

## DEVELOPMENT OF MPACT FOR FULL-CORE SIMULATIONS OF MAGNOX GAS-COOLED NUCLEAR REACTORS

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### ABSTRACT

The MPACT code, jointly developed by Oak Ridge National Laboratory and University of Michigan, is designed to perform high-fidelity light water reactor (LWR) analysis using whole-core pin-resolved neutron transport calculations on modern parallel-computing hardware. MPACT uses the subgroup method for resonance self-shielding, while the primary neutron transport solver uses a 2D/1D method that is based on the method of characteristics (MoC) for the x-y planes coupled with a 1D diffusion or transport solver in the axial dimension. Additional geometry capabilities are currently being developed in MPACT to support hexagonal-pitched lattices, as well as interstitial geometry (i.e., control rods at the corner of four adjacent pin cells). In this research, the MPACT method is tested on gas-cooled reactors by applying MPACT to full-core MAGNOX reactor test problems. MAGNOX test problems were chosen due to the availability of high-quality reactor design and validation data (available through an ongoing collaboration with the National Nuclear Laboratory in the United Kingdom) and the existence of a relatively complex axial power shape that is expected to challenge the MPACT method. MPACT's convergence for partial- and full-core problems will be tested and verified. MPACT will be compared with high-fidelity continuous-energy Monte Carlo simulations to verify core reactivity, power distributions, and performance of the available cross section data libraries and energy group structures.

KEYWORDS: MAGNOX, full-core neutron transport, gas-cooled reactor

### 1. INTRODUCTION

MPACT is a state-of-the-art neutron transport code developed jointly at Oak Ridge National Laboratory and the University of Michigan to perform high-fidelity analysis using whole-core, three-dimensional (3D), pin-resolved neutron transport calculations on modern parallel computing hardware. MPACT was originally developed to model light water reactors (LWRs) [1,2], but the two-dimensional–one-dimensional (2D-1D) neutron transport method [3,4] underlying the core simulator is agnostic to reactor type. Provided the core

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has a geometry extruded in the axial ( $z$ ) dimension, as is the case for many reactors, MPACT should be capable of performing neutronics calculations for non-LWR cores.

The capability of MPACT are being extended to simulate gas-cooled, graphite-moderated cores such as MAGNOX reactors [5]. Several advanced reactor concepts depend on gas coolants and/or graphite moderators [6]. MAGNOX reactors were operated in the United Kingdom for nearly 60 years (1956–2015), so a large volume of operational data is potentially available for validation purposes. Before MPACT can be validated against operational data, it first should be verified using code-to-code comparisons.

Work to methodically benchmark MPACT's neutronic calculations for MAGNOX reactors against reference solutions computed using an independent code base and methodology is summarized in these proceedings [7]. Additional work summarizing the development of a new MPACT cross section library for MAGNOX reactors [8] as well as development of AGREE for a thermal modeling capability [9] is also provided in these proceedings. The research described herein is focused on the ability of MPACT to converge for large 3D MAGNOX simulations and on the comparison of the pin power and eigenvalue ( $k_{\text{eff}}$ ) results to full-core Monte Carlo reference solutions. The full-core reference solutions summarized herein were generated using Shift [10], a newly developed Monte Carlo code for fixed source and eigenvalue calculations designed to be scalable to very large computational clusters.

### 1.1. MAGNOX Reactor Design

MAGNOX reactors are graphite-moderated,  $\text{CO}_2$ -cooled systems that use natural uranium metal fuel clad in magnesium. MAGNOX cores primarily consist of a large graphite structure (“pile”) constructed by stacking graphite blocks vertically within the core vessel. Vertical channels in the graphite blocks house five to six fuel elements stacked atop one another. More modern MAGNOX fuel elements use a “herringbone” fin pattern on the fuel elements to enhance cooling. A control rod channel is located at the center of each  $4 \times 4$  set of fuel pins (a  $4 \times 4$  set of pins is typically referred to as a “charge pan”). For the research summarized herein, the Calder Hall design [5] was used, which contains three different radial zones with different cooling channel sizes to allow more coolant to flow through the center of the reactor and less coolant to flow through the outer channels. The varying coolant channel size also changes the neutron spectrum throughout the system, as there is less graphite to moderate neutrons in the center of the reactor versus the periphery of the reactor. Exact design dimensions of the fuel elements, cooling channels, control rods, etc., can be found elsewhere [5].

Of particular interest in this work is the method of stacking fuel slugs atop one another in MAGNOX reactors, which creates an unfueled region between fuel slugs due to the presence of the fuel end cap. The unfueled regions yield increased moderation of neutrons at the axial ends of the fuel slugs that results in power peaking. MPACT, which uses a 1D axial coupling method in the  $z$ -dimension [3], has been primarily developed for modeling LWRs, which have a smoother axial power shape (with exception of grid spacers). A primary research question to resolve is the capability of the 1D axial coupling methods to model this complex axial power shape.

## 2. MAGNOX REACTOR TEST PROBLEMS

Several test problems covering a wider range of conditions, but smaller geometries, is provided in Ref. 7. The test problems developed for this work specifically test MPACT's ability to simulate and predict  $k_{\text{eff}}$  and pin power at the core level. For these studies, a full-length  $\frac{1}{4}$ -core model was developed. A number of control rod insertion layouts were selected for testing, and two control rod depths within these layouts were tested.

## 2.1. Calder Hall Quarter-Core Models

The Calder Hall  $\frac{1}{4}$ -core model was developed using the native MPACT input, which allows the user full control of the geometry construction, including radial rings, axial levels, radial and azimuthal meshing, etc. The corresponding Shift reference solution model was constructed using the SCALE generalized geometry. The true Calder Hall geometry was simplified somewhat for these studies. Fuel end plugs were assumed to consist of magnesium, conserving the overall mass and axial length of the end plugs. The fuel elements were assumed to rest on a graphite axial reflector, while in the true geometry, the fuel elements rest on a specially designed bottom support that contains a mixture of materials including graphite and steel, which in turn rests on the core support plate. A graphite top axial reflector was also assumed through which the fuel channels extend to the top of the model.

The MPACT model contains 11 axial regions per fuel slug and 10 radial regions within each fuel pin for mesh refinement and future depletion analysis. The Shift model contains 11 axial regions per fuel slugs (same axial boundaries as the MPACT model) with a single radial ring. A figure showing the MPACT fuel pin and charge pan meshing can be found in Figure 1. When comparisons are made, the power over the 10 radial fuel rings in the MPACT is integrated to yield a pin-averaged power. One difference between the MPACT and Shift models is the way the radial reflector is treated. MPACT currently uses a “blocked” radial reflector boundary that has a jagged boundary made up of square reflector blocks, while the Shift model uses a true cylinder for the radial reflector, as shown in Figure 2. Also note that although the models in Figure 2 appear to be  $\frac{1}{8}$ <sup>th</sup> symmetric, they are not—the southwest corner of the geometry contains a number of five-slug fuel channels that the corresponding northeast channels do not.

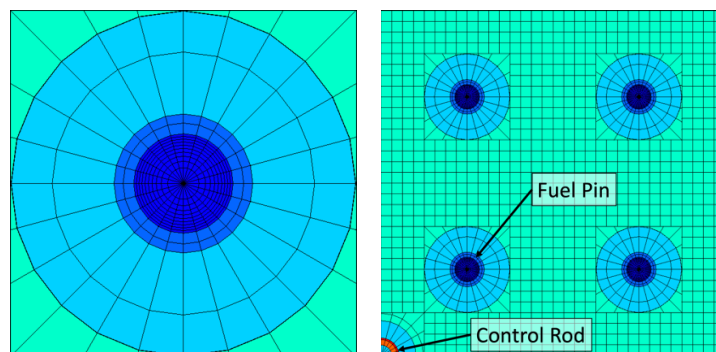


Figure 1. MPACT model meshing in the fuel pin (left) and charge pan (right).

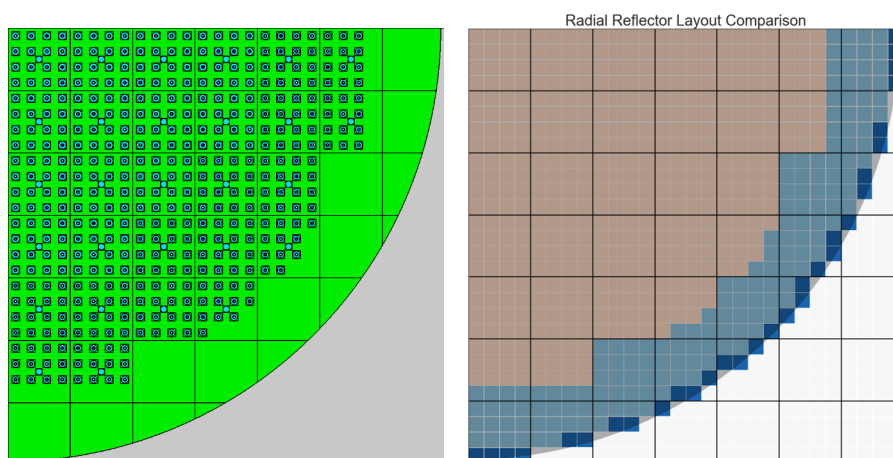


Figure 2. Plot of an axial slice in the Shift model (left) and comparison of radial reflector layout between MPACT and Shift (right) showing “clipped” reflector blocks in dark blue.

For Shift, the continuous-energy ENDF/B-VII.1 cross section library that is deployed with the SCALE [11] code system was chosen. All MPACT simulations herein use the new specially-developed 69-group MAGNOX cross section library; further details of the cross section processing method and cross section library can be found elsewhere in the proceedings [7,8].

## 2.2. Control Rod Insertion Maps

In addition to a model with no control rods inserted, nine control rod insertion maps (CRMs) were chosen for MPACT and Shift comparisons. Within these nine control rod maps, insertion depths of 50% and 100% were simulated in both MPACT and Shift. CRM-1 – CRM-4 used a single control rod inserted along the diagonal symmetry plane (from northwest to southeast corner in Figure 2 and Figure 3), while CRM-5 – CRM-9 have more than a single rod inserted. Graphical depictions of the tested control rod maps are shown in Figure 3. CRM-1, 2, 3, and 4 are all shown in the figure (upper left: red, blue, green, yellow, respectively), and for each different color, only that particular rod is inserted.

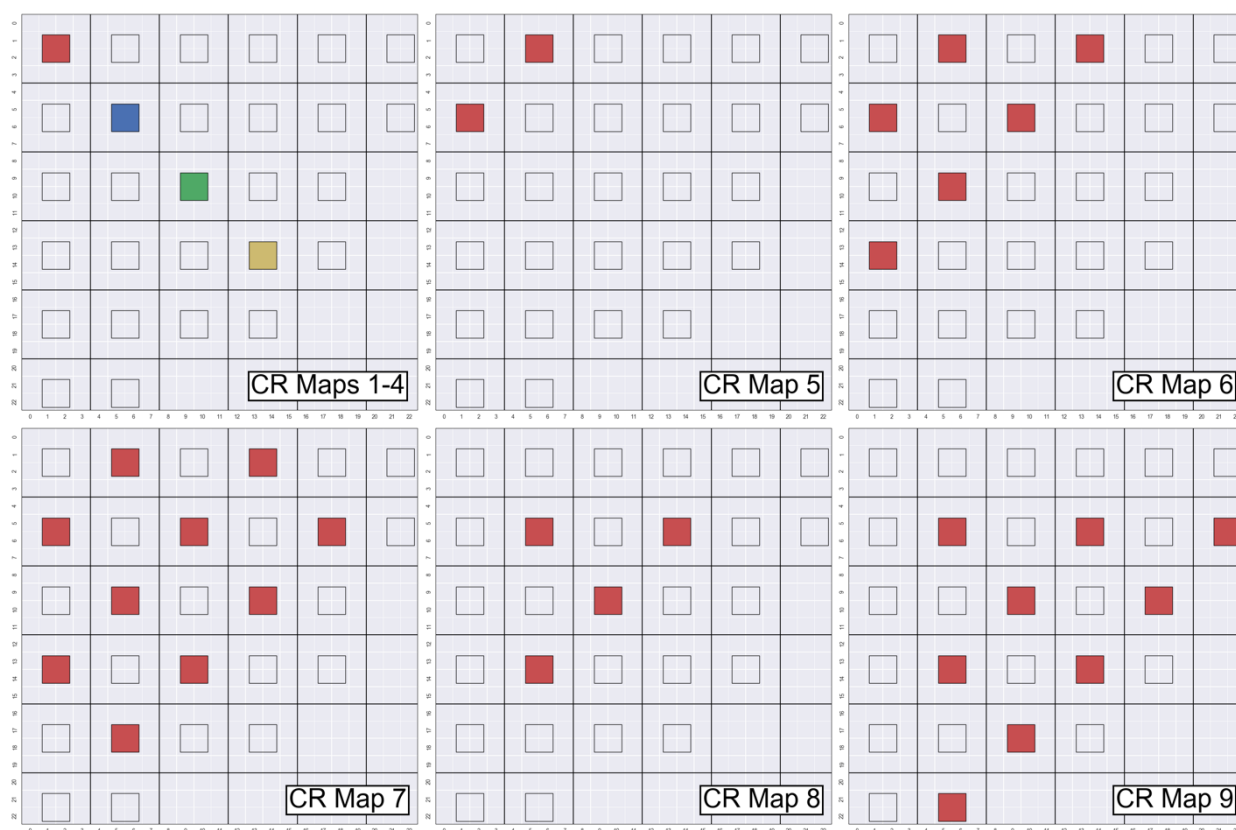


Figure 3. Control rod maps tested. CRM-1 – CRM-4 are shown in the same figure (upper left).

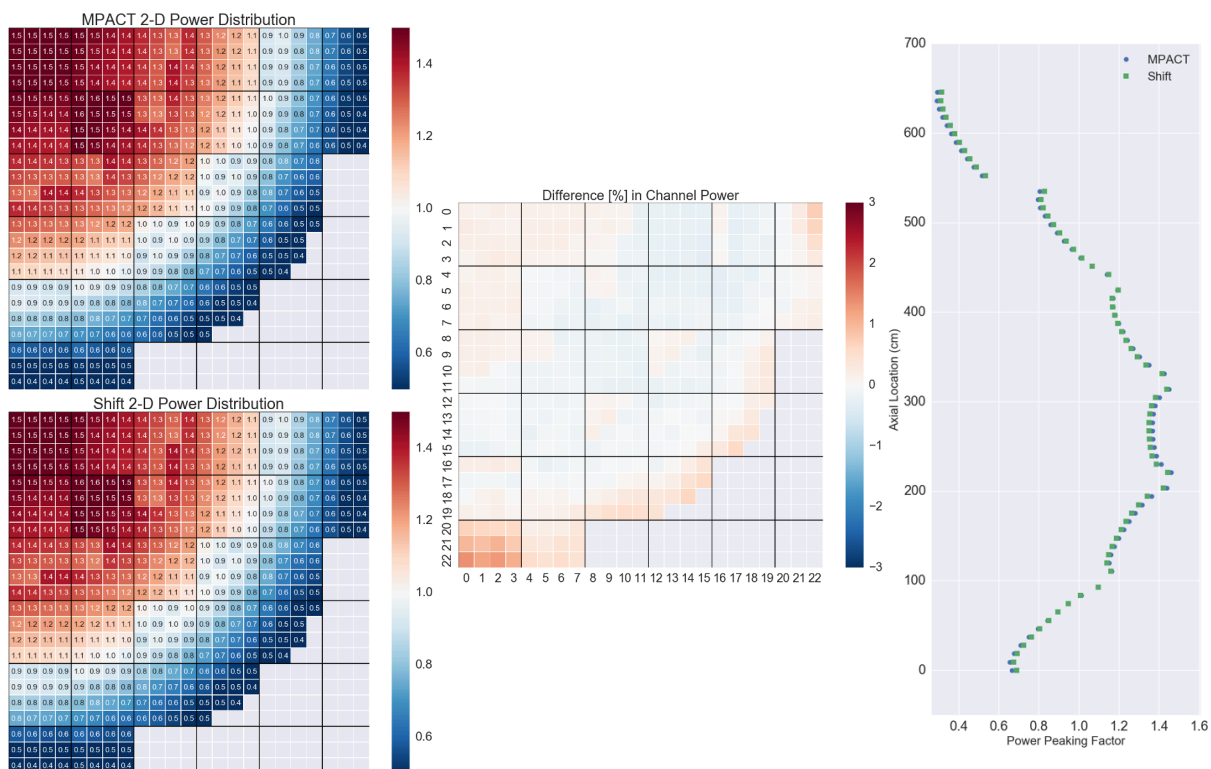
## 3. RESULTS

Quantities of interest (QOIs) for these analyses are primarily  $k_{eff}$ ,  $\Delta k_{eff}$  from the rods-out case, and root-mean-square (RMS) deviation for fuel region power distribution. For the RMS comparisons, axial, radial, and 3D RMS values are calculated and provided. The axial RMS values are calculated by integrating each 2D core slice to yield a core level axial power profile, and the RMS is then calculated between those two axial profiles. The radial RMS is calculated by integrating the axial power profile in each fuel channel, and

the RMS is then calculated between the MPACT and Shift solutions. The 3D RMS is calculated over all fuel regions in the models.

### 3.1. Rods Out Results

The BOL control-rods-out simulations yield  $k_{\text{eff,MPACT}} = 1.03085$  and  $k_{\text{eff,Shift}} = 1.03381$ , and a  $\Delta k_{\text{eff}} = -296$  percent mille ( $1 \text{ pcm} = 10^{-5}$ ). All Shift calculated  $k_{\text{eff}}$  values have an estimated standard deviation of less than 2 pcm. The MPACT and Shift axially integrated channel peaking factors can be found in Figure 4, along with a comparison (percent difference) for the power distributions. The largest channel-power-distribution differences are observed along the southwest corner of the model. This particular location contains a number of channels in which five fuel slugs are stacked instead of the normal six fuel slugs; however, there are a number of other channels in the model that contain five slugs instead of six that do not yield large differences in power. Larger channel power differences are also observed for the radial periphery of the reactor than for pins internal to the reactor. Overall, the radial power distributions compare very well, with a difference of less than 0.2% in most channels. Comparison of the axial power shape indicates that MPACT accurately predicts the overall axial power shape; however, slightly larger relative biases are observed at the axial ends of the top and bottom of the reactor than in the center of the reactor. Overall, MPACT predicts a slightly more center peaked power distribution than Shift. The overall radial, axial, and 3D pin power RMS values are 0.20%, 1.26%, and 1.38%, respectively.



**Figure 4. Radial and axial power distribution comparison for all control rods removed.**

### 3.2. Control Rod Insertion $k_{\text{eff}}$ Results

The control rod insertion  $k_{\text{eff}}$  values and control rod worths are summarized in Table I. The results of these comparisons are very good—MPACT agrees with the Shift reference solution within less than 305 pcm for all 50% insertion cases (average of 288 pcm) and less than 385 pcm for all 100% insertion cases (average of 331 pcm). The computed control rod worths for Shift and MPACT agree very well—less than 50 pcm

for all 50% insertion cases and less than 100 pcm for all 100% insertion cases. These results indicate that MPACT is accurately predicting the worth of inserted control rods when compared with a Shift reference solution. It should be noted that one MPACT cases failed to converge (CRM-7 at 100% insertion); the cause and potential solution of these convergence issues are still being investigated.

**Table I. Summary of control rod insertion  $k_{\text{eff}}$  results and rod worths.**

CRM	Depth	MPACT $k_{\text{eff}}$	Shift $k_{\text{eff}}$	M-S $\Delta k^2$ (pcm)	Worth <sup>1,2</sup> (pcm)	M-S $\Delta$ Worth <sup>2</sup> (pcm)
1	50%	1.02753	1.03058	-305	324	8
2	50%	1.02733	1.03030	-297	351	0
3	50%	1.02851	1.03148	-297	234	0
4	50%	1.03000	1.03295	-295	86	-1
5	50%	1.02461	1.02757	-296	624	0
6	50%	1.01743	1.02016	-274	1365	-23
7	50%	1.01473	1.01728	-255	1653	-42
8	50%	1.02215	1.02504	-290	877	-7
9	50%	1.02064	1.02350	-286	1031	10
<b>Average (sd)</b>				-288 (15)		-6 (16)
1	100%	1.02352	1.02673	-321	709	24
2	100%	1.02258	1.02574	-317	807	20
3	100%	1.02568	1.02876	-307	506	11
4	100%	1.02911	1.03213	-303	168	6
5	100%	1.01655	1.01991	-335	1391	39
6	100%	0.99137	0.99522	-385	3859	89
7	100%	DNF	0.97583	—	5799	—
8	100%	1.00768	1.01115	-346	2267	50
9	100%	1.00308	1.00668	-359	2714	63
<b>Average (sd)</b>				-331 (28)		34 (28)

<sup>1</sup>CR worth as calculated by Shift

<sup>2</sup>Some values differ by 1 pcm compared to associated  $k_{\text{eff}}$  values due to the amount of significant digits shown in the table

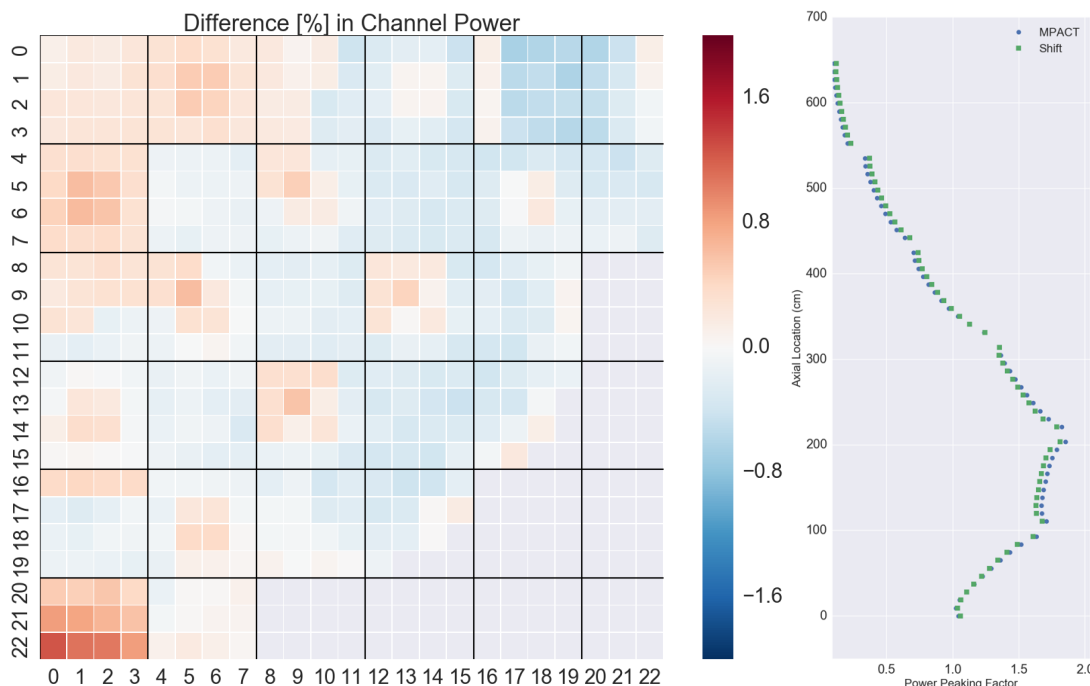
### 3.3. Control Rod Insertion Pin Power Results

A summary of the control rod insertion pin power results can be found in Table II. These results indicate that in addition to being able to accurately predict the reactivity effect of the control rods, MPACT can also accurately predict the pin power distribution under these scenarios. In general, MPACT more accurately predicts the pin power distribution under fully inserted control rod cases than for partially inserted cases. This is expected as partially inserted control rods yield a more complex axial power shape for which the 1D axially coupling method may have more difficulty than when the control rods are fully inserted. For the cases with many rods inserted to half-depth, the axial and 3D pin power RMS nears 3.0%. However, for the fully inserted cases, the pin power RMS results are on the same level of accuracy as the rods-out case (Section 3.1).

Figure 5 shows the difference in radial and axial pin power distribution for CRM-7 at 50% insertion depth. Figure 5 indicates that MPACT, as in the control rods out case, struggles to predict the radial power distribution in the southwest corner of the problem. There are a few reasons MPACT may be struggling in this region. The results presented herein show that MPACT has more difficulty predicting the axial power shape for five-slug channels than for six-slug channels and more difficulty in predicting the power in the radial periphery of the reactor. The southwest corner of this geometry contains both of these issues. This could also be due in part to Monte Carlo statistics—this region is a particularly low power regions, so larger pin power uncertainties exist for this region. However, all estimated pin power uncertainties are less than 1%, and running selected additional cases to great precision did not reduce this bias significantly. Regardless, further investigation of this issues is planned.

**Table II. Summary of control rod insertion pin power results.**

CRM	50% Insertion			100% Insertion		
	Radial RMS	Axial RMS	3D RMS	Radial RMS	Axial RMS	3D RMS
1	0.32%	1.40%	1.54%	0.26%	1.27%	1.36%
2	0.30%	1.44%	1.57%	0.29%	1.28%	1.38%
3	0.22%	1.30%	1.41%	0.21%	1.24%	1.35%
4	0.22%	1.31%	1.42%	0.19%	1.25%	1.37%
5	0.51%	1.77%	1.95%	0.33%	1.32%	1.42%
6	0.61%	2.64%	2.79%	0.49%	1.35%	1.48%
7	0.29%	2.84%	2.93%	—	—	—
8	0.23%	2.11%	2.21%	0.22%	1.27%	1.39%
9	0.32%	2.23%	2.35%	0.23%	1.21%	1.39%



**Figure 5. Radial and axial power distribution comparison for CRM-7 at 50% insertion depth.**

### 3.4. Computational Performance

Comparison of the computational speed between MPACT and Shift is somewhat difficult for these models as the models use the same axial mesh in the fuel elements, but a different radial mesh within the fuel pin. The MPACT calculations use 10 radial rings in the fuel (spatial detail inside the pin is being used for other ongoing studies), while the Shift calculations use a single radial region within the pin. As a result, the MPACT models contain 10 times the number of spatial regions in the fuel when compared to the Shift models. In addition, these calculations were run on different computer clusters, with slightly different architecture and performance. Within this work, Shift is used only to provide a reference solution for overall performance metrics, and MPACT will be used for detailed depletion studies. Regardless of the differences, comparison of the computational performance of the two codes can be useful.

All Shift calculations were run on 192 CPUs, and generally require on the order of 10 hours of CPU time. These calculations use 2 million particles per cycle, for 1200 total cycles with the first 200 cycles skipped for fission source convergence (total of 2.4 billion total particle histories). These calculations include tallying the power distribution over the more than 27000 fuel cell regions. The average, minimum, and maximum estimated standard deviation associated with these tallies are 0.30%, 0.18%, and 0.66%, respectively. All MPACT calculations were run on 384 CPUs and required an average of 5.6 hours of CPU time. The MPACT calculations use convergence criteria of  $1.0E-6$  for eigenvalue and  $1.0E-5$  for region flux. Multiplying CPU time by the total number of CPUs used yields 1920 CPU-hours for the Shift calculations and 2227 CPU-hours for the MPACT calculations. Of course, these numbers change significantly if Shift is run so that tallies reach lower estimated standard deviations or tighter convergence criteria are used for the Shift calculations.

These simulations only compare beginning-of-life (BOL) states, however, over depletion calculations, the MPACT simulation far outperforms the Shift calculations in terms of computational performance. Once the fuel mixtures are depleted and contain a number of isotopes, the Shift Monte Carlo performance degrades significantly. However, MPACT uses the previous flux and power distribution as a starting point for the next depletion step, and as a result, subsequent depletion steps (transport calculations) typically require only ~30% of the time required for the initial transport calculation.

## 4. CONCLUSIONS

MPACT has been extended to simulate gas-cooled, graphite-moderated cores such as MAGNOX reactors [7,8,9]. Using Calder Hall [5] as a test bed, the full-core performance of MPACT has been tested using a computational reference solution from the Shift Monte Carlo neutron transport code. The results indicated that MPACT can accurately predict both the reactivity ( $k_{\text{eff}}$ ) and pin power distribution for cases in which control rods are removed, inserted partially, and inserted to full depth as compared to the reference solution. MPACT predicted control rod worth values within 100 pcm of Shift for all cases. The 3D pin power distributions all yielded RMS errors of less than 3.0% for the partially inserted control rod cases and less than 1.5% for all the fully inserted control rods cases.

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