

Transition Core Modeling for Extended Enrichment, Accident Tolerant Fuel Using PARCS/Polaris

Muhammad Rizki Oktavian¹, Ugur Merturek², and Yunlin Xu¹

¹School of Nuclear Engineering, Purdue University
516 Northwestern Ave., West Lafayette, IN 47906, USA

²Oak Ridge National Laboratory
1 Bethel Valley Rd., Oak Ridge, TN 37831, USA

rizkiokt@purdue.edu, mertureku@ornl.gov, yunlin@purdue.edu

[leave space for DOI, which will be inserted by ANS]

ABSTRACT

Current plans and efforts from reactor operators and vendors to include extended enrichment (EE) and accident-tolerant fuel (ATF) in current reactor fleets motivate the study of these changes in reactor physics analysis. This work uses the US Nuclear Regulatory Commission core simulator PARCS to do the core calculation and SCALE Polaris lattice physics code to generate the required homogenized, few-group constants. The lattice model used is based on the GE-14 10×10 assemblies with UO_2 fuels. Both nominal core and transition core are studied in this work, and both cores use GE-14 10×10 assemblies with UO_2 fuel. The nominal core uses regular UO_2 fuel with a maximum enrichment of 5 wt % and ZIRC-2 cladding. The ATF transition core uses FeCrAl cladding and regular UO_2 fuel with a maximum enrichment of 5 wt %, while the EE-ATF transition core uses FeCrAl cladding with UO_2 fuel with 8 max wt % enrichment. The accuracy presented in the colorset models verified the capability of the PARCS/Polaris procedures for the transition core analysis. For the whole core calculation, the ATF and EE-ATF transition core models were made in addition to the nominal core model. The core parameters to study are the core power distribution and power peaking factor, doppler temperature coefficients, and control rod worth at cold zero power and hot full power. Comparing the core parameters of the transition cores with the nominal core in PARCS, the results suggest that there is no unexpected outcome for the implementation of ATF and EE fuels.

KEYWORDS: transition core, extended enrichment, accident-tolerant fuel, PARCS, Polaris

1. INTRODUCTION

Commercial light water reactor (LWR) vendors and operators plan to include the extended enrichment (EE) and accident-tolerant fuel (ATF) designs in the current fleets of nuclear power plants. The additional fuel

* 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>).

enrichment in EE fuel designs (5–10% ^{235}U) has the main purpose to improve fuel economy in the current reactor fleet, enabling higher burnup than that of typical reactor fuels [1–2]. The ATF designs are used to improve the safety level of the fuel system under accident conditions [3].

Several types of ATF designs are being developed by various industry vendors, for either near-term or longer-term deployment. These designs include chromium-coated cladding, FeCrAl cladding, and doped fuels. Westinghouse is developing Advanced Doped Pellet Technology in chromium-coated zirconium alloy cladding [4]. Framatome, on the other hand, continues to develop chromium-coated M5 cladding with chromia-enhanced uranium oxide [5]. Global Nuclear Fuels (GNF) is developing FeCrAl alloy cladding and Abrasion Resistant, More Oxidation Resistant coating design for zirconium alloy [6].

Economic analysis of the ATF designs on an LWR-type reactor core suggests that the ATF implementation provides a positive impact on fuel cycle economics. The favorable impacts are seen not only in the equilibrium ATF core but also in the transition cycle from standard fuels. Better improvement is also observed in the economic analysis of the 24-month transition cycle, which will be the recommended path in future LWR development [7].

There is an ongoing project sponsored by the US Nuclear Regulatory Commission to prepare and support the deployment of ATF and EE fuels in selected LWR designs. The project's Phase I goal is to evaluate lattice physics parameters and fuel isotopic changes for standard boiling water reactor (BWR) [1] and pressurized water reactor (PWR) [2] models. Two report documents have been published for the EE designs for those two models, and another report focusing on the ATF features has been published [3].

The previous works were conducted on the assembly-level assessment using SCALE [8] for EE and ATF designs in PWR and BWR lattices. In summary, no anomalous trend was observed in the study because the EE and ATF implementation resulted in expected effects. Some ATFs, like FeCrAl cladding, introduced a reactivity penalty and thus should be considered in the fuel designs [3].

This paper represents parts of Phase II efforts with an objective to investigate the core-level performance of ATF and EE fuels in a transition cycle using the US Nuclear Regulatory Commission's PARCS core simulator [9]. Some core parameters like power distribution, control rod worth (CRW), and doppler temperature coefficients (DTC) are compared between the nominal and transition cores. The SCALE/Polaris code [10], which is used for the previous lattice physics work, is utilized to provide the homogenized few-group constants for PARCS.

2. METHODOLOGY

As explained in the previous section, this work utilized SCALE/Polaris to perform lattice calculations on assembly models and the PARCS core simulator to perform the core physics calculations. The lattice model is based on the GE-14 fuel assembly, and the core simulation utilized the Hatch reactor core-like model. This section provides details for the methodology used in this work.

2.1. Lattice Model

The lattice models used are based on the dominant region of the GE-14 BWR fuel assembly design. To model the transition core in PARCS, the cross sections from different types of fuel assemblies need to be generated from Polaris. Therefore, several different lattice designs are modeled in Polaris: nominal, ATF, and EE-ATF fuel assembly designs. Detailed parameters of the designs are presented in Table I.

In the design specification shown in Table I, the ATF pin rods have a larger pellet radius and thinner cladding materials than standard fuel pins. This design is made as a mitigation of the parasitic effect in

FeCrAl cladding to maintain the reactivity of the lattice model. The larger fuel radius and thinner FeCrAl; cladding layer has comparable reactivity with the nominal fuel assembly designs. The EE-ATF assemblies use higher enrichment (8 max wt % of ^{235}U) than the non-EE assembly designs.

Table I. Specification of lattice design modeled in Polaris

Parameter	Nominal	ATF	EE-ATF
Lattice Size	10 × 10		
Assembly Pitch	14.8945 cm		
Fuel Rod Pitch	1.2954 cm		
Cladding Material	ZIRC-2	FeCrAl	FeCrAl
Fuel Pellet Radius	0.438 cm	0.4655 cm	0.4655 cm
Gap Thickness	0.009 cm	0.009 cm	0.009 cm
Cladding Thickness	0.066 cm	0.0385 cm	0.0385 cm
Fuel Enrichment	5 max wt % 4.4 av wt %	5 max wt % 4.4 av wt %	8 max wt % 7.2 av wt %

Notes: ATF = accident-tolerant fuel; EE = extended enrichment.

Figure 1 presents the pin map of lattice models from Polaris. The lattices consist of various types of fuel rods with different ^{235}U enrichment and gadolinia concentration shown in Table II. In the nominal and ATF lattices, the fuel enrichment ranges from 1.6 wt % to 5.0 wt % of ^{235}U with some pins containing between 6 wt % and 8 wt % of Gd_2O_3 . For the EE-ATF lattice with 8 max wt % of enriched uranium, the fuel pin enrichment ranges from 2.6 wt % to 8.0 wt % with gadolinia concentration of 7–9 wt %.

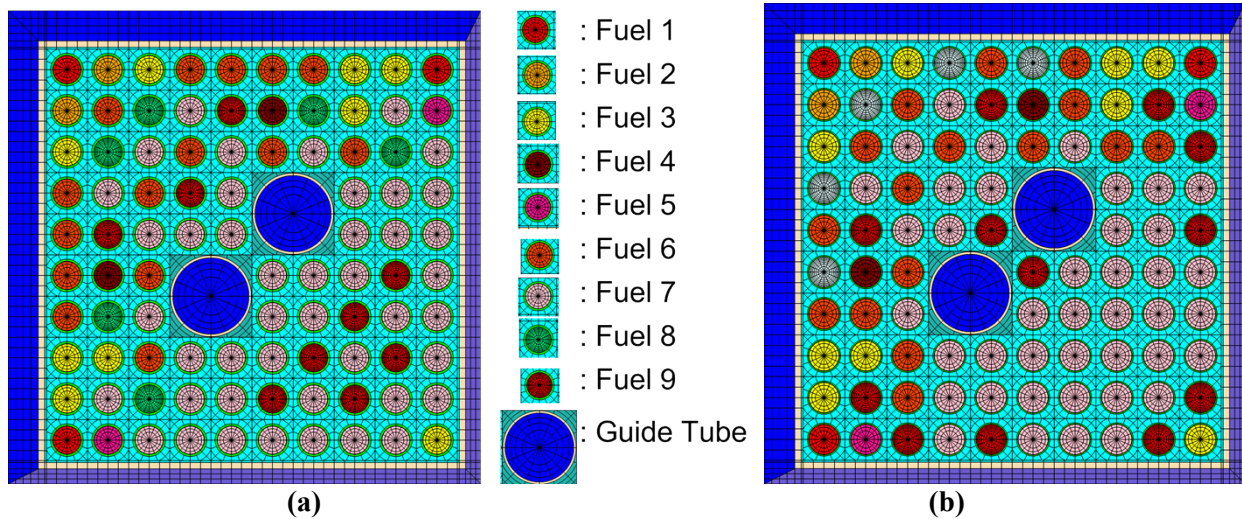


Figure 1. Pin maps of boiling water reactor fuel assembly models in Polaris for (a) nominal and accident-tolerant fuel lattice and (b) 8 max wt % extended enrichment accident tolerant fuel lattice

Table II. Uranium enrichment and gadolinia concentration for each type of fuel pins

Type	Note	Fuel 1	Fuel 2	Fuel 3	Fuel 4	Fuel 5	Fuel 6	Fuel 7	Fuel 8	Fuel 9
5 max wt % lattice	U^{235}	1.6 %	2.8 %	3.2 %	3.6 %	3.9 %	4.4 %	5.0 %	4.4 %	5.0 %
	GAD	0.0 %	0.0 %	0.0 %	0.0 %	0.0 %	0.0 %	0.0 %	6.0 %	8.0 %
8 max wt % lattice	U^{235}	2.2 %	3.3 %	4.3 %	4.8 %	6.4 %	7.2 %	8.0 %	7.2 %	7.2 %
	GAD	0.0 %	0.0 %	0.0 %	0.0 %	0.0 %	0.0 %	0.0 %	7.0 %	9.0 %

2.2. Core Model

The core model used is based on the geometry and size of the Edwin I. Hatch reactor core. The core map was simplified from the original core to facilitate the implementation in PARCS. Figure 2 presents the quarter core map of the reactor model used. This core map is based on the three cycles of fuel loading patterns. In the actual PARCS simulation, the whole core model is used to account for the fuel shuffling mechanism in the multi-cycle calculation.

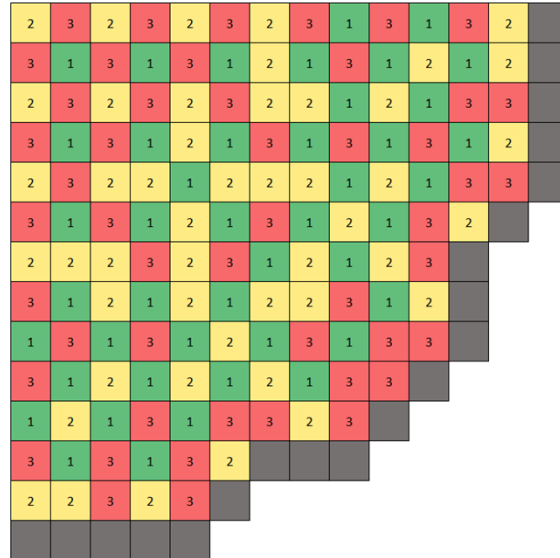


Figure 2. Quarter core map of a boiling water reactor with three cycles of fuel loading, modeled in PARCS. The numbering represents the cycle number of each fuel assembly.

2.3. Calculation Procedure

The calculation procedure involved the lattice physics calculation in Polaris for the different types of assemblies. To generate cross sections for reflectors, standard Polaris simulations employing fuel assembly and parts of reflector geometry were performed. These assembly-level simulations produced the homogenized, few-group, cross section data that can be used to construct the whole core model. Before the cross section data from Polaris can be utilized by PARCS, they need to be converted using the GenPMAXS processing code to generate PMAXS files [11]. The core simulation was then performed in PARCS using the assembly-wise, few-group constants in PMAXS files.

The multi-cycle calculation was performed in PARCS to handle the fuel shuffling and loading in the core model. Each cycle includes an 18-month reactor operation with 532.5 days of full reactor power operation.

Using this approach, a transition core can be modeled by replacing some of the fuels with the ATF and EE-ATF fuel assemblies. In this work, three different core simulations were conducted in PARCS:

1. Nominal core, which includes the standard 5 max wt % with ZIRC-2 cladding fuel assemblies
2. ATF transition core, which replaces some fuel assemblies in the nominal core with the 5 max wt % fuels and FeCrAl cladding fuel assemblies
3. EE-ATF transition core, which replaces some fuel assemblies in the nominal core with the 8 max wt % fuels and FeCrAl cladding fuel assemblies

3. POLARIS/PARCS VERIFICATION ON COLORSET MODELS

Before performing the whole core calculation using PARCS/Polaris, it is important to verify the procedure using a simpler model. A 2×2 fuel assemblies colorset model of BWR was constructed in Polaris and PARCS, as shown in Figure 3. Polaris was designed as a lattice calculation code, but with some modifications to the pin map, a multi-assembly model may be built. This setup allows an excellent verification procedure for this problem. Because Polaris is used to generate the cross sections, PARCS results should be comparable to the Polaris calculation of the same model.

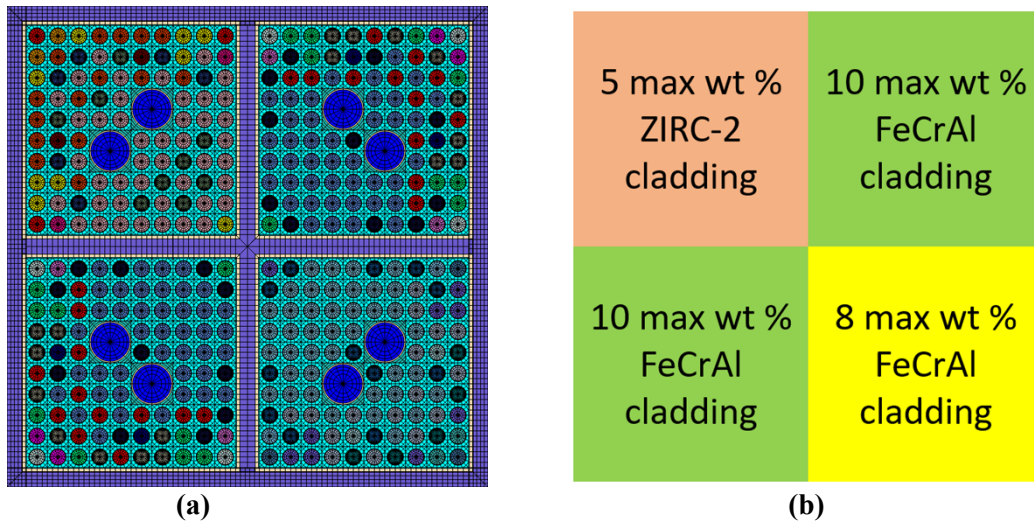


Figure 3. A 2×2 colorset model of boiling water reactor assemblies with (a) a heterogeneous model in Polaris and (b) a homogeneous model in PARCS

Table III provides the PARCS/Polaris colorset results with various few-group structures. All errors shown in the table are compared with the Polaris multi-assembly calculation. A high-resolution Monte Carlo code, Serpent [12], is used to provide additional results to verify the PARCS/Polaris calculation.

Table III. Verification of PARCS/Polaris colorset results with various few-group structures

Model	k	k Differences (pcm)	Avg. Assembly Power Differences	Max Assembly Power Differences	Avg. Pin Power Differences	Max Pin Power Differences
Polaris	1.00819	-	-	-	-	-
Serpent	1.00921±0.00002	102.0	0.10%	0.20%	0.41%	2.06%
PARCS 2G	1.009706	151.6	0.93%	1.50%	0.92%	5.86%
PARCS 4G	1.009605	141.5	0.77%	1.37%	0.76%	4.70%
PARCS 8G	1.009573	138.3	0.79%	1.40%	0.80%	4.66%

Based on the table, the Polaris result matches closely with the Serpent simulation, with very small differences in the assembly power error and pin power error. The multiplication differs around 100 pcm, which is still acceptable for this case. Compared with the Polaris results, the results from the PARCS calculation have observable eigenvalue error, assembly power error, and pin power error. The larger group structure used did not provide significant improvement to the nodal diffusion calculation. This is because the transport effect might be more prominent in the larger group structure, and the group structure, therefore, needs to be optimized to better improve the results. However, in this case, the 2G result is still acceptable in terms of the error introduced, so this structure was used in the next step of this work.

The next verification step was to test the transition core model using the 2×2 colorset in Polaris and PARCS. The colorset model was run in three reactor cycles, with each cycle lasting for 18 months. For each cycle, the colorset configuration is described as follows:

- Initially, the model consists of all nominal fuel assemblies containing fresh fuels with 5 max wt % enrichment and ZIRC-2 cladding. This colorset is then burned twice (2x18-month cycle).
- For the next cycle, three assemblies were replaced by fresh EE-ATF assemblies and formed the configuration as shown in Figure 3 with the standard fuel assembly already burned twice

The multi-cycle calculation was conducted in both Polaris and PARCS to obtain the comparison shown in Figure 4. The multiplication factor in PARCS matched the Polaris result with some observable discrepancy between cycles and in the last step of the calculation. At the end of cycle (EOC) of the last cycle, the assembly power error is around 0.3% for the 5 max wt % and 10 max wt % fuel assemblies and around 0.9% for the 8 max wt % assembly. These results gave the confidence to carry out the same procedure to simulate the transition cycle analysis for the whole core model.

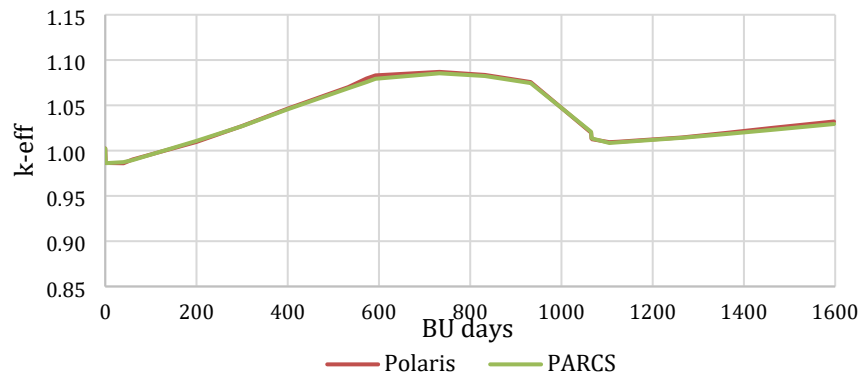


Figure 4. Transition models for boiling water reactor colorset compared between Polaris and PARCS for each burnup step

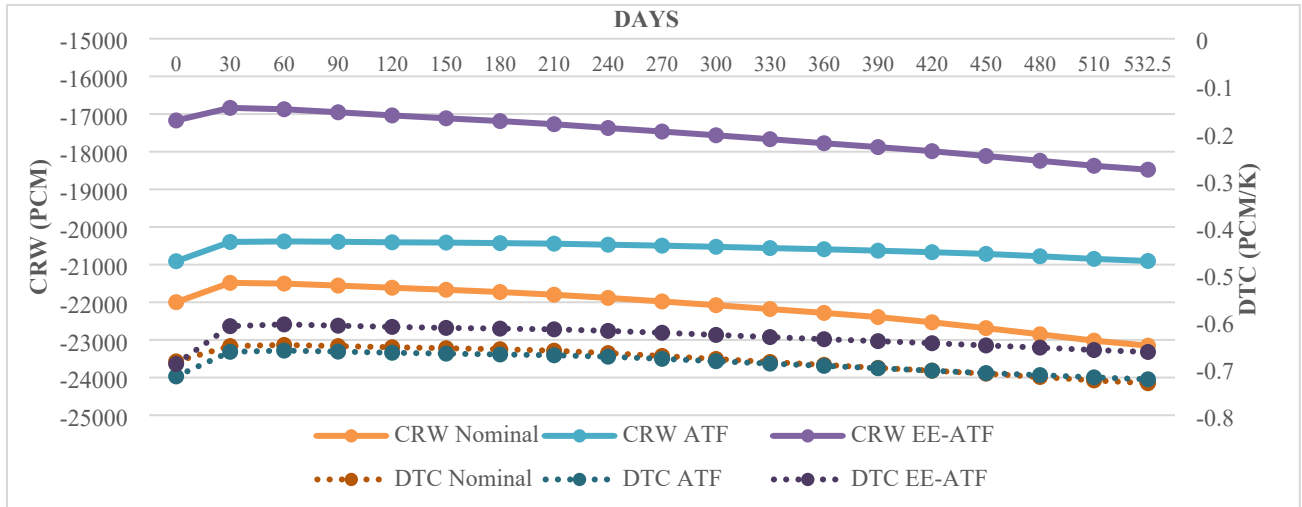


Figure 5. Control rod worth (CRW) and Doppler temperature coefficient (DTC) at hot full power (HFP) for the 2x2 colorset model in a transition cycle

Before implementing the PARCS/Polaris transition cycle calculation on the whole core model, a similar approach is implemented for the colorset model. Similar to the previous simulation, after the initial assemblies burned twice, the transition colorset is used. The transition colorset replaces three of the initial fuel assemblies with transition fuels, which include the ATF assemblies with nominal enrichment or EE-ATF assemblies. The comparison of these transition colorset models with the nominal colorset results is presented in Figure 5.

4. WHOLE CORE CALCULATION RESULTS

The calculation procedures verified in Section 3 for colorset models can be used to simulate the transition calculation for the whole BWR core model. The delta approach is utilized to analyze the effects of implementing ATF and EE fuels in an LWR core.

4.1. Core Power Distribution

One of the most interesting parameters to compare in this case is the power distribution in the reactor. The assembly power is calculated as the fission energy released data (obtained from Polaris lattice calculation) multiplied by the neutron scalar flux and the node volume, then summed for all energy groups. In PARCS, the power distribution is normalized so that the average core power for each assembly is unity.

Figure 6 presents the core power distribution at beginning of cycle (BOC) for the three reactor cores. Visually, the ATF transition core pattern for the power distribution is similar to the nominal core pattern. The higher enrichment in the EE-ATF transition core seems to introduce a checkerboard-like pattern near the core center. This can be understood because the larger yield of ^{235}U in the EE-ATF assemblies can provide a higher fission reaction rate and, thus, higher power.

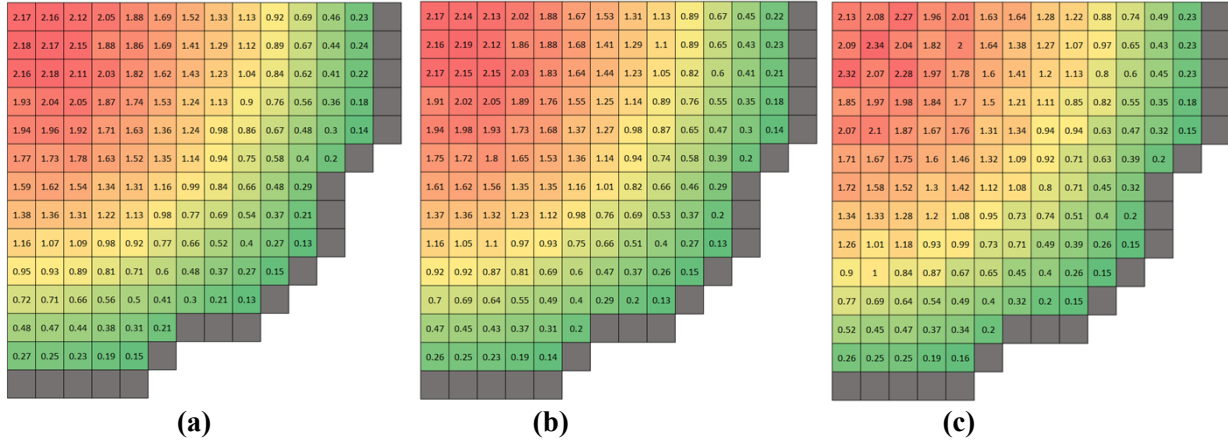


Figure 6. Radial core power distribution at beginning of cycle for the (a) nominal core, (b) accident-tolerant fuel transition core, and (c) extended enrichment accident tolerant fuel transition core

At the EOC, the radial core distribution has a different pattern because the fuels were depleted to a certain level. Because the core center typically has a larger neutron flux than that of other parts of the core, the assemblies located there were depleted faster than ones located anywhere else in the core. As presented in Figure 7, the largest assembly power is located a few assemblies away from the center core.

Based on this power distribution, the radial power peaking factor (PPF) can be compared among those three cores. The PPF can be defined as the maximum power divided by the core-averaged power. Because the core-averaged power was already normalized to unity, the PPF is the maximum power presented in Figures 6 and 7. Table IV summarizes these values. Based on the table, the BOC PPF is observed to be significantly higher than the EOC PPF. Also, the ATF transition core has a slightly higher PPF compared with the nominal core PPF, which can be attributed to the parasitic effect of FeCrAl cladding. Adding the extended enrichment fuels made the PPF significantly higher in the EE-ATF transition core. The reason is that the higher fuel enrichment caused higher fission power generated by the respective fuel assemblies.

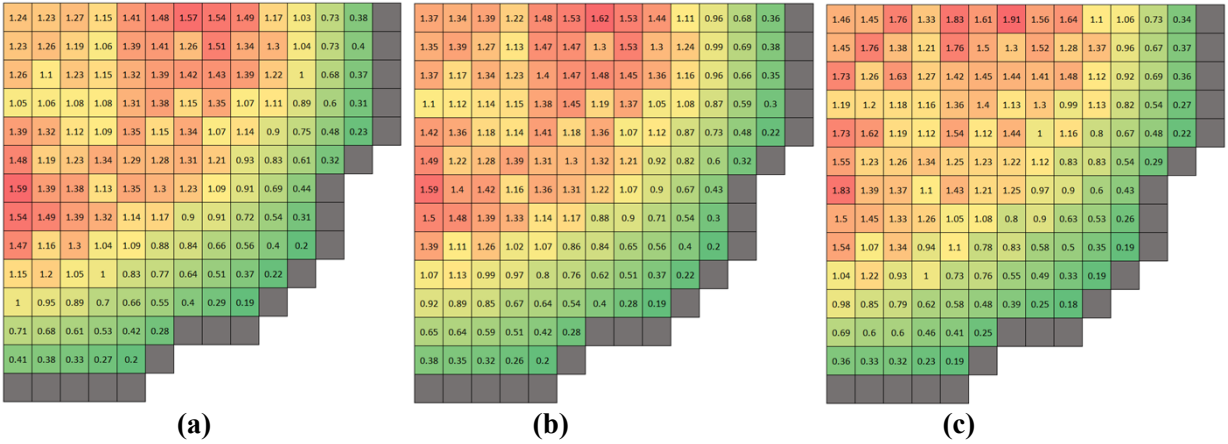


Figure 7. Radial core power distribution at end of cycle for the (a) nominal core, (b) accident-tolerant fuel transition core, and (c) extended enrichment accident tolerant fuel transition core

Table IV. Radial power peaking factor (PPF) at beginning of cycle (BOC) and end of cycle (EOC)

Core	BOC PPF	EOC PPF
Nominal Core	2.178	1.588
ATF Transition Core	2.194	1.617
EE-ATF Transition Core	2.343	1.906

Table V. Doppler temperature coefficients (DTC) and control rod worth (CRW) at beginning of cycle

Core	CZP CRW (pcm)	HFP CRW (pcm)	DTC (pcm/K)
Nominal Core	-19434	-19265	-0.391
ATF Transition Core	-19073	-18907	-0.380
EE-ATF Transition Core	-17177	-17070	-0.329

Notes: CZP = cold zero power; HFP = hot full power.

4.2. Reactivity Coefficients and Control Rod Worth

Reactivity coefficients and CRW are important parameters in the reactor safety analysis. In this work, DTC and CRW at cold zero power (CZP) and hot full power (HFP) are compared for the three core models. These results at BOC are presented in Table V. The introduction of the ATF transition core caused the DTC, CZP CRW, and HFP CRW to be slightly less negative (smaller in magnitude) compared with the nominal core. This is in line with the previous work on assembly-level calculation [3] that FeCrAl-cladded fuel assemblies with larger fuel pellets have slightly higher CRW and DTC. On the other hand, the introduction of higher enrichment fuels in the EE-ATF transition core made the CRW and DTC significantly smaller than the nominal and ATF transition cores. This is also in agreement with the previous work on the extended enrichment fuel assemblies [1–2].

Figures 8 and 9 present the results at HFP for the 18-month cycle of BWR operation. Similar patterns are observed for the transition cores. The EE-ATF transition core has significantly smaller DTC and CRW along the operation cycle. The ATF transition core also tends to have smaller DTC and CRW, but the difference with the nominal core is smaller than when the extended enriched fuels are added into the reactor core. These trends were also observed in the transition colorset model shown in Figure 5. However, in terms of overall magnitude, the whole core model has a smaller DTC than the colorset model. In means that this parameter is not conserved in the colorset model.

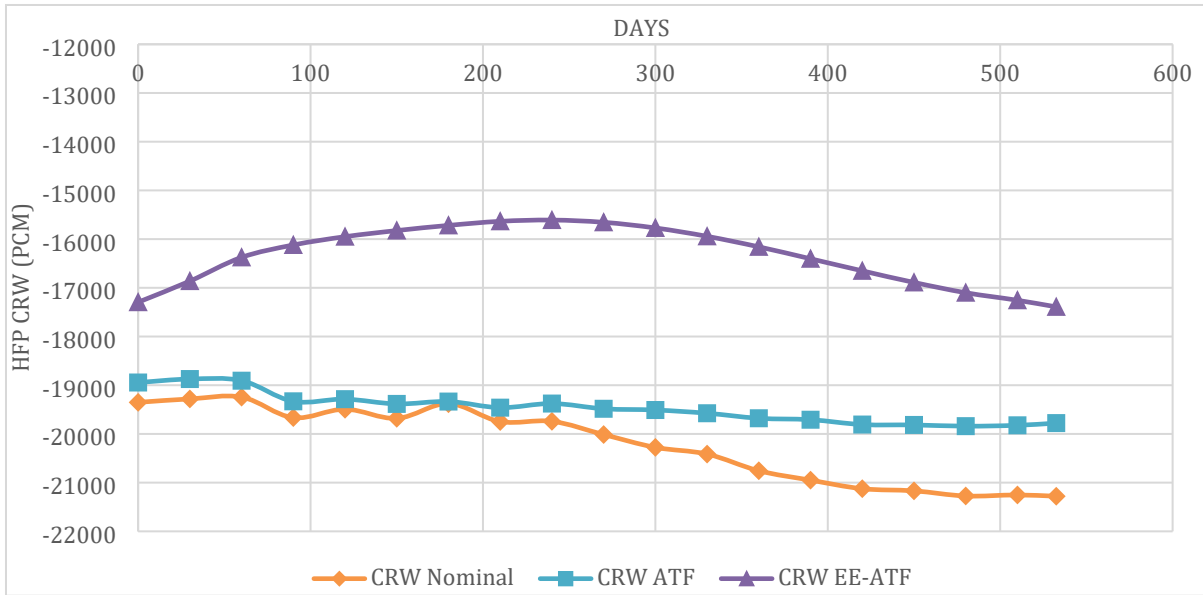


Figure 8. Control rod worth (CRW) at hot full power (HFP)

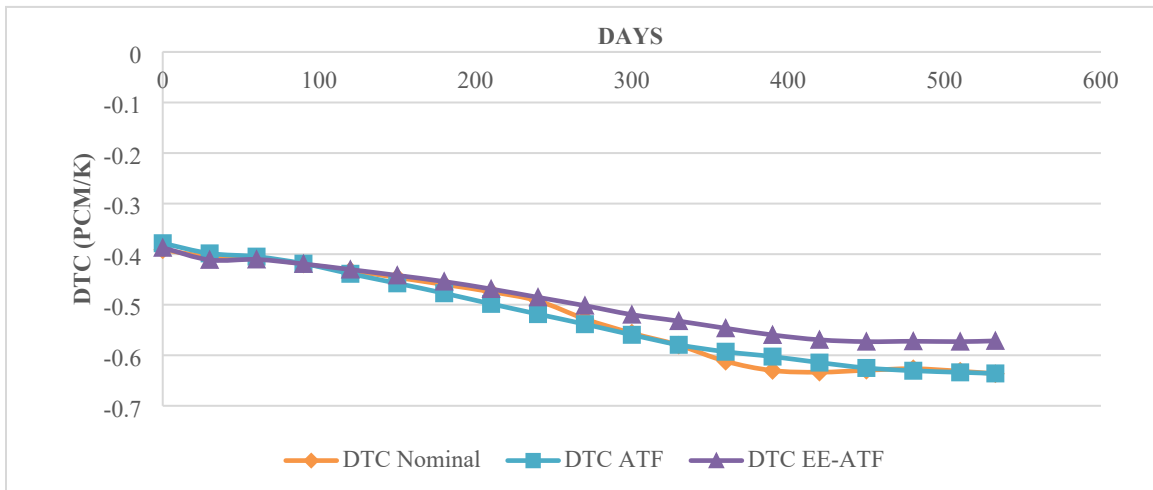


Figure 9. Doppler temperature coefficient (DTC) at hot full power (HFP)

5. CONCLUSIONS

Based on the results presented, the PARCS/Polaris calculation procedures can be used to analyze the transition core for the extended enrichment and accident-tolerant fuels. The introduction of the ATF and EE can cause some core parameters in the reactor to change, but these changes are mostly not significant. Based on the tests that were performed, ATF and ATF-EE fuel perform as expected and no significant differences were observed in Polaris/PARCS results compared to reference results. The results for the transition cycle analysis in the colorset models also have mostly similar trends with the whole core calculation. Future works will assess similar transition cores using the actual reactor data to produce a more realistic analysis for this matter.

ACKNOWLEDGMENTS

This research was supported in part by an appointment to the Oak Ridge National Laboratory Virtual Graduate Research Summer Internship, sponsored by the U.S. Department of Energy and administered by the Oak Ridge Institute for Science and Education.

REFERENCES

1. R. Cumberland, R. Sweet, U. Mertyurek, R. Hall, and W. A. Wieselquist, "Isotopic and Fuel Lattice Parameter Trends in Extended Enrichment and Higher Burnup LWR Fuel Volume II: BWR Fuel," ORNL/TM-2020/1835, Oak Ridge National Laboratory, Oak Ridge, TN (March 2021).
2. R. Hall, R. Cumberland, R. Sweet, and W. A. Wieselquist, "Isotopic and Fuel Lattice Parameter Trends in Extended Enrichment and Higher Burnup LWR Fuel Volume I: PWR Fuel," ORNL/TM-2020/1833, Oak Ridge National Laboratory, Oak Ridge, TN (February 2021).
3. R. Hall, R. Sweet, R. Belles, and W. A. Wieselquist, "Extended-Enrichment Accident-Tolerant LWR Fuel Isotopic and Lattice Parameter Trends," ORNL/TM-2021/1961, Oak Ridge National Laboratory, Oak Ridge, TN (March 2021).
4. WEC (Westinghouse Electric Company), "Westinghouse Advanced Doped Pellet Technology (ADOPT™) Fuel," WCAP-18482-NP, Rev. 0 (2020).
5. S. E. Cole, et al., "AREVA Optimized Fuel Rods for LWRs," *Top Fuel Reactor Fuel Performance 2012 Transactions*, Manchester, United Kingdom, September 2–6, 2012 (2012).
6. Y. Lin, R. M. Fawcett, S. S. DeSilva, et al., "Path Towards Industrialization of Enhanced Accident Tolerant Fuel," *Proceeding of TOPFUEL 2018*, Prague, Czech Republic, September 30–October 4, 2018, A0141 (2018).
7. F. Francheschini, et al., "Transition Cycle Analysis for Optimum ATF Implementation in Current PWRs," *Proceeding of TOPFUEL 2018*, Prague, Czech Republic, September 30–October 4, 2018, A0001 (2018).
8. W. A. Wieselquist, R. A. Lefebvre, and M. A. Jessee, Eds., *SCALE Code System*, ORNL/TM-2005/39, Version 6.2.4, Oak Ridge National Laboratory, Oak Ridge, TN (2020).
9. T. Downar, Y. Xu, and V. Seker, "PARCS v3.0 U.S. NRC Core Neutronics Simulator User Manual," 3.0, University of Michigan, Ann Arbor (2010).
10. M. A. Jessee, et al., "Polaris: A new two-dimensional lattice physics analysis capability for the SCALE code system," *PHYSOR 2014*, The Westin Miyako, Kyoto, Japan, September 28–October 3, 2014 (2014).
11. A. Ward, Y. Xu, and T. Downar, "Code for Generating the PARCS Cross Section Interface File PMAXS," *GenPMAXS-v6.3 Release*, University of Michigan (2020).
12. J. Leppanen, et al., "The Serpent Monte Carlo code: Status, development and applications in 2013," *Annals of Nuclear Energy* **82**, 142 (2015).