MPACT VERIFICATION WITH MAGNOX REACTOR NEUTRONICS PROGRESSION PROBLEMS

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ABSTRACT

MPACT is a state-of-the-art core simulator designed to perform high-fidelity analysis using whole-core, three-dimensional, pin-resolved neutron transport calculations on modern parallel computing hardware. MPACT was originally developed to model light water reactors, and its capabilities are being extended to simulate gas-cooled, graphite-moderated cores such as Magnox reactors. To verify MPACT's performance in this new application, the code is being formally benchmarked using representative problems. Progression problems are a series of example models that increase in complexity designed to test a code's performance. The progression problems include both beginning-of-cycle and depletion calculations. Reference solutions for each progression problem have been generated using Serpent 2, a continuous-energy Monte Carlo reactor physics burnup calculation code.

Using the neutron multiplication eigenvalue k_{eff} as a metric, MPACT's performance is assessed on each of the progression problems. Initial results showed that MPACT's multigroup cross section libraries, originally developed for pressurized water reactor problems, were not sufficient to accurately solve Magnox problems. MPACT's improved performance on the progression problems is demonstrated using this new optimized cross section library.

KEYWORDS: Magnox, MPACT, MOC, 2D-1D, Serpent

1. INTRODUCTION

MPACT is a state-of-the-art core simulator 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

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was originally developed to model light water reactors (LWRs) [1], but the two-dimensional–one-dimensional (2D-1D) neutron transport method [2] underlying the core simulator is agnostic to reactor type. Provided the core has a geometry extruded in the axial (z) dimension, as is the case for many reactors, a modified version of MPACT should be capable of performing neutronics calculations for non-LWR cores.

MPACT is being extended to simulate gas-cooled, graphite-moderated cores such as Magnox reactors. Several advanced reactor concepts depend on gas coolants or graphite moderators, and some concepts rely on both [3]. 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 the modified MPACT code can be validated against operational data, it first should be verified using code-to-code comparisons.

The purpose of this work is to methodically benchmark MPACT's neutronic calculations for Magnox reactors against reference solutions computed using an independent code base and methodology. A series of progression problems have been created for Magnox reactors. A similar series of progression problems describing pressurized water reactor problems was prepared during the initial stages of the Consortium for Advanced Simulation of LWRs project [4]. These problems evolve from simple 2D pin-cells through more complicated geometries and conditions to a 3D full core. The reference solutions for these progression problems have been computed using Serpent 2, a continuous-energy Monte Carlo reactor physics burnup calculation code developed at VTT Technical Research Centre of Finland Ltd. [5]. Presented herein are the k_{eff} results for the 2D progression problems; the results for the 3D core simulation are presented elsewhere in these proceedings [6].

2. PROGRESSION PROBLEMS

The progression problems are organized primarily by geometry. Problem category 1 is the collection of all 2D pin-cell calculations. Although Magnox reactors use stackable fuel elements rather than fuel pins, a single fuel channel model is analogous to a single LWR fuel pin. Problem category 2 is the collection of problems that model slightly more complex 2D geometry—a collection of 16 fuel channels with a central control rod channel known as a *charge pan*. This problem category is analogous to an LWR fuel lattice, except Magnox cores do not employ variable enrichments and burnable absorbers in a charge pan. Problem category 3 is the collection of problems that model a 2D symmetric quarter core with graphite reflector geometry. The geometries for the three progression problem categories are shown in Figure 1.

Secondarily, the progression problems are organized by the type of calculation being performed. Problem type 1 calculations are single state point problems, such as those at beginning-of-cycle (BOC), middle-of-cycle (MOC), and end-of-cycle (EOC). Problem type 2 computations are depletion calculations. Depletion problems for MPACT and Serpent 2 use the same number and size of time steps, and the k_{eff} values are compared at the same burnup. A burnup interval weighted root-mean discrepancy value is computed using Eqs. 1 and 2, where N is the total number of burnup steps, B_i is the burnup at step i, $k_{\text{eff}}^{(\text{MPACT})}(B_i)$ is eigenvalue computed by MPACT at burnup step

(a) Problem 1: Pin-Cell   (b) Problem 2: Charge Pan   (c) Problem 3: Quarter Core
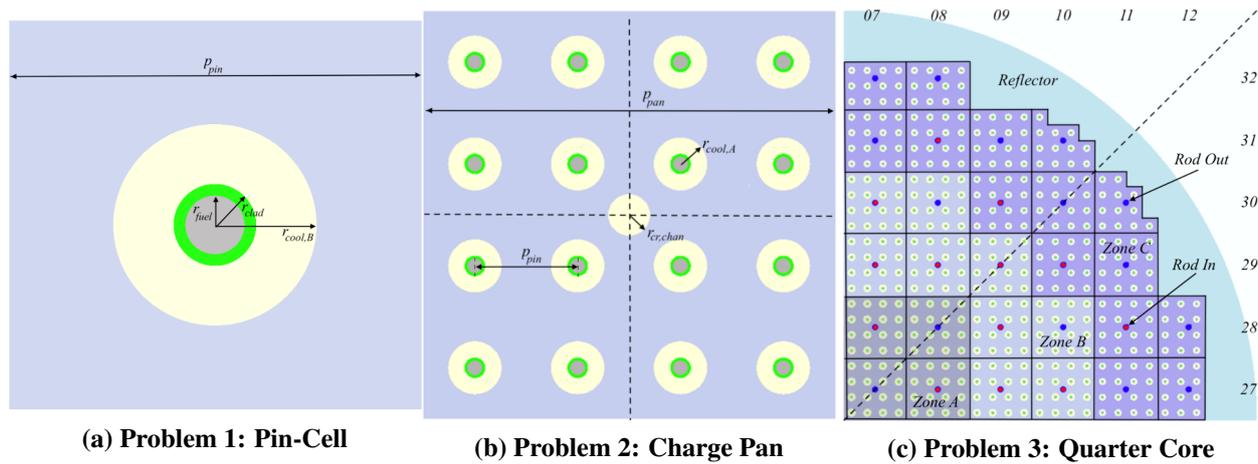
Figure 1: Magnox progression problem geometries.

i, and $k_{\text{eff}}^{(\text{Serpent})}(B_i)$ is the reference eigenvalue computed by Serpent 2.

$$\Delta k_i^2 = \left(k_{\text{eff}}^{(\text{MPACT})}(B_i) - k_{\text{eff}}^{(\text{Serpent})}(B_i) \right)^2 \qquad\qquad i = 1, 2..., (N) \tag{1}$$

$$\overline{\Delta k} = \left(\frac{1}{2B_N} \left(B_1 \Delta k_0^2 + \left(\sum_{i=1}^{N-1} [B_{i+1} - B_{i-1}] \Delta k_i^2 \right) + [B_N - B_{N-1}] \Delta k_N^2 \right) \right)^{1/2} \tag{2}$$

The $\overline{\Delta k}$ value will always be positive regardless of the sign of the discrepancy at each burnup state point.

A nomenclature is now defined to describe the progression problems. All pin-cell problems are numbered 1.x with single state point problems are numbered 1.1, and depletion problems are numbered 1.2. Charge pan single state point problems are numbered 2.1, and charge pan problems depletion are numbered 2.1. Quarter core single state point problems are numbered 3.1, and quarter core depletion problems are numbered 3.2. Problems are further organized by minor modifications to geometry, temperature, burnup, enrichment, and the presence or absence of control rods. These modifications extend the nomenclature. For example, a BOC pin-cell problem using temperature profile I is problem 1.1.06, but a BOC pin-cell problem using a temperature profile II is problem 1.1.07.

The geometry variations in these progression problems are based on documentation for the Calder Hall 1 reactor at the Sellafield site near Seascale in the United Kingdom [7]. The core has three radial zones, each with a different coolant channel outer radius: zone A is 5.28 cm, zone B is 5.02 cm, and zone C is 4.58 cm. Each coolant channel radius is in its own case within pin cell and charge pan problems.

To test the full range of expected temperatures, five temperature profiles are used. The temperature profiles are shown in Table 1. Profile I corresponds to typical operating temperatures, and profile II corresponds to cold zero-power temperatures. Profiles III, IV, and V test a range of fuel temperatures while keeping the clad, coolant, and moderator temperatures constant. Serpent 2 uses

Table 1: Temperature Profiles

Temperature Profile	Fuel (K)	Clad (K)	Coolant (K)	Moderator (K)
I	698.15	533.59	511.15	523.15
II	300.00	300.00	300.00	300.00
III	600.00	600.00	600.00	600.00
IV	900.00	600.00	600.00	600.00
V	1200.00	600.00	600.00	600.00

300 K, 600 K, 900 K, and 1200 K library temperatures, so direct comparisons to the Monte Carlo solutions can be made without on-the-fly Doppler broadening.

The pin-cell problems also include variation due to burnup and enrichment (^{235}U wt%). Magnox reactors are typically fueled with natural uranium, but low-enriched fuel is used in some pin-cell progression problems to verify the robustness of the cross section library over the expected range of enrichments. Single state points include the following burnups: BOC at 0.0 MWd/MtU, MOC at 600.0 MWd/MtU, and EOC at 1200.0 MWd/MtU. Table 2 lists the enrichment and burnup variations for the pin-cell progression problems.

Table 2: Single State Point Pin-Cell Problem Variations

Problem #	Coolant Zone	Temp. Profile	Burnup $\left(\frac{\text{MWd}}{\text{MtU}}\right)$	^{235}U (wt%)	Problem #	Coolant Zone	Temp. Profile	Burnup $\left(\frac{\text{MWd}}{\text{MtU}}\right)$	^{235}U (wt%)
1.1.01	A	I	0.0	0.711	1.1.17	B	II	600.0	0.711
1.1.02	A	II	0.0	0.711	1.1.18	B	III	600.0	0.711
1.1.03	A	III	0.0	0.711	1.1.19	B	IV	600.0	0.711
1.1.04	A	IV	0.0	0.711	1.1.20	B	V	600.0	0.711
1.1.05	A	V	0.0	0.711	1.1.21	B	I	1200.0	0.711
1.1.06	B	I	0.0	0.711	1.1.22	B	II	1200.0	0.711
1.1.07	B	II	0.0	0.711	1.1.23	B	III	1200.0	0.711
1.1.08	B	III	0.0	0.711	1.1.24	B	IV	1200.0	0.711
1.1.09	B	IV	0.0	0.711	1.1.25	B	V	1200.0	0.711
1.1.10	B	V	0.0	0.711	1.1.26	B	IV	0.0	1.000
1.1.11	C	I	0.0	0.711	1.1.27	B	IV	0.0	2.000
1.1.12	C	II	0.0	0.711	1.1.28	B	IV	0.0	3.000
1.1.13	C	III	0.0	0.711	1.1.29	B	IV	0.0	4.000
1.1.14	C	IV	0.0	0.711	1.2.01	A	IV	Depletion	0.711
1.1.15	C	V	0.0	0.711	1.2.02	B	IV	Depletion	0.711
1.1.16	B	I	600.0	0.711	1.2.03	C	IV	Depletion	0.711

An additional problem variation used is the presence of control rods for the charge pan and quarter core geometries. Control rods used in the Calder Hall reactor are axially heterogeneous, with steel composed of 3 wt% and steel composed of 4 wt% absorber regions and a stainless steel tip. The rodded charge pan problems use all 3 types of material, while the all-rods-in (ARI) quarter core problems use the steel composed of 3 wt%. The all-rods-out (ARO) problems use only coolant in the control rod channel. Table 3 lists control rod and other variations for the charge pan progression problems, and Table 4 lists the quarter core problems.

Table 3: Natural Uranium Charge Pan BOC Problems

Problem #	Coolant Zone	Temp Profile	Control Rod	Problem #	Coolant Zone	Temp. Profile	Control Rod
2.1.01	A	I	None	2.1.16	A	IV	Stainless Steel
2.1.02	A	II	None	2.1.17	A	IV	Steel (Boron 3%)
2.1.03	A	III	None	2.1.18	A	IV	Steel (Boron 4%)
2.1.04	A	IV	None	2.1.19	B	IV	Stainless Steel
2.1.05	B	V	None	2.1.20	B	IV	Steel (Boron 3%)
2.1.06	B	I	None	2.1.21	B	IV	Steel (Boron 4%)
2.1.07	B	II	None	2.1.22	C	IV	Stainless Steel
2.1.08	B	III	None	2.1.23	C	IV	Steel (Boron 3%)
2.1.09	B	IV	None	2.1.24	C	IV	Steel (Boron 4%)
2.1.10	B	V	None	2.2.01	A	IV	None
2.1.11	C	I	None	2.2.02	B	IV	None
2.1.12	C	II	None	2.2.03	C	IV	None
2.1.13	C	III	None	2.2.04	B	IV	Stainless Steel
2.1.14	C	IV	None	2.2.05	B	IV	Steel (Boron 3%)
2.1.15	C	V	None	2.2.06	B	IV	Steel (Boron 4%)

Table 4: Natural Uranium Quarter Core BOC Problems

Problem #	Temp. Profile	Control Rod	Problem #	Temp. Profile	Control Rod
3.1.1	III	ARO	3.1.4	III	ARI
3.1.2	IV	ARO	3.1.5	IV	ARI
3.1.3	V	ARO	3.1.6	V	ARI

Reference solutions were computed using Serpent 2.1.31. Monte Carlo convergence of k_{eff} eigenvalues varied by problem. The least converged problem had a standard error of 24 pcm, the most converged problem had a standard error of 7 pcm, and the average standard error of all problems is 20 pcm. Power normalization and fission heating terms are set in Serpent to be the same as those used by MPACT to ensure valid comparisons between the two codes throughout depletion.

3. COMPARISON OF MPACT RESULTS WITH REFERENCE SOLUTIONS

Initial MPACT calculations computed k_{eff} eigenvalues using the multigroup cross section libraries with 47 and 51 energy groups developed for LWRs during the Consortium for Advanced Simulation of LWRs project. This proved inadequate as k_{eff} eigenvalues were discrepant by > 1000 pcm (percent mille), i.e. a descrepancy of 1%, for even simple pin-cell calculations. This initiated development of a new 69-group cross section library designed specifically for Magnox reactors [8].

A comparison of MPACT's computed k_{eff} eigenvalues with reference solutions computed by Serpent 2 is shown in Figure 2. These results were computed using the 69-group cross section library, and the agreement with the reference solutions is significantly better than values computed with the multigroup libraries developed for LWR analysis.
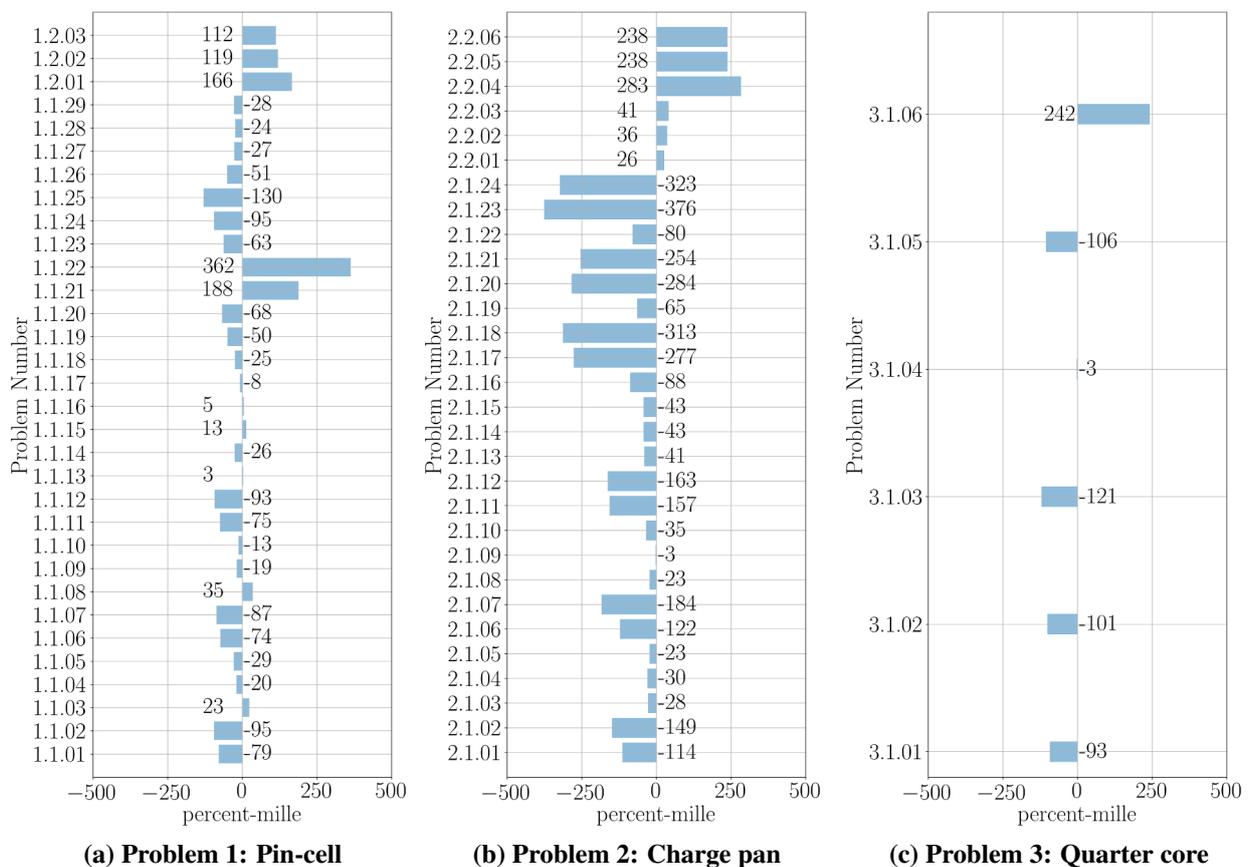

(a) Problem 1: Pin-cell   (b) Problem 2: Charge pan   (c) Problem 3: Quarter core

Figure 2: Comparison of k_{eff} values.

4. CONCLUSIONS AND FUTURE WORK

For the pin-cell problems, the greatest k_{eff} discrepancies between MPACT and the reference solutions occur at the lower temperature profiles II (problems 1.1.02, 1.1.07, and 1.1.12) and I (prob-

lems 1.1.01, 1.1.06, and 1.1.11). This is consistent for zones A, B, and C. Differences in k_{eff} within a specified temperature profile among zones is minimal, but agreement improves slightly as the coolant channel radius decreases (e.g., compare problems 1.1.05, 1.1.10, and 1.1.15). For zone B, the discrepancy decreases at MOC for temperature profiles III, IV, and V, and then it slightly increases at EOC. For temperature profiles I and II, the results change from a negative at BOC to a positive bias at MOC, which becomes even greater at EOC. The enriched fuel problems show generally better agreement at greater enrichments (problems 1.1.26–1.1.29). Except for problems using the lowest temperature profile II, all other pin-cell problems demonstrate reasonable agreement with the reference solutions. Recall that temperature profile II is cold zero-power conditions, so actual fuel depletion using these temperatures is unphysical (isotopics used in problems 1.1.17 and 1.1.22).

For the charge pan problems, similar trends to the pin-cell cases are seen in the the unrodded problems (2.1.01–2.1.15) as expected. For the rodded BOC problems (2.1.16–2.1.24), agreement with the reference solutions generally decreases as boron weight percent increases. There is no clear trend across the three coolant channel radii. In the unrodded depletion problems (2.2.01 and 2.2.03) for zones A and C, the burnup interval averaged root-mean discrepancy $\overline{\Delta k}$ is nearly the same the BOC value (problems 2.1.04 and 2.1.14), implying the bias is nearly constant over the cycle. The $\overline{\Delta k}$ value from the unrodded zone B depletion problem (2.2.02) is noticeably larger than the BOC value (problem 2.1.09). The reason for this is unclear, but it may be due to Monte Carlo statistics because both the $\overline{\Delta k}$ and BOC k_{eff} are in excellent agreement with the reference solutions. In the rodded charge pan depletion problems (2.2.04–2.2.06), the $\overline{\Delta k}$ is less than the BOC discrepancy for each rod type, implying that the bias decreases with burnup.

For the quarter core unrodded BOC problems (3.1.1–3.1.3), all discrepancies are less than 125 pcm, with the greatest agreement (101 pcm) at temperature profile IV, which is near to nominal operating temperatures. The full core problem discrepancies are generally consistent with the charge pan and pin cell problems, and the biases are acceptably low.

These progression problems demonstrate that the MPACT and the newly developed 69-group library are generally excellent for unrodded Magnox reactor analysis over a range of operating conditions. They also demonstrate that computations using temperatures significantly lower than operating temperatures may have unacceptably large k_{eff} biases. The rodded cases deviate from the reference solutions more than unrodded problems so further development of the 69-group cross-section library may be needed for rodded cases.

Further refinement of the cross section library for better agreement with the rodded problems is an area for future work. Additionally, other metrics, such as power distributions and isotopic concentrations during depletion, will be used to verify MPACT is accurate for Magnox reactor analysis. This verification effort only considered neutronic calculations, but MPACT is a core simulator capable of neutronic feedback from a coupled thermal code. A specially developed thermal code called AGREE has been developed for this purpose. Future work will include verification of a coupled MPACT-AGREE code for Magnox reactor analyses. After these verification efforts are complete, future work includes validation of MPACT-AGREE using operational cycle data from the Calder Hall 1 reactor.

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