MPACT VERIFICATION WITH MAGNOX REACTOR NEUTRONICS PROGRESSION PROBLEMS

Nicholas P. Luciano, Brian J. Ade, Kang Seog Kim, Andrew J. Conant*  
Oak Ridge National Laboratory  
PO Box 2008, MS6165 Oak Ridge, TN 37831-6165  
lucianonp@ornl.gov, adebj@ornl.gov, kimk1@ornl.gov, conantaj@ornl.gov

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 $k_{\text{eff}}$ 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

*Notice: This manuscript has been authored by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the US Department of Energy (DOE). The US government retains and the publisher, by accepting the article for publication, acknowledges that the US government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this manuscript, or allow others to do so, for US government purposes. DOE will provide public access to these results of federally sponsored research in accordance with the DOE Public Access Plan (http://energy.gov/downloads/doe-public-access-plan).

© The Authors, published by EDP Sciences. This is an open access article distributed under the terms of the Creative Commons Attribution License 4.0 (http://creativecommons.org/licenses/by/4.0/).
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 re-
actors. 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 valida-
tion 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 Mag-
nox reactors against reference solutions computed using an independent code base and methodol-
gy. 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 Ser-
pent 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 \(k_{\text{eff}}\) 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 col-
lection 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 collec-
tion 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 enrich-
ments 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 deple-
tion calculations. Depletion problems for MPACT and Serpent 2 use the same number and size of
time steps, and the \(k_{\text{eff}}\) 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
i, and $k_{\text{eff}}^{(\text{Serpent})}(B_i)$ is the reference eigenvalue computed by Serpent 2.

$$\Delta k_i^2 = \left( k_{\text{eff}}^{(\text{MPACT})}(B_i) - k_{\text{eff}}^{(\text{Serpent})}(B_i) \right)^2$$

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

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 (MWd/MtU) | $^{235}$U (wt%) | Problem # | Coolant Zone | Temp. Profile | Burnup (MWd/MtU) | $^{235}$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.

| 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%) |

| 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 $k_{\text{eff}}$ 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 $k_{\text{eff}}$ 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 $k_{\text{eff}}$ eigenvalues were discrepant by $>1000$ pcm (percent mille), i.e. a discrepancy 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 $k_{\text{eff}}$ 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.

![Figure 2: Comparison of $k_{\text{eff}}$ values.](image)

4. CONCLUSIONS AND FUTURE WORK

For the pin-cell problems, the greatest $k_{\text{eff}}$ 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 $k_{\text{eff}}$ 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 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 $\Delta k$ is nearly the same as the BOC value (problems 2.1.04 and 2.1.14), implying the bias is nearly constant over the cycle. The $\Delta k$ 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 $\Delta k$ and BOC $k_{\text{eff}}$ are in excellent agreement with the reference solutions. In the rodded charge pan depletion problems (2.2.04–2.2.06), the $\Delta k$ 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 $k_{\text{eff}}$ 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.
ACKNOWLEDGEMENTS

This work was funded by the Office of Defense Nuclear Nonproliferation Research and Development (NA-22), within the US Department of Energy’s National Nuclear Security Administration.

REFERENCES

[1] B. Collins, S. Stimpson, B. Kochunas, and T. Downar. “Assessment of the 2D/1D Implementation in MPACT.” In Proceedings of The International Conference on the Physics of Reactors PHYSOR 2014 - The Role of Reactor Physics towards a Sustainable Future. Kyoto, Japan (2014).

[2] B. Collins, S. Stimpson, B. Kelley, M. Young, B. Kochunas, A. Graham, E. Larsen, T. Downar, and A. Godfrey. “Stability and Accuracy of 3D Neutron Transport Simulations using the 2D/1D Method in MPACT.” Journal of Computational Physics, volume 326 (2016). URL https://doi.org/10.1016/j.jcp.2016.08.022.

[3] D. A. Arostegui and M. Holt. “Advanced Nuclear Reactors: Technology Overview and Current Issues.” Technical Report R45706, US Congressional Research Service, Washington, DC (2019). URL https://crsreports.congress.gov/product/pdf/R/R45706.

[4] A. T. Godfrey. “VERA Core Physics Benchmark Progression Problem Specifications.” Technical Report CASL-U-2012-0131-004, Oak Ridge National Laboratory, Oak Ridge, TN (2014). URL https://www.casl.gov/sites/default/files/docs/CASL-U-2012-0131-004.pdf.

[5] J. Leppnen, M. Pusa, T. Viitanen, V. Valtavirta, and T. Kaltiaisenaho. “The Serpent Monte Carlo Code: Status, Development and Applications in 2013.” Annals of Nuclear Energy, volume 82, pp. 142–150 (2015). URL http://www.sciencedirect.com/science/article/pii/S0306454914004095.

[6] B. J. Ade, N. P. Luciano, C. Gentry, S. Simpson, B. Collins, and R. Mills. “Development of MPACT for Full-Core Simulations of MAGNOX Gas-Cooled Nuclear Reactors.” In Proceedings of Physics of Reactors (PHYSOR) 2020: Transition to a Scalable Nuclear Future. University of Cambridge, UK (2020).

[7] S. E. Jensen and E. Nonbl. “Description of the Magnox Type of Gas Cooled Reactor (MAGNOX).” Technical Report NKS-2 ISBN 87-7893-050-2, Ris National Laboratory, Roskilde, Denmark (1998). URL https://inis.iaea.org/collection/NCLCollectionStore/Public/30/052/30052480.pdf.

[8] K. S. Kim, B. J. Ade, and N. P. Luciano. “Development of the MPACT 69-Group Library for the Magnox Reactor Analysis Using CASL VERA.” In Proceedings of Physics of Reactors (PHYSOR) 2020: Transition to a Scalable Nuclear Future. University of Cambridge, UK (2020).