 2D MOC sweeper to solve multiple planes, the source term in the MOC sweeper is also be altered to account for axial leakage. The assumption in the baseline 2D/1D method is that the axial source is isotropic. Although some angular information is available concerning the axial leakage, the isotropic assumption provides significant improvements in speed and memory for the 2D MOC solution if the source is not angle dependent. Ongoing research is investigating computationally efficient methods to include the angular shape of the axial leakage in the 2D/1D solution.

The axial direction is solved using a low order approximation to the transport equation. MPACT has several nodal diffusion kernels implemented but currently only the 2-node Nodal Expansion (NEM) kernel is implemented in the 2D/1D solver. The NEM kernel assumes the intranodal flux is a fifth order Legendre polynomial in space and then enforces current and flux continuity between nodes. The remaining coefficients are solved using a set of three weighted residual equations. The 2-node nodal formulation is used to enhance the stability of the global method. In the 2-node formulation, a NEM system is constructed for every axial interface and the current and surface flux are solved at the interface of the 2 nodes. The boundary condition for the 2 node problem is the average flux in both of the adjacent nodes. Fixing the average flux of each node serves to stablize the local iteration and helps to prevent the 2-nodes solutions from becoming out of phase with the global solution. Since the dominant parallel docomposition in the 2D/1D problem is by axial planes, the axial solution is highly decomposed. In the axial iteration scheme, the shape of the source, cross-sections, and the average flux are passed via MPI communication to the processor which will solve the 2 node problem and then the flux shape and interface current are passed back. In MPACT, the convention is used that each process will solve the interface on the top of its subdomain. In the case of the bottom boundary of the core, the processor who owns the bottom node will also solve for that interface.

The CMFD acceleration scheme not only accelerates the convergence of the entire solution but also provides stability to the radial and axial sweeps. Since the radial and axial equations are solved alternately, the tendency is for data propagation in the axial direction to become very slow as the planes become thin. CMFD helps couple all of the planes together by solving a global diffusion-like system of equations. The elliptic nature of the diffusion system tightly couples the interior of the core to the boundary. It should also be noted that if nonlinear correction factors are not added in the axial direction, the CMFD accelerator can be used as a finite difference axial solution which no longer requires an axial solver if finite difference accuracy is acceptable.

The global iteration scheme used for the baseline 2D/1D scheme is to use the CMFD system to accelerate the calculation of the eigenvalue and eigenvector of the system. Once CMFD has sufficiently converged, the fission source is fixed and the axial solution is performed. The axial solver obtains estimations for the axial leakage which is then used in the 2D MOC planar solutions. Once the leakage source is fixed, the 2D MOC solver is called to determine the new flux distribution. Once the planar MOC solutions are complete, the homogenized cross-sections and nonlinear correction factors for CMFD are updated and the iteration continues. The iteration is complete when the eigenvalue and flux are sufficiently converged.

ASSESSMENT OF MPACT FOR 3D CORE PROBLEMS

C5G7 Benchmark

The C5G7 benchmark [#,#] is a numerical benchmark that is widely used to assess the accuracy of transport codes. The benchark contains two 17x17 assemblies, one UO2 and one MOX. They are arranged in a checkerboard pattern and surrounded by water. Figure 1 shows the model geometry. Cross-sections are specified for fuel, guide tube, instrument tube, moderator, and control rod in a 7 group format.

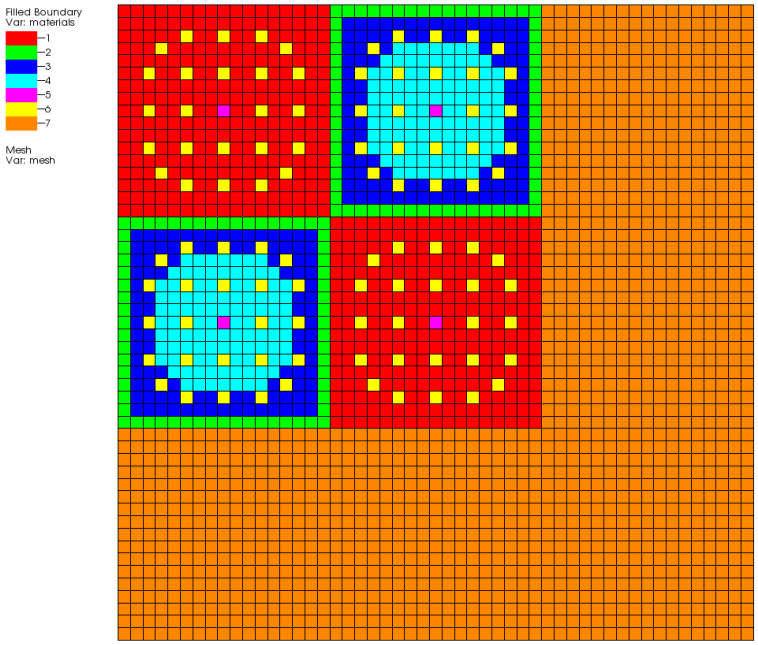

Figure 1: C5G7 Benchmark Problem Geometry

The reference solution for the C5G7 benchmark is a multigroup MCNP5 solution. In a previous milestone report, the 2D solver in MPACT was compared to the reference solution of the benchmark. There are four different 3D models that can be evaluated using the 2D/1D solver. The first model is close to a standard full height assembly. The fuel is 385.56 cm high with 21.42 cm of water above and below the fuel. The 3D model is shown in figure 2.

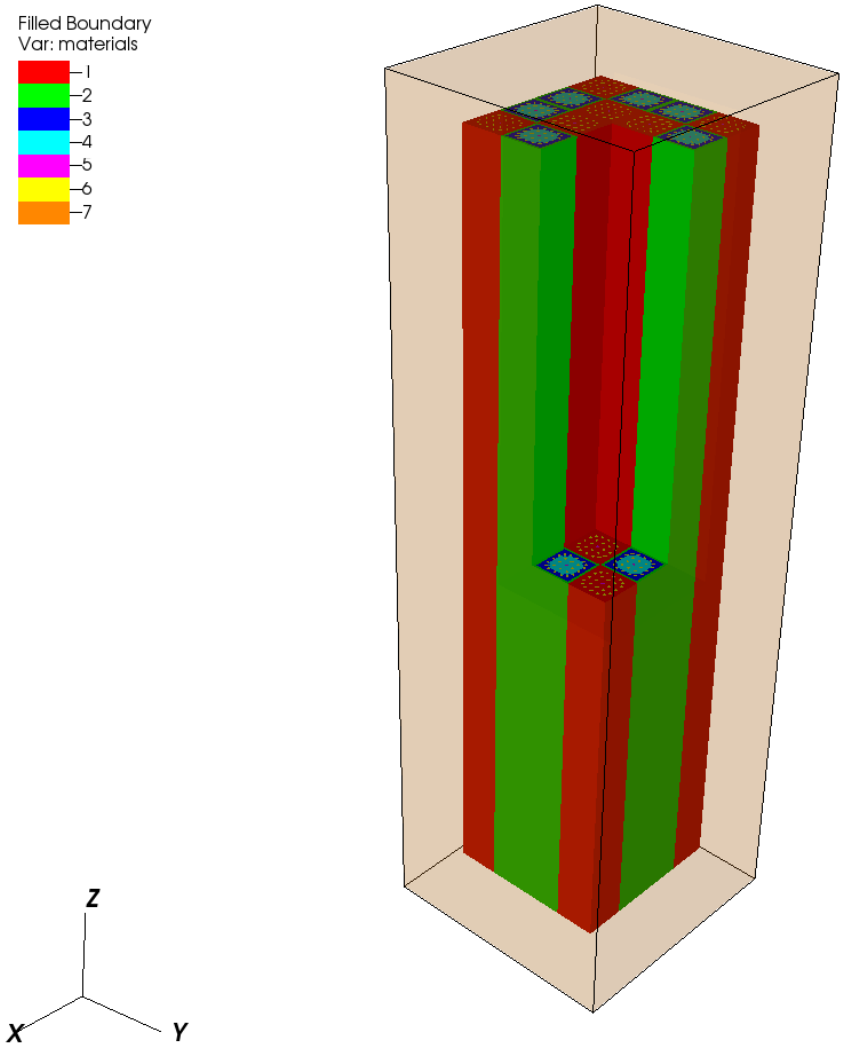

Figure 2: C5G7 Benchmark 3D Problem Geometry

Several years after the original C5G7 benchmark was released, an extension of the benchmark was published to investigate the effects of modeling control rods in a similar geometry. In order to reduce the computational cost, the height of the fuel was decreased to 128.52 cm and the model was assumed symmetric across the centerplane in the axial direction. There are three configurations in the benmark; the unrodded case where the control rods are only in the upper reflector; rodded configuration A which has the control rod inserted 1/3 of the way into the center UO2 assemblies, and rodded configuration B which has the control rod inserted 2/3 of the way into the center UO2 assemblies and another rod inserted 1/3 of the way into the MOX assemblies. Rod configuration B is shown in Figure 3.

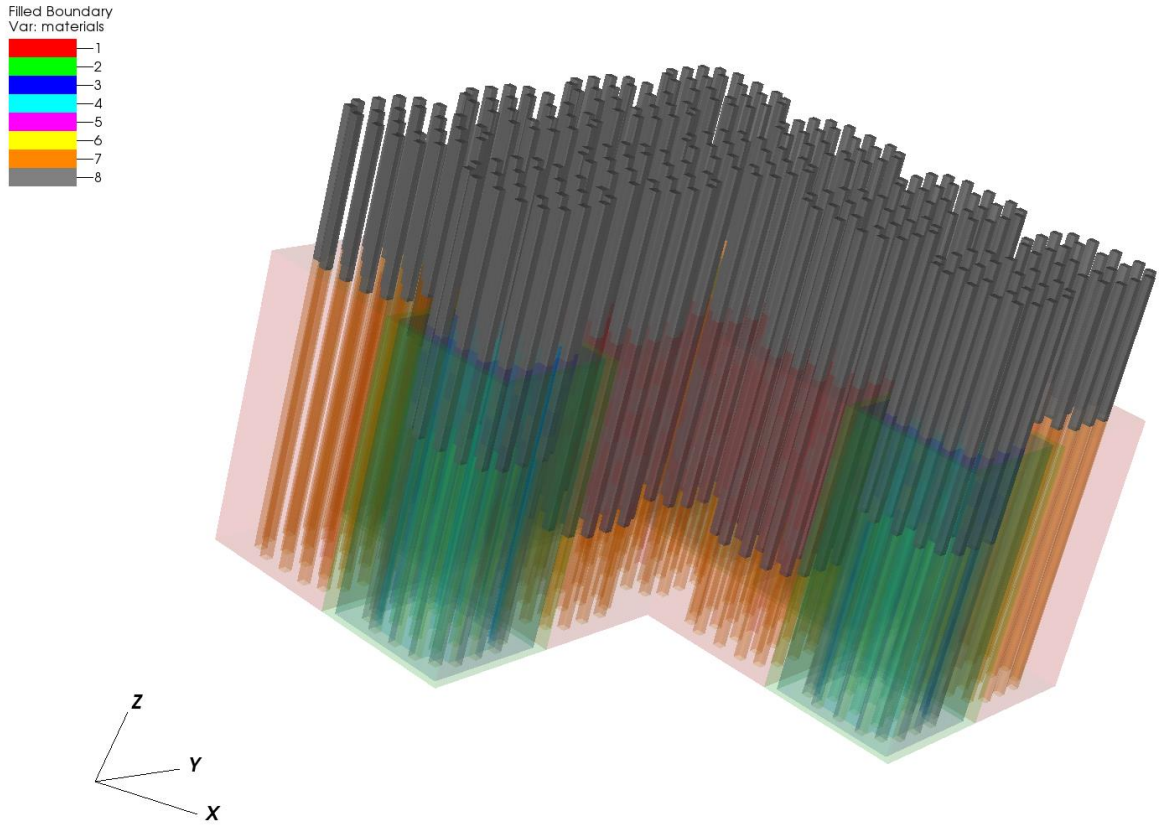

Figure 3: C5G7 Benchmark Control Rod Configuration for Problem B

The reference solution for the C5G7 problems provide maximum pin and assembly axially averaged powers. The extended C5G7 problems also provide the powers for 3 axial slices. The full height assembly comparisons are shown in Table 1.

Table 1 MPACT C5G7 Results for Rodded Configuration B

		Axially Integrated Powers					
		keff	min	max	Inner UO2	MOX	Outer UO2
Original 3D	MPACT	1.18390	0.24	2.49	491.62	211.80	140.10
	Error	-9	2.38%	-0.41%	-0.26%	0.16%	0.36%

The agreement for this case is very good although there axial data was not provided in the Benchmark for detailed 3D comparison. The only result that is significantly different from the 2D results is the minimum power. All of the errors are of the same order as the other participants in the benchmark.

The extended C5G7 benchmark results are shown in Table 2.

Table 2 MPACT C5G7 Results for Unrodded and Rodded Configuration A

		Axially Integrated Powers						Slice Power Errors				
		keff	min	max	Inner UO2	MOX	Outer UO2	Slice	max	Inner UO2	MOX	Outer UO2
Unrodded	MPACT	1.14170	0.24	2.48	490.07	212.89	140.15	1	-0.78%	-0.78%	-1.38%	-1.64%
	Error	138	--	-0.18%	-0.23%	0.09%	0.54%	2	-0.17%	-0.24%	-0.82%	-0.91%
								3	3.07%	3.35%	4.00%	2.75%
Rodded A	MPACT	1.12744	0.26	2.25	461.13	221.62	151.63	1	-0.02%	-0.22%	-0.80%	-0.98%
	Error	62	--	0.05%	-0.02%	-0.04%	0.15%	2	-0.98%	-0.83%	-0.61%	-0.60%
								3	2.62%	3.67%	3.71%	2.87%
Rodded A	MPACT	1.07751	0.35	1.83	395.24	236.73	187.30	1	-0.70%	-0.60%	-0.47%	-0.59%
	Error	26	--	-0.16%	-0.04%	0.05%	0.00%	2	-0.16%	0.39%	-0.70%	-0.37%
								3	3.73%	3.12%	3.64%	2.63%

In all cases, the axially integrated powers agree very well but the axial power shape suggests some shortcomings in the axial diffusion solution. Even though the power in the slice close to the reflector has larger errors, it is consistent with other codes with axial diffusion solvers like DeCART. And similar to the approach used in DeCART, the implementation of an axial transport solver such as SP3 in MPACT should reduce the errors in slice 3 near the reflector.

VERA Core Physics Benchmark Progression Problems – Problem 3: 3D Assembly

The VERA Progression problems were developed in order to provide guidelines for the development of reactor physics modeling. Previous reports have focused on MPACT's perfromance for 2D coases (Problems 1 and 2). Problem 3 extends the 2D lattices into a full assembly shown in figure 4. Two different configurations are compared. The first is a nominal assembly and the second has a PYREX rod cluster insterted. Both assemblies are at cold conditions without thermal hydraulic feedback.

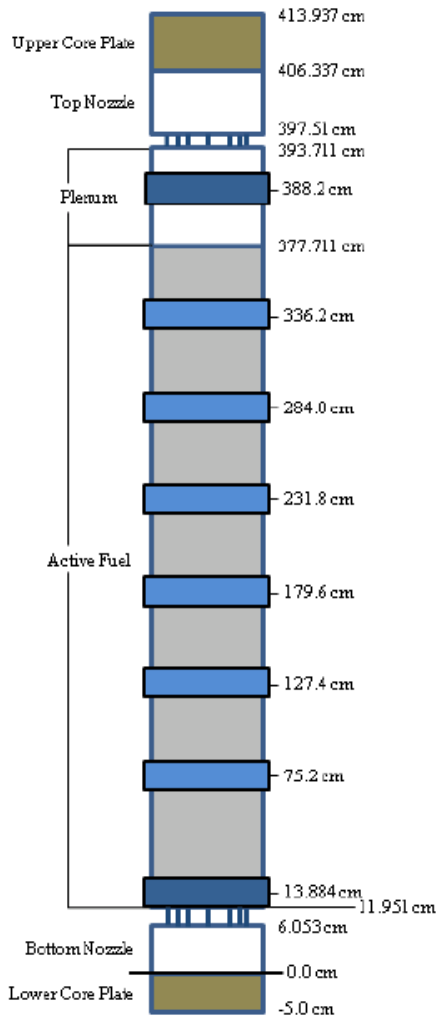

Figure 4: VERA Progression Problem 3 Geometry

The reference case for both assemblies are generated using the KENO continuous energy monte carlo code. Both eigenvalue and fission distribution are compared. Table # shows the comparison between MPACT and KENO for both cases. Figures # and # show the axial power comparison for both cases.

Table 1: VERA Progression Problem 3 Results

	3a	3b
Eigenvalue	1.17584	1.00113
Difference [pcm]	-45	-40
Pin Power RMS [%]	0.185	0.259
Pin Power Max [%]	0.651	1.367

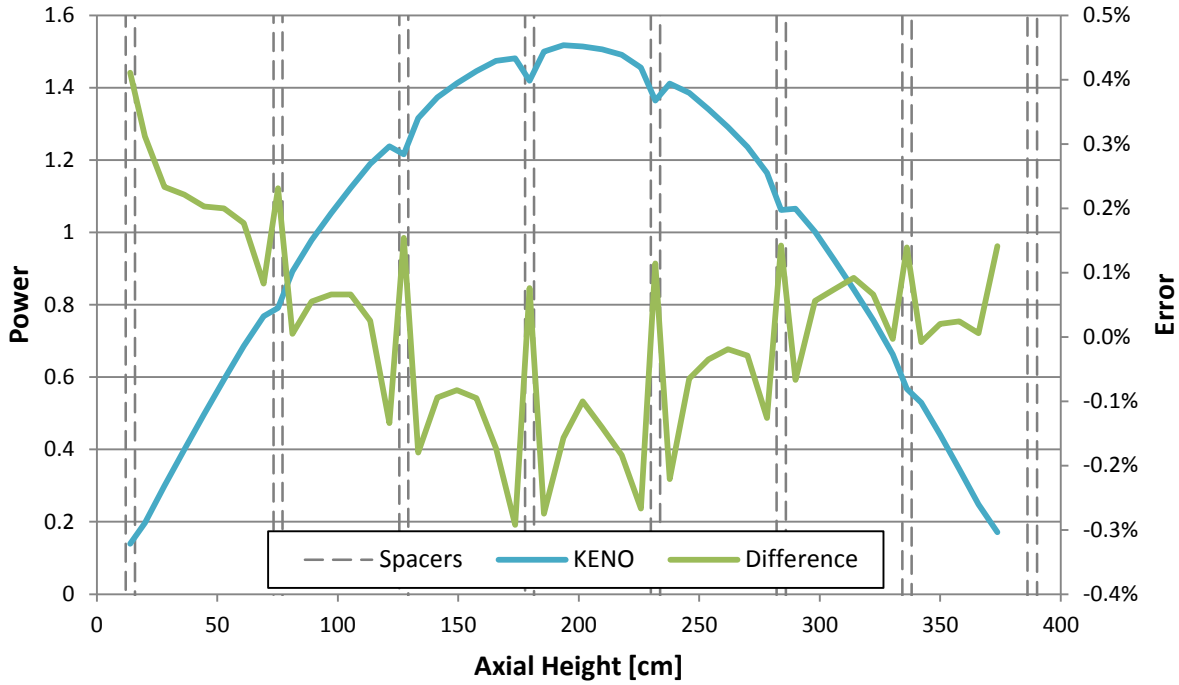

Figure 1: VERA Progression Problem 3a Axial Power Comparison

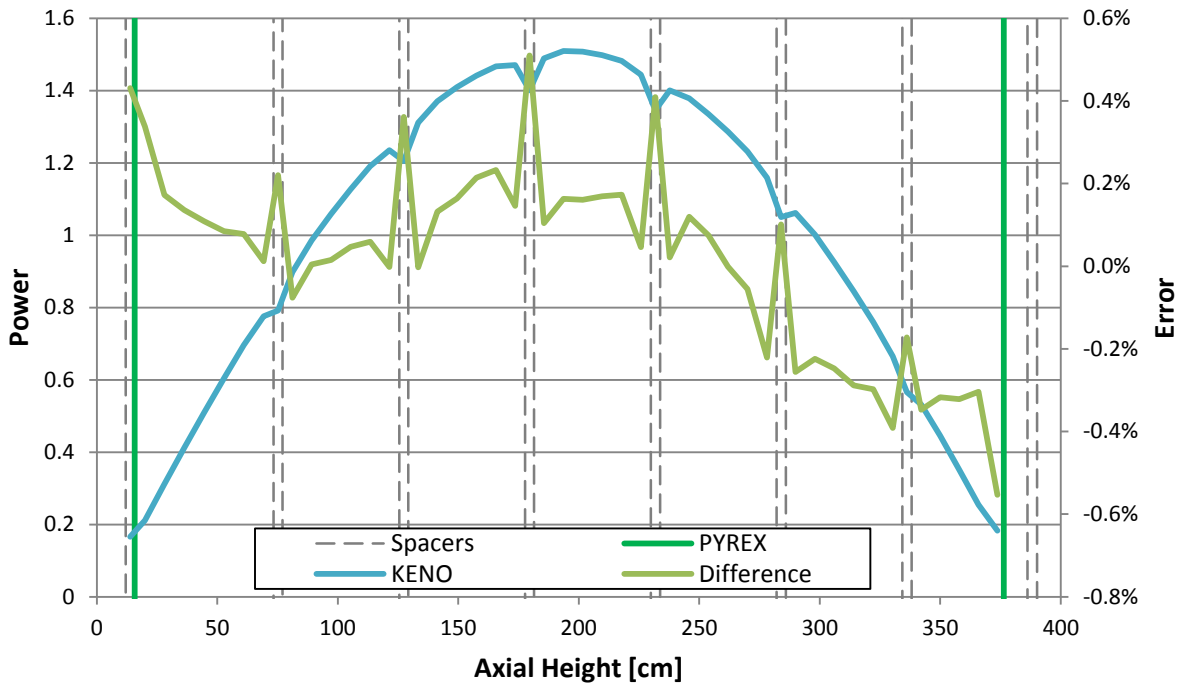

Figure 2: VERA Progression Problem 3b Axial Power Comparison

In both cases, the comparison to KENO show good results. For the PYREX cases, the power shape errors are higher than the nominal case. The majority of the larger errors occur round the tip of the pyrex rod. Also, the differences in the the spacer grid pins in both cases can be attributed to differences in the way the grid spacers are modeled between the two codes.

VERA Core Physics Benchmark Progression Problems – Problem 4: 3D Color-sets

The next VERA Progression problem is a 3D 3x3 assembly case with a control rod cluster inserted into the ceter assembly as shown in Figure #.

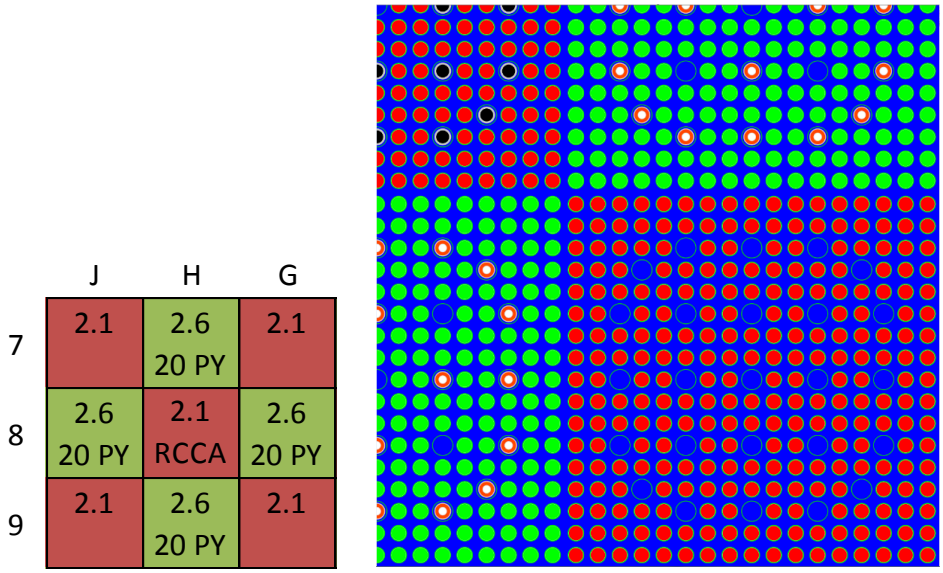

Figure 3: VERA Progression Problem 4 Color-set

There are two components to this problem. The first component is a comparison of the control rod worth as the rod is withdrawn 10% at a time. The KENO reference solution provides the rod worth for each case but does not provide a pin power distribution. Figure # shows the comparison of the rod worths between MPACT and the reference solution. The total rod worth is predicted very well, but around 20% withdrawn, the rod worth has larger error. The major factor for the larger error is the homogenization of the control rod tip inside the 2D MOC plane. This is a limitation of the current implementation of the 2D/1D method in MPACT. Further research is needed to implement a better model for determining control rod worth.

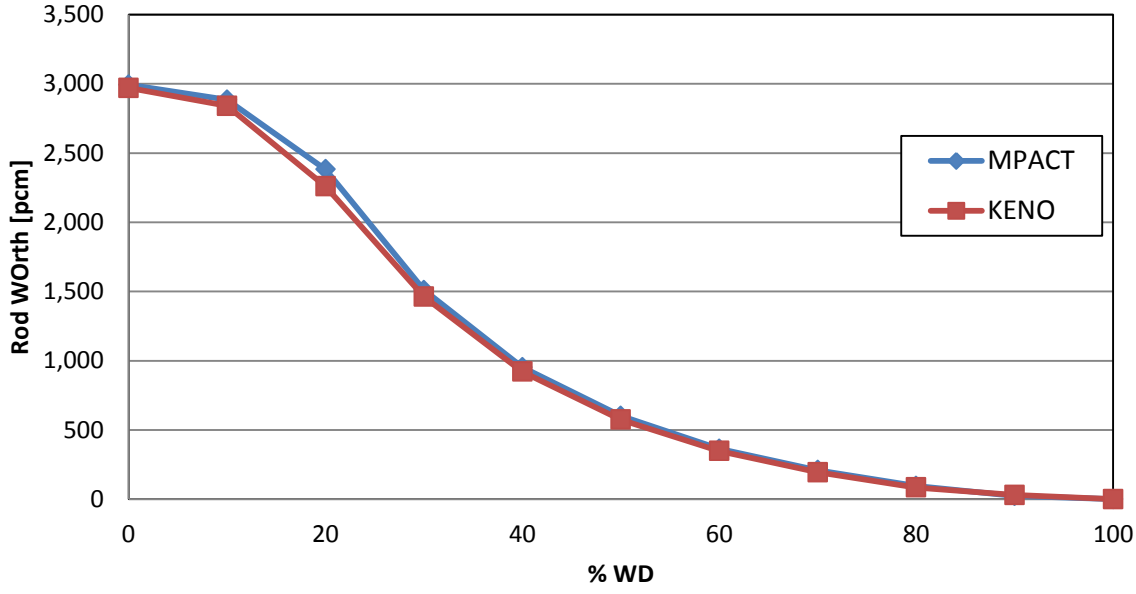

Figure 4: Integral Rod Worth Curve

The second component is a partially rodded case in which both the eigenvalue and pin power distribution are compared to the reference solution. Table # shows the comparison of MPACT to the reference solution and Figure # shows the axial power profile.

Table 2: VERA Progression Problem 4a Results

	4a
Eigenvalue	0.99797
Difference [pcm]	-199
Pin Power RMS [%]	1.051
Pin Power Max [%]	2.347

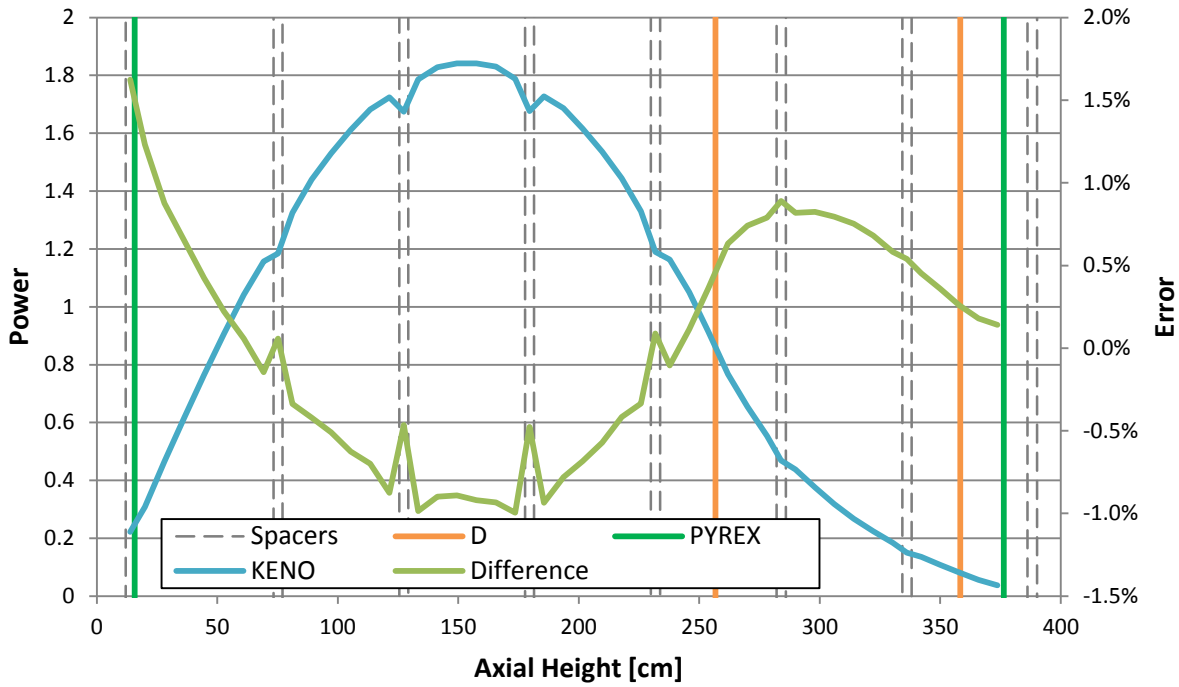

Figure 5: VERA Progression Problem 4a Power Shape Comparison

VERA Core Physics Benchmark Progression Problems – Problem 5: Hot Zero Power (HZP) Full Core

The final comparison is the HZP full core comparisons. The shear size of this problem prohibits a reference solution for the pin power, but eigenvalue comparison can be made against CE KENO results and the critical configurations of the startup core. There are 10 critical configurations that are compared here: the initial critical, the All Rods Out (ARO) critical, and each of the 8 rod banks inserted into the core. These 10 critical configurations are shown in Table #. In addition, calculation of the differential boron worth and isothermal temperature coefficient are also calculated. The differential boron worth is calculated by taking the ARO critical and perturbing the boron concentration to 1271 pcm and calculating the difference in reactivity. The isothermal temperature coefficient is calculated by doing both a positive and negative 5 K perturbation on the temperature from the ARO position and changing the fluid density appropriately. The three points were used to determine the reactivity coefficient using a forward, backward, and central difference. The reactivity coefficients are given in Table #.

Table 3: VERA Progression Problem 5 Results

	Bank Position										
	A	B	C	D	SA	SB	SC	SD	Boron	keff	Difference [pcm]
Initial Critical	--	--	--	167	--	--	--	--	1285	0.99810	190
ARO Critical	--	--	--	--	--	--	--	--	1291	0.99857	143
Bank D Critical	--	--	--	18	--	--	--	--	1170	0.99720	280
Bank SA Critical	--	--	--	69	0	--	--	--	1170	0.99675	325
Bank SB Critical	--	--	--	134	--	0	--	--	1170	0.99728	272
Bank SC Critical	--	--	--	71	--	--	0	--	1170	0.99740	260
Bank SD Critical	--	--	--	71	--	--	--	0	1170	0.99736	264
Bank A Critical	0	--	--	97	--	--	--	--	1170	0.99675	325
Bank B Critical	--	0	--	113	--	--	--	--	1170	0.99687	313
Bank C Critical	--	--	0	119	--	--	--	--	1170	0.99697	303

The critical configurations are compared to an eigenvalue of unity. The eigenvalue bias with control rods in constant around 200-300 pcm. There are a few contributers to this including deficiencies of diffusion theory, not accounting for thermal expansion of the fuel, and bias casued by the cross-section library and cross-section processing.

Table 4: VERA Progression Problem 5 Reactivity Coefficients

	Boron [ppm]	Temperature [^{o}F]	keff	Reactivity Worth	
ARO Critical	1291	557.33	0.99857	--	
DBW	1271	557.33	1.00060	-10.12	pcm/ppmB
ITC -Forward	1291	566.33	0.99820	-4.17	pcm/^{o}F
Backward	1291	548.33	0.99890	-3.64	pcm/ ^{o}F
Central				-3.90	pcm/ ^{o}F

The boron worth calculation agrees very well with the measured value of -10.8 pcm/ppmB but the isothermal temperature coefficient is about twice the measured value of -2.2 pcm/^{o}F. Although the difference is larger than expected, it is consistent to the other VERA codes. Further analysis into the ITC is needed to better understand the differences.

SUMMARY AND CONCLUSIONS

This report outlined the extension of the 2D MOC capability in MPACT into a baseline 3D capability using the 2D/1D solution. The C5G7 benchmark has been used to compare the accuracy of the 2D/1D capability with Monte Carlo solutions and other benchmark participants using deterministic codes. In addition, MPACT was used to model the VERA Core Physics Benchmark Progression Problems 3, 4, and 5. Overall the comparisons to the reference solutions are very good. The C5G7 results show a good comparison without rods but show larger pin power differences when control rods are inserted. The VERA progression problems also show good comparison to the reference without strong absorbers. The control rod cases have larger pin power error. The rod worth comparisons also uncover issues when the control rod is partially inserted into a 2D plane. The full core cases show a consistent 200 to 300 pcm bias. Further investigation is required to better understand this bias.

FUTURE WORK

Although the implementation of the 2D/1D method has been demonstrated in this report, there are a few components that require further work in order for MPACT to meet the requirements for a VERA core simulator.

1. Improve axial solution. The current diffusion coefficient when using P2 scattering is inconsistent with the radial solution. The diffusion coefficient needs to be improved or a higher order transport method is required
2. Memory requirements for large cases. The current CMFD methodology uses a considerable amount of memory. The full matrix method was reduced to a group by group sweep which ultimately hurts convergence rates and increases run time.
3. Run times for large cases. In addition to memory requirements, the run times are still excessive for useful reactor analysis. A detailed profiling of the code and adjustments made to increase the computational performance.

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