Enhanced Accident-Tolerant Fuel Performance and Reliability for Aggressive iPWR/SMR Operation

Fuel Cycle Research and Development

Ivan Maldonado
University of Tennessee, Knoxville

Frank Goldner, Federal POC
Kurt Terrani, Technical POC
Enhanced Accident-Tolerant Fuel Performance and Reliability for Aggressive iPWR/SMR Operation

Prepared by:

Dr. G. Ivan Maldonado (PI) (Ivan.Maldonado@utk.edu)

Department of Nuclear Engineering
University of Tennessee
315 Pasqua Engineering Bldg
Knoxville, TN 37996-2300

Performed Under:
NEUP 14-6893
Under Prime Contract No. DE-NE0008290
(UT Proposal 14-1479, UT Award A15-0356-001)

Technical POC: Kurt Terrani
National Technical Director: Jon Carmack
Federal Manager: Frank Goldner
HQ Program Manager: Dave Henderson

Rev. 0
August 2018
## Table of Contents

List of Figures ................................................................................................................................. iv  
List of Tables ................................................................................................................................. vi  
3. Executive Summary ..................................................................................................................... 8  
4. Global Objective of this Project ................................................................................................. 8  
5. Status of Milestones .................................................................................................................... 8  
5.1 Task 1: Analysis of large PWR with current fuels and current operating regime ............... 9  
   5.1.a Stated Objective of Task 1 ............................................................................................... 9  
   5.1.b Report on Task 1 ............................................................................................................ 10  
5.2 Task 2: Analysis of large PWR with current fuels and aggressive operating regime .......... 17  
   5.2.a Stated Objective of Task 2 ............................................................................................ 17  
   5.2.b Report on Task 2 ........................................................................................................... 17  
5.3 Task 3: Analysis of SMR with standard fuels and operating regime .................................. 27  
   5.3.a Stated Objective of Task 3 ............................................................................................ 27  
   5.3.b Report on Task 3 ........................................................................................................... 27  
5.4 Task 4: MOOSE/BISON evaluation and development for ATFs ........................................ 36  
   5.4.a Stated Objective of Task 4 ............................................................................................ 36  
   5.4.b Report on Task 4 ........................................................................................................... 37  
5.5 Task 5: Analysis of large PWR with leading ATF concepts ................................................ 47  
   5.5.a Stated Objective of Task 5 ............................................................................................ 47  
   5.5.b Report on Task 5 ........................................................................................................... 47  
5.6 Task 6 Analysis of SMR with leading ATF concepts ............................................................. 74  
   5.6.a Stated Objective of Task 6 ............................................................................................ 74  
   5.6.b Report on Task 6 ........................................................................................................... 74  
5.7 Task 7 Integration and Conclusions ...................................................................................... 78  
   5.7.a Stated Objective of Task 7 ............................................................................................ 78  
   5.7.b Report on Task 7 ........................................................................................................... 78  
6. References .................................................................................................................................. 79  
7. Students and Personnel .............................................................................................................. 80  
8. Publication Legacy ...................................................................................................................... 81  
   8.1.a List of Journal Publications Inspired by NEUP Project ................................................... 81  
   8.1.b List of Conference Publications Inspired by NEUP Project ........................................ 81
List of Figures

Figure 5-1. Project Overview of Tasks, Specific Objectives, Milestones, and Deliverables .............. 9
Figure 5-2. Core configuration and poison loading pattern for WBNS1C1........................................ 11
Figure 5-3. Model input for reactor power relative to actual operational power ............................ 11
Figure 5-4. CASMO-4 output for one 2.11% enriched fuel branch.............................................. 12
Figure 5-5. CASMO-4 output for 3.1% enriched and AIC rodded fuel (2.11% for Zirconium and SiC) ................................................................. 12
Figure 5-6. Base NESTLE case ................................................................................................. 13
Figure 5-7. NESTLE output using 100 µm clad thickness (excluding Zirconium and SiC) ............ 14
Figure 5-8. NESTLE output for 50% increase in enrichment (excluding Zirconium and SiC) ...... 14
Figure 5-9. k-effective versus burnup for the 500 µm cases..................................................... 15
Figure 5-10. Plot of the fast flux pin power reconstructed function for sample problem ............. 17
Figure 5-11. Predicted Difference in Planar Relative Power between NESTLE and MPACT for WBNS1 .................................................................................. 20
Figure 5-12. Predicted Axial Power for WBNS1 (NESTLE and KENO results) ......................... 21
Figure 5-13. Bank D Control Rod Worth Results for NESTLE and CASL KENO ...................... 22
Figure 5-14. Enrichment adjustments required for various ATF claddings at 570 µm thickness .. 22
Figure 5-15. Enrichment adjustments required for various ATF claddings at 500 µm thickness .. 23
Figure 5-16. Enrichment adjustments required for various ATF claddings at 366 µm thickness .. 23
Figure 5-17. Equilibrium Core Loading Pattern (Obtained Manually) .................................... 25
Figure 5-18. Multicycle EOC Core Exposure versus Cycle Number ....................................... 26
Figure 5-19. Multicycle EOC F-Delta-h Values versus Cycle .................................................. 26
Figure 5-20. Soluble boron concentration for Cycle 6 ............................................................... 27
Figure 5-21. Best SMR loading pattern found by LWROpt using only the loading pattern optimization ........................................................................................................... 28
Figure 5-22. Constraint values vs burnup for the best LP/CRP for the individual searches case .... 30
Figure 5-23. Control rod patterns generated for the best LP/CRP for the individual searches case (notches withdrawn, 40 total notches) ........................................................................ 31
Figure 5-24. Best SMR loading pattern found by LWROpt using the coupled LP/CRP optimization .............................................................. 32
Figure 5-25. Constraint values as a function of burnup for best LP/CRP for the coupled searches ........................................................................... 33
Figure 5-26. Control rod patterns generated for the coupled LP/CRP search (notches withdrawn, 40 total notches) ........................................................................... 34
Figure 5-27. Peak and Average Fuel Centerline for SMR with Zirc-4 (1400 EFPD) ................. 35
Figure 5-28. Cladding Axial (left) and Radial (right) Displacements for SMR with Zirc-4 (1400 EFPD) ........................................................................... 36
Figure 5-29. Maximum Cladding Hoop Stress for SMR with Zirc-4 (1400 EFPD) .................... 36
Figure 5-30. Crack growth rate for various temperatures total ................................................... 39
Figure 5-31. Crack growth rate for load ratio 0.1 and 0.5 at 25 and 300C .................................. 39
Figure 5-32. Crack length for the 5x5x50mm bar with 1250 and 1800 mesh elements ............ 40
Figure 5-33. Failure profile for the bar using signed von Mises and max principal criterion ...... 41
Figure 5-34. Maximum and Average Power Histories for 366µm FeCrAl cladded rods for ~450 days .............................................................. 42
Figure 5-35. Average vs Peak Fuel Centerline Temperature ...................................................... 43
Figure 5-36. Maximum Radial Displacement (left) and Maximum Hoop Stress (right) in the Cladding ................................................................. 44
Figure 5-37. Fuel Rod Plenum Volume ................................................................................................................................. 44
Figure 5-38. Fission Gas Release (left) and Plenum Pressure (right) ............................................................................................ 44
Figure 5-39. Peak and Average Fuel Centerline for SMR with Zirc-4 (1400 EFPD) ................................................................. 45
Figure 5-40. Cladding Axial (left) and Radial (right) Displacements for SMR with Zirc-4 (1400 EFPD) ................................................................. 46
Figure 5-41. Maximum Cladding Hoop Stress for SMR with Zirc-4 (1400 EFPD) ................................................................. 46
Figure 5-42. Core Map Illustrating Selection of Limiting Linear Heat Rates .................................................................................. 48
Figure 5-43. Relative Power for Limiting Pin Selected .................................................................................................................. 48
Figure 5-44. Axial Linear Power Density for FeCrAl Claddings at Varying Enrichments/Thicknesses .......................................................... 49
Figure 5-45. Multi-Cycle Linear Power Density for FeCrAl Claddings at Varying Enrichments/Thicknesses .......................................................... 49
Figure 5-46. Axial Linear Power Density for Zirc and SiC Claddings at Varying Enrichments/Thicknesses .......................................................... 50
Figure 5-47. Multi-Cycle Linear Power Density for Zirc and SiC Claddings at Varying Enrichments/Thicknesses .......................................................... 50
Figure 5-48. Average fuel centerline temperatures for Zirc and FeCrAl cladding materials ............................................................ 51
Figure 5-49. The maximum radial displacement of Zirc and FeCrAl cladding materials ............................................................ 52
Figure 5-50. Core map in quarter symmetry (4.6% test location highlighted in orange) ............................................................ 53
Figure 5-51. Assembly lattice map in quarter symmetry ................................................................................................................ 53
Figure 5-52. Average 2D relative power of standard assembly vs. 5.0% U-235 FeCrAl assembly ............................................................. 55
Figure 5-53. The rod average linear heat rate of the fuel rods as a function of time ............................................................................. 57
Figure 5-54. The peak fuel centerline temperatures over the fuel lifetime ..................................................................................... 58
Figure 5-55. The average fuel centerline temperatures over time ................................................................................................. 58
Figure 5-56. The cladding axial elongation ................................................................................................................................. 59
Figure 5-57. Thermal expansion versus time ................................................................................................................................. 59
Figure 5-58. The maximum cladding hoop stress versus time ......................................................................................................... 60
Figure 5-59. The percentage of fission gas released versus time ........................................................................................................ 61
Figure 5-60. Sample illustration of ParaView/VisIt graphic capabilities for LPD (kw/ft) ................................................................. 62
Figure 5-61. Bank D rod insertion steps during load-following maneuver ........................................................................................ 63
Figure 5-62. Base case: Linear heat rate with load following at BOC ................................................................................................. 63
Figure 5-63. Base case: Linear heat rate with load following at MOC ................................................................................................. 64
Figure 5-64. Base case: Linear heat rate with load following at EOC ................................................................................................. 64
Figure 5-65. Base case linear heat rate with load following at BOC ................................................................................................. 64
Figure 5-66. Base case linear heat rate with load following at MOC ................................................................................................. 65
Figure 5-67. Base case linear heat rate with load following at EOC ................................................................................................. 65
Figure 5-68. Base vs ATF cases linear heat rate with load following at EOC .................................................................................. 65
Figure 5-69. Energy production in kW/ft for all of the pins in a node for test case ........................................................................... 66
Figure 5-70. Fast flux fit function for test case ................................................................................................................................. 67
Figure 5-71. This is a representation of the mesh used for the FCM pellet in a LWR environment .................................................. 68
Figure 5-72. This figure illustrates the effects of constant volume growth versus large volumetric swelling in the PyC irradiation induced dimensional change.................................................................69
Figure 5-73. Vertical slices of the hoop stress through the FCM pellet.................................................................71
Figure 5-74. Effects of using a stress limited PyC IIDC ........................................................................................72
Figure 5-75. A comparison of the maximum matrix hoop stress using four different distributions for the debonding threshold values............................................................................................................................73
Figure 5-76. Comparison of SMR lattice power peaking between CASMO-4 and TRITON....................................75
Figure 5-77. Comparison of SMR lattice k-infinity between CASMO-4 and TRITON............................................76
Figure 5-78. Temperature distribution of a rod within a RELAP5 assembly..............................................................76
Figure 5-79. Thermal Hydraulic relationships obtained by RELAP5........................................................................77
Figure 5-80. Updated k-effective behavior for SMR core........................................................................................78

List of Tables
Table 5.1. Combinations of clad thicknesses and enrichment..................................................................................15
Table 5.2. Simulation of a Typical French Power Plant Load-Follow Maneuver .........................................................18
Table 5.3. Bank D Control Rod Worth Calculations with NESTLE compared to CASL KENO data...............21
Table 5.4. Constraint values for the baseline design and each of the SMR optimizations ........................................28
Table 5.5 Material constants used to calculate the crack growth per cycle............................................................39
Table 5.6. Fuel rod parameters for power histories studied with BISON................................................................42
Table 5.7. Rod Geometry and Characteristics for BISON Calculations...............................................................51
Table 5.8. $F_{\text{DIH}}$ values for 570 $\mu$m, 4.6% U-235 case.......................................................................................54
Table 5.9. $F_{\text{DIH}}$ values for select FeCrAl cases – hot location ‘A’ .........................................................................54
Table 5.10. $F_{\text{DIH}}$ values for select FeCrAl cases - cold location ‘B’ .................................................................55
Table 5.11. $F_{\text{DIH}}$ values for 366 $\mu$m 4.6% FeCrAl single rod and whole assembly ........................................56
Table 5.12. Summary of Simulations for BISON Parametric Analysis.................................................................56
Table 5.13. Sample text output from NESTLE for pin power reconstruction.......................................................62
Table 5.14. The geometry for a TRISO-III fuel pellet intended for use in LWRs....................................................68
3. **Executive Summary**

This report describes the progress achieved during full period of NEUP Project 14-6893, which corresponds to 01 October 2014 through 31 December 2017. The material presented in this report is cumulative and describes the progress achieved during the full term of the grant.

4. **Global Objective of this Project**

This project will develop a process that evaluates the whole-core operational and safety performance of a reactor-and-fuel combination by integrating core-wide three-dimensional neutronics with Moose/Bison and Peregrine multi-physics fuel performance assessments using explicit time and space dependent fuel rod operational power histories generated in the whole-core analysis. Demonstration of the process will target large contemporary PWRs with traditional UO2 fuel and Zircaloy cladding to establish a baseline analysis, while the innovative application of this project will extend the developed process to evaluate operational and safety performance, via reactor physics and fuel performance analyses, of key emerging/leading concepts of enhanced Accident Tolerant Fuels (ATFs) within increasingly aggressive operational scenarios such as load-follow maneuvers in PWRs and long-cycle rodded and unborated operation in small modular reactors (SMRs). The ATFs to be considered include standard UO2 fuel pellets cladded with advanced iron-based alloys (FeCrAl) as well as particle-based Fully Ceramic Microencapsulated (FCM) fuels with FeCrAl or Zircaloy cladding, but the process being developed and demonstrated could ultimately be applied to any candidate ATF concept in a light water reactor. In fact, given that ATF R&D priorities are in a dynamic state, the scope related to ATFs will be targeted for the second half of this three-year project so to provide some opportunity to strengthen the programmatic alignment of this project with the DOE Fuels Campaign, by identifying the most promising and relevant ATFs at that time for further evaluation, while the early part of the project will focus upon fine-tuning the process herein developed and upon generating the baseline analyses against which a larger scope of ATF concepts can be compared.

5. **Status of Milestones**

Figure 5-1 presents the projected layout of activities for this project, divided into 7 tasks. These tasks have each been converted into project milestones. These tasks are listed below.

- **Task 1**: Analysis of large PWR with current fuels and current operating regime
- **Task 2**: Analysis of large PWR with current fuels and aggressive operating regime
- **Task 3**: Analysis of SMR with standard fuels and operating regime
- **Task 4**: MOOSE/BISON evaluation and development for ATFs
- **Task 5**: Analysis of large PWR with leading ATF concepts
- **Task 6**: Analysis of SMR with leading ATF concepts
- **Task 7**: Integration and Conclusions

The status of those milestones is described in the subsections that follow.
5.1 Task 1: Analysis of large PWR with current fuels and current operating regime

5.1.a Stated Objective of Task 1

This task will define and establish realistic, representative “baseline” design for a large standard PWR, using current UO2-Zircaloy fuels. Activities include modeling and simulation of full-core 3-D neutronics and fuel performance analysis. The generated, representative fuel pin power history from the neutronics will feed into the fuel performance analysis, hence the phasing of the work. Since this task involves gathering the data, and establishing the base models, additional time is allocated for the early setup tasks. Analysis of steady state, key operational and safety parameters will be completed in the reactor physics/neutronics section, and once a viable core design established, the resulting power histories will be used in the fuel performance assessment. Key thermo-mechanical fuel performance analysis such as rod internal pressure, fuel temperatures and fission gas release will be evaluated. The linking between fuel performance codes and the neutronics for the pin power histories is being developed in Task 4, and will be used in this Task.
5.1.b Report on Task 1

*Employing a PWR Model of Watts Bar Unit 1 to Evaluate Various AFT Claddings*

The neutronic evaluations for this project were carried out with the NESTLE code, a 3-D nodal simulator originally developed at NC State University [1] currently maintained and enhanced at the University of Tennessee, Knoxville [2]. This project is using NESTLE to simulate Cycle 1 of the Watts Bar Nuclear Unit 1 (WBN1C1) Pressurized Water Reactor (PWR) as part of a DOE NEUP project to develop a process to evaluate the multi-physics performance of various reactor/fuel/clad combinations intended to evaluate enhanced accident tolerance. The two main areas of evaluation herein targeted are 3-D neutronics and fuel performance. The latter is to be handled using the BISON-CASL code [3,4] for fuel performance evaluations. BISON-CASL (formerly Peregrine) expands on material libraries implemented in the BISON fuel performance code [5] and the MOOSE framework [6] by providing problem specific material data.

This section of the report focuses upon the NESTLE work, which investigated the result of changing the zirconium cladding used in WBN1C1 to five different claddings of enhanced accident tolerance: 304 stainless steel (304ss), 310 stainless steel (310ss), iron-chromium-aluminum (FeCrAl), APMT™, and silicon carbide (SiC). The goal of these full-core 3-D simulations was to try to match the End of Cycle (EOC) $k_{eff}$ values of the zirconium alloy cladding “base case” by thinning the ATF cladding thicknesses and compensating heavy metal mass by increasing the fuel pellet outer radius and enrichment for these proposed cladding options. This work found that varying pellet radius only, while keeping gap thickness and outer clad diameter constant, was not enough to match the EOC reactivity of the base case zirconium alloy for neither the two steels nor the two ferritic alloys, thus, increases in enrichment were necessary. Conversely, SiC, as expected, exceeded the reactivity performance of Zirconium throughout the cycle length. These results show consistent trends with previous studies carried out on the basis of lattice physics calculations on PWR bundles (i.e., not full core analysis) [7], and also representative of full-core studies performed on a BWR [8,9].

The NESTLE code is a few-group diffusion code that utilizes the Nodal Expansion Method (NEM) to calculate 3-D power/flux distributions as a function of burnup. NESTLE couples the neutronics with thermal hydraulics, using either a Homogeneous Equilibrium Model (HEM) for PWRs or the two-phase flow Drift Flux method for BWRs, for single or two-phase flow conditions, respectively. For this study, the bundle homogenized few-group cross-sections were evaluated by the lattice physics code Casmo-4 [10] to supply the cross-section data.

The Watts Bar Nuclear Plant Unit 1 is a PWR rated for 3411 MWth. The unit specifications have been made public as a result of the work of the Consortium of the Advanced Simulation of Light Water Reactors (CASL), and can be found in full in Reference [11]. The initial core is composed of three regions with enrichments of 2.11%, 2.6%, and 3.1%. The fuel assemblies are Westinghouse 17x17 bundles utilizing Pyrex burnable absorbers and AIC/B4C control rods. The core is quarter symmetric and the assembly arrangement can be seen in Figure 1, while Figure 2 shows the modeled reactor power conditions versus measured. The EOC exposure was 16.939 GWd/MTU. Future results intend to employ an equilibrium core model of WBN1C1 which would be more representative of a current operational plant/cycle.
Approach to Analysis

Before varying the cladding type, a base NESTLE case using standard Zircaloy/UO2 fuel had to first be established as a reference point for the newly proposed claddings. Casmo-4 calculations were then performed with the new cladding types to obtain a preliminary neutronics comparison. One branch is shown in Figure 3 for the 2.11% bundle with specific state point parameters of 565 K for moderator and fuel, 1300 ppm boron concentration, and 0.661 g/cc moderator density. A total of 17 branches (8 for unrodded bundles) were used in CASMO in order to fully capture the possible state values at which cross sections would be needed in the full-core simulation. Fuel radii and enrichment values were increased for the four less reactive claddings to match k-effective values to
those of Zirconium (see Figure 4). Because SiC trended so well with Zirconium, no additional cases needed to be tested; thus, the base Zirconium and SiC cases were included on Figure 4. It was deemed very helpful to use Casmo-4 to find the optimal parameters given its much faster run relative to the run time of NESTLE.

After producing cross sections using Casmo-4, NESTLE was run for the various ATF cases. For each case, the full core 3D cases were run for the entire cycle length without a critical boron search in order to best compare the clad types in terms of cycle length.

![Figure 5-4. CASMO-4 output for one 2.11% enriched fuel branch](image)

![Figure 5-5. CASMO-4 output for 3.1% enriched and AIC rodded fuel (2.11% for Zirconium and SiC)](image)

**Results**

Figures 5-6 through 5-8 show three different NESTLE cases. Figure 5-6 represent the base cases, where the only changes made were in the cladding compositions. Figures 5-7 and 5-8 are the results of varying the fuel pellet radii and enrichment, respectively, for the four less reactive...
cladding types. The base Zircaloy and SiC cases were included on each plot for reference. As can be seen from the plots, the SiC cladding performed just as well as the Zirconium, and even showed a slightly higher reactivity at every depletion step in the cycle. Figure 5 shows the results for when the fuel radius is at its maximum size (100 μm) given a constant gap thickness and cladding outer diameter; it is evident that merely increasing the pellet radius alone is not sufficient for matching the EOC reactivity of Zircaloy for any of the four alternate cladding types. Figure 6 is a plot of an approximately 50% increase in U235 concentration in each of the three assembly types. The other nuclides were adjusted using the following relationships [11].

\[
\begin{align*}
U^{234} &= 0.007731 \times w^{1.0837} \\
U^{236} &= 0.0046 \times w \\
U^{238} &= \text{balance}
\end{align*}
\]

Given that the highest enrichment of the three assembly types is approximately 4.6% U235, there is still available opportunity for finer adjustments such that the reactivity exactly matches that of Zirconium while staying below the 5% mark.

![Figure 5-6. Base NESTLE case](image-url)
Three different cladding thicknesses were tested in NESTLE for the five different cladding types of 304ss, 310ss, FeCrAl, APMT, and SiC, and the enrichments at which each type matched the cycle k-eff of Zirconium were determined. Table 5.1 below lists, for each of the three cladding thicknesses of 570 μm, 500 μm, and 366 μm, the optimal enrichment values (within a tenth of a weight percent 235U) for the low, medium, and high enrichment assembly types of the WBN1 Cycle 1 core. The base Zirconium enrichment values were 2.11, 2.6, and 3.10 % 235U, and the cladding thickness used in WBN1C1 was 570 μm. Figure 8 below shows the k-effective as the cycle progresses for the 500 μm case set and includes the base Zirconium case as a reference. No burnable absorbers were used in order to best compare the cladding types. The figure shows that unity is crossed at the same burnup step for each of the different cladding types.
Figure 5-9. k-effective versus burnup for the 500 μm cases

Table 5.1. Combinations of clad thicknesses and enrichment

<table>
<thead>
<tr>
<th>Thickness</th>
<th>Clad type</th>
<th>Assembly type by U235 enrichment</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>low (%)</td>
<td>mid (%)</td>
</tr>
<tr>
<td>570 μm</td>
<td>304ss</td>
<td>3.5</td>
</tr>
<tr>
<td></td>
<td>310ss</td>
<td>3.7</td>
</tr>
<tr>
<td></td>
<td>FeCrAl</td>
<td>3.1</td>
</tr>
<tr>
<td></td>
<td>APMT</td>
<td>3.5</td>
</tr>
<tr>
<td></td>
<td>SiC</td>
<td>2</td>
</tr>
<tr>
<td>500 μm</td>
<td>304ss</td>
<td>3.4</td>
</tr>
<tr>
<td></td>
<td>310ss</td>
<td>3.5</td>
</tr>
<tr>
<td></td>
<td>FeCrAl</td>
<td>2.9</td>
</tr>
<tr>
<td></td>
<td>APMT</td>
<td>3.3</td>
</tr>
<tr>
<td></td>
<td>SiC</td>
<td>2</td>
</tr>
<tr>
<td>366 μm</td>
<td>304ss</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>310ss</td>
<td>3.1</td>
</tr>
<tr>
<td></td>
<td>FeCrAl</td>
<td>2.7</td>
</tr>
<tr>
<td></td>
<td>APMT</td>
<td>2.9</td>
</tr>
<tr>
<td></td>
<td>SiC</td>
<td>2.11</td>
</tr>
</tbody>
</table>

Conclusions

Given that SiC is nearly transparent to thermal neutrons, it is quite reasonable to see it have a similar neutronic performance as Zirconium. As a result, no further cases using SiC needed to be run. The other four, however, were not nearly as neutronically economical and each required significant changes to the enrichments and/or pellet radii in order to match the EOC reactivity of...
Zircaloy clad. Fortunately, the reactivity could be matched while staying below the 5% enrichment mark for the highest enriched “fresh” fuel assembly. Additionally, the outer cladding diameter did not need to be increased for any of the EOC keff-matched cases, which is certainly a key constraint for modern nuclear power utilities, the potential employers of these new cladding types. Given that the model used to compare the cladding types was an actual operating nuclear reactor, with reliable measured data to draw from, should lend further confidence in the performance trends observed from these early results. These results provide quantitative support to what has been previously understood about ATF, and future work on this project will more precisely evaluate the optimal clad parameters for matching, at the least, the neutronic performance of Zirconium.

The full paper version of this work reported a summary of the fuel performance characteristics of the base case versus the FeCrAl clad (a popular material currently being considered for enhancing accident tolerance) using the BISON-CASL code.

**NESTLE software updates: Pin Power Reconstruction for Cartesian geometry**

As reported previously, the initial implementation of pin power reconstruction for Cartesian models in NESTLE is mostly complete. The method being implemented was originally developed for SIMULATE-3 [21]. This method was selected because of its’ simplicity and the detailed description available in the literature.

The fast flux fit is an x, y polynomial with terms up to the fourth power but cross terms only include terms up to the second power. The thermal flux includes a multiple of the fast flux and has a similar structure to the fast flux but uses hyperbolic sine and cosine terms. The plotting functionality in NESTLE has been expanded to generate plots of many important quantities in the pin power reconstruction process. Sample plot of the fast flux is shown in Figure 5-10. We are still working on improving the thermal flux results and need to benchmark against lattice physics and operating data as available. The implementation of this feature into NESTLE is crucial for the proper determination of localized power histories for subsequent fuel performance evaluations with BISON or other codes that will require this information.
5.2 Task 2: Analysis of large PWR with current fuels and aggressive operating regime

5.2.a Stated Objective of Task 2

Using the base data and analysis generated in Task 1 (hence the phasing of the tasks), a 3D neutronics analysis will be completed, but using a more aggressive operating strategy for a large PWR i.e. load following (therefore, more onerous fuel performance), and longer cycle lengths. Again, the fuel used will be UO2-Zircaloy. The key safety parameters from the neutronics will be compared with the PWR baseline case above. The resulting power history will then be used in a fuel performance analysis to determine the effect of the more aggressive fuel operating history. This will indicate the key phenomena affected by moving to more aggressive regimes, and where the fuel performance analysis gaps, or changes in phenomena are affected.

5.2.b Report on Task 2

*Update on Evaluating Aggressive Load-Follow Operation on a Modern US PWR (WBN1C1)*

A part of the evaluation of enhanced Accident Tolerant Fuels involved the study of aggressive operational scenarios in PWRs, such as load following. The method used in the study was based off of how the French Nuclear Power Plants (NPPs) are authorized to operate. Due to nuclear power sharing more than 75% of the total electrical output in France, French NPPs cannot be run at 100% power on a daily basis [12]. As a result, a typical scheme involves daily power...
changes from 100 to 50% reactor power at a rate usually no greater than 1.5% per minute. The scheme chosen in this evaluation used the “12-3-6-3” scheme [13], where the PWR operates at 100% for 12 hours, ramps to 50% over 3 hours, holds at 50% for 6 hours, and finally ramps back to 100% over the last 3 hours of the day.

The same model that was used for evaluating the performance of ATFs during normal reactor operation, Watts Bar Nuclear Unit 1 Cycle 1, was used for studying aggressive operation. The major change incorporated in the NESTLE model for the latter case was including a transient solver for Xenon and Samarium, since the depletion steps were to be solved at much shorter intervals. In addition, since WBN1C1 did not perform load following, the determination was made to begin the “12-3-6-3” scheme at the point in WBN1’s first cycle where 100% power was first reached. The control rod bank at this depletion step was used for every subsequent step at 100% power. The control rod group D (the only control rods used to control power [11]) insertion used at each 50% power step was determined by performing a linear extrapolation using the two reactivity worths of the depletion step where 100% was first reached (1229 MWd/MTU) and where 65% was reached (346 MWd/MTU). With the two group D insertion lengths determined, the cycling between 100% and 50% power could then be performed. No boron search was used in NESTLE in order to assess the most limiting case. The table below lists how the relevant parameters change during the maneuver. The results are being evaluated still before they can be submitted for thermal mechanical performance analysis.

**Table 5.2. Simulation of a Typical French Power Plant Load-Follow Maneuver**

<table>
<thead>
<tr>
<th>Time (hours)</th>
<th>Power (%)</th>
<th>Bank D Position (inches above core)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>100</td>
<td>138.7</td>
</tr>
<tr>
<td>12</td>
<td>100</td>
<td>138.7</td>
</tr>
<tr>
<td>15</td>
<td>50</td>
<td>114.2</td>
</tr>
<tr>
<td>21</td>
<td>50</td>
<td>114.2</td>
</tr>
<tr>
<td>24</td>
<td>100</td>
<td>138.7</td>
</tr>
<tr>
<td>36</td>
<td>100</td>
<td>138.7</td>
</tr>
<tr>
<td>39</td>
<td>50</td>
<td>114.2</td>
</tr>
<tr>
<td>45</td>
<td>50</td>
<td>114.2</td>
</tr>
<tr>
<td>48</td>
<td>100</td>
<td>138.7</td>
</tr>
</tbody>
</table>

The pertinent neutronic data from this case, as well as from a case utilizing soluble boron, will be used in BISON to assess fuel failure mechanisms such as PCI, fission gas buildup, creep/swelling, etc.

**Updated PWR Model of Watts Bar Unit 1 with NESTLE**

In previous reports, the Watts Bar core model was described in detail. In summary, the Watts Bar Nuclear Plant Unit 1 is a PWR rated for 3411 MWth. The unit specifications have been made public as a result of the work of the Consortium of the Advanced Simulation of Light Water Reactors (CASL), and can be found in full in Reference [11]. The initial core is composed of three regions with
enrichments of 2.11%, 2.6%, and 3.1%. The fuel assemblies are Westinghouse 17x17 bundles utilizing Pyrex burnable absorbers and AIC/B4C control rods.

updated results for base case using albedo approach to model reflector

The original calculations presented for WBNS1 included excellent agreements between the zero power physics tests simulations with NESTLE and those evaluated with a high-fidelity KENO calculation published by CASL [11]. However, some of the rod worth predictions by NESTLE appeared to require further examination, as well as the “at power” power and reactivity predictions by NESTLE. Much of this was believed to be attributable to a poor representation of the core/reflecto interface cross sections that inherently introduce a power tilt if not treated properly. Accordingly, the use of an albedo boundary condition was pursued to manually adjust the leakage. This albedo adjustment approach dates to the days when explicit reflector cross-section models were not common practice. The idea of this method is to adjust the core/reflecto interface cross-sections so that one can predict a more accurate neutron leakage at the core boundary relative to a measured/operational or high-fidelity trusted results. This generally translates into improved agreement for relative power distributions, reactivity predictions, and control rod worth calculations.

The first step in the process is to select a reflective boundary condition. The idea is to allow neutrons to pass through the reflector and reflect back to the core. The reflector, then, needs to be modified to be a pure absorber. The NESTLE cross-section file was modified so that the values of the fission cross-section and \(v\) were zero. The assembly discontinuity factors are also set to 1.0. Now all that remains is to modify the absorption and transport cross-sections that lead to an accurate simulation of the reflection. In previous calculations, the peripheral nodes were all too hot, so the absorption needed to be increased. A trial-and-error process was applied and the resulting difference between NESTLE and a trusted calculation from the CASL team calculated with the MOC transport-based code MPACT yielded an RMS error of 1.84% in the planar power distribution. These results are shown in Figure 5-11 and provide additional confidence in the actual conditions to be employed while testing the various accident tolerant fuel scenarios. Furthermore, the axial power shapes were also compared between NESTLE and data obtained from KENO, of which one such result is shown in Figure 5-12 and also shows a reasonable trend. It should be noted that the CASL calculation done with KENO includes effects caused by the spacer grids. Therefore, these differences are more visible at those particular locations.

Finally, in addition to evaluating these at-power results, reactivity calculations were carried out with the newly adjusted model. This was done for all zero power criticals, as well as for control rod worth. The results in Table 5.3 and Figure 5-13 show an excellent agreement relative to previous results with the old model.
### MPACT PREL @ 1.919 GWd/MTU -- Eighth Core Reported was Expanded

<table>
<thead>
<tr>
<th></th>
<th>MPACT PREL</th>
<th>NEUSTLE PREL</th>
<th>NESTLE PREL</th>
<th>MPACT PREL</th>
<th>NEUSTLE PREL</th>
<th>RMS Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.195</td>
<td>1.128</td>
<td>1.180</td>
<td>1.130</td>
<td>1.181</td>
<td>1.075</td>
<td>1.012</td>
</tr>
<tr>
<td>1.128</td>
<td>1.180</td>
<td>1.073</td>
<td>1.191</td>
<td>1.127</td>
<td>1.142</td>
<td>0.995</td>
</tr>
<tr>
<td>1.180</td>
<td>1.073</td>
<td>1.182</td>
<td>1.135</td>
<td>1.190</td>
<td>1.119</td>
<td>1.002</td>
</tr>
<tr>
<td>1.130</td>
<td>1.191</td>
<td>1.135</td>
<td>1.195</td>
<td>1.104</td>
<td>1.087</td>
<td>0.944</td>
</tr>
<tr>
<td>1.181</td>
<td>1.127</td>
<td>1.190</td>
<td>1.104</td>
<td>1.212</td>
<td>0.867</td>
<td>0.833</td>
</tr>
<tr>
<td>1.075</td>
<td>1.142</td>
<td>1.119</td>
<td>1.087</td>
<td>0.867</td>
<td>0.839</td>
<td>0.562</td>
</tr>
<tr>
<td>1.012</td>
<td>0.995</td>
<td>1.002</td>
<td>0.944</td>
<td>0.833</td>
<td>0.562</td>
<td></td>
</tr>
<tr>
<td>0.716</td>
<td>0.797</td>
<td>0.712</td>
<td>0.583</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### NESTLE PREL @ 1.919 GWd/MTU -- Quarter Core Results

<table>
<thead>
<tr>
<th></th>
<th>MPACT PREL</th>
<th>NEUSTLE PREL</th>
<th>NESTLE PREL</th>
<th>MPACT PREL</th>
<th>NEUSTLE PREL</th>
<th>RMS Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.177</td>
<td>1.149</td>
<td>1.158</td>
<td>1.150</td>
<td>1.163</td>
<td>1.099</td>
<td>1.004</td>
</tr>
<tr>
<td>1.150</td>
<td>1.162</td>
<td>1.099</td>
<td>1.172</td>
<td>1.146</td>
<td>1.131</td>
<td>1.019</td>
</tr>
<tr>
<td>1.166</td>
<td>1.099</td>
<td>1.163</td>
<td>1.153</td>
<td>1.165</td>
<td>1.123</td>
<td>0.994</td>
</tr>
<tr>
<td>1.150</td>
<td>1.169</td>
<td>1.153</td>
<td>1.170</td>
<td>1.116</td>
<td>1.066</td>
<td>0.945</td>
</tr>
<tr>
<td>1.162</td>
<td>1.146</td>
<td>1.172</td>
<td>1.118</td>
<td>1.185</td>
<td>0.882</td>
<td>0.811</td>
</tr>
<tr>
<td>1.097</td>
<td>1.121</td>
<td>1.125</td>
<td>1.070</td>
<td>0.887</td>
<td>0.837</td>
<td>0.553</td>
</tr>
<tr>
<td>1.014</td>
<td>1.019</td>
<td>1.003</td>
<td>0.945</td>
<td>0.797</td>
<td>0.543</td>
<td></td>
</tr>
<tr>
<td>0.743</td>
<td>0.797</td>
<td>0.735</td>
<td>0.577</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### NESTLE Difference from MPACT (NESTLE PREL - MPACT PREL)

<table>
<thead>
<tr>
<th></th>
<th>NESTLE PREL</th>
<th>MPACT PREL</th>
<th>RMS Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>-1.8%</td>
<td>2.1%</td>
<td>-2.1%</td>
<td>2.0%</td>
</tr>
<tr>
<td>2.2%</td>
<td>-1.8%</td>
<td>2.6%</td>
<td>-1.9%</td>
</tr>
<tr>
<td>-1.4%</td>
<td>2.6%</td>
<td>-1.9%</td>
<td>1.8%</td>
</tr>
<tr>
<td>2.0%</td>
<td>-2.2%</td>
<td>1.8%</td>
<td>-2.5%</td>
</tr>
<tr>
<td>-1.9%</td>
<td>1.9%</td>
<td>-1.8%</td>
<td>1.4%</td>
</tr>
<tr>
<td>2.2%</td>
<td>-2.0%</td>
<td>0.6%</td>
<td>-1.7%</td>
</tr>
<tr>
<td>0.2%</td>
<td>2.4%</td>
<td>0.0%</td>
<td>0.1%</td>
</tr>
<tr>
<td>2.7%</td>
<td>0.0%</td>
<td>2.3%</td>
<td>-0.6%</td>
</tr>
</tbody>
</table>

**NESTLE RMS Error:** 1.84%

*Figure 5-11. Predicted Difference in Planar Relative Power between NESTLE and MPACT for WBNS1*
Figure 5.12. Predicted Axial Power for WBNS1 (NESTLE and KENO results)

Table 5.3. Bank D Control Rod Worth Calculations with NESTLE compared to CASL KENO data

<table>
<thead>
<tr>
<th>Bank D Position</th>
<th>% Withdrawn</th>
<th>KENO keff</th>
<th>NESTLE k-eff</th>
<th>Δp (pcmΔk)</th>
<th>Rod Worth KENO (pcm)</th>
<th>Rod Worth ALBEDO NESTLE</th>
<th>Δworth (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.992755</td>
<td>0.988754</td>
<td>-400.1</td>
<td>-1383.9</td>
<td>-1420.1</td>
<td>-36.2</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>0.993162</td>
<td>0.989194</td>
<td>-396.8</td>
<td>-1342.6</td>
<td>-1375.1</td>
<td>-32.5</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>0.994555</td>
<td>0.990681</td>
<td>-387.4</td>
<td>-1201.6</td>
<td>-1223.4</td>
<td>-21.8</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>0.997369</td>
<td>0.993467</td>
<td>-390.2</td>
<td>-917.9</td>
<td>-940.3</td>
<td>-22.4</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>1.000279</td>
<td>0.996391</td>
<td>-388.8</td>
<td>-626.2</td>
<td>-644.9</td>
<td>-18.7</td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>1.002542</td>
<td>0.998652</td>
<td>-389.0</td>
<td>-400.5</td>
<td>-417.7</td>
<td>-17.1</td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>1.004163</td>
<td>1.000315</td>
<td>-384.8</td>
<td>-239.5</td>
<td>-251.2</td>
<td>-11.7</td>
<td></td>
</tr>
<tr>
<td>70</td>
<td>1.005300</td>
<td>1.001466</td>
<td>-383.4</td>
<td>-126.9</td>
<td>-136.3</td>
<td>-9.4</td>
<td></td>
</tr>
<tr>
<td>80</td>
<td>1.006073</td>
<td>1.002236</td>
<td>-383.7</td>
<td>-50.5</td>
<td>-59.6</td>
<td>-9.1</td>
<td></td>
</tr>
<tr>
<td>90</td>
<td>1.006468</td>
<td>1.002692</td>
<td>-377.6</td>
<td>-11.5</td>
<td>-14.2</td>
<td>-2.8</td>
<td></td>
</tr>
<tr>
<td>100</td>
<td>1.006584</td>
<td>1.002835</td>
<td>-374.9</td>
<td>0.0</td>
<td>0.0</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>
Recalculation of the previous reactivity assessments of the various ATF claddings reported in the previous quarterly report (FY2015-Q4) was performed. As expected, the results showed similar trends of enrichment adjustments required for the various ATF cladding options at various clad thicknesses. For completeness, these newly revised results for clad thicknesses of 570µm, 500µm, and 366µm are presented in Figure 5-14, Figure 5-15, and Figure 5-16, respectively.

**Figure 5-13. Bank D Control Rod Worth Results for NESTLE and CASL KENO**

**Figure 5-14. Enrichment adjustments required for various ATF claddings at 570 µm thickness**
Figure 5-15. Enrichment adjustments required for various ATF claddings at 500 µm thickness

<table>
<thead>
<tr>
<th>Clad type</th>
<th>low (%)</th>
<th>mid (%)</th>
<th>high (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>304ss</td>
<td>3.4</td>
<td>4.1</td>
<td>4.6</td>
</tr>
<tr>
<td>310ss</td>
<td>3.5</td>
<td>4.3</td>
<td>5.0</td>
</tr>
<tr>
<td>FeCrAl</td>
<td>2.9</td>
<td>3.9</td>
<td>4.5</td>
</tr>
<tr>
<td>APMT</td>
<td>3.3</td>
<td>4.0</td>
<td>4.6</td>
</tr>
</tbody>
</table>

Figure 5-16. Enrichment adjustments required for various ATF claddings at 366 µm thickness

<table>
<thead>
<tr>
<th>Clad type</th>
<th>low (%)</th>
<th>mid (%)</th>
<th>high (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>304ss</td>
<td>3.0</td>
<td>3.8</td>
<td>4.4</td>
</tr>
<tr>
<td>310ss</td>
<td>3.1</td>
<td>3.9</td>
<td>4.6</td>
</tr>
<tr>
<td>FeCrAl</td>
<td>2.7</td>
<td>3.6</td>
<td>4.4</td>
</tr>
<tr>
<td>APMT</td>
<td>2.9</td>
<td>3.8</td>
<td>4.5</td>
</tr>
</tbody>
</table>
**Update on Development of Equilibrium Core Design for Base Studies**

The cases previously studied employed the initial cycle of Watts Bar Unit 1 as a reference case. However, upon initial evaluations of this cycle, it was decided that a better option for reference studies would be an equilibrium core instead. In other words, the initial core generally employs lower enrichment bundles, all fresh, and typically runs for a shorter and “less aggressive” scheme. Therefore, the team put special emphasis upon the development of an equilibrium core design for the base studies. Two paths were followed, one was to develop a new option in the LWROpt code to automatically generate equilibrium patterns with NESTLE for the WB1 cycles, the second path was to manually generate an equilibrium core employing the CASMO/SIMULATE code suite employing a representative example. Both of these are described below.

**LWROpt Generation of Equilibrium Patterns with NESTLE**

For the implementation of equilibrium cycle determination in LWROpt a new LP generation method, the shuffle operator, was developed. The shuffle operator exactly duplicates the shuffling of the used fuel and the new fuel LP in contrast with the traditional LP operator which duplicates the new fuel LP but loads the used fuel based on the value of a sorting parameter (exposure or k-infinity) for each assembly. For actual equilibrium cycles there should be little difference between the methods, but there are likely to be major differences between the methods during the search for an equilibrium LP. Using the LP operator is expected to minimize the differences between equilibrium cycles, but at the expense of not using the actual equilibrium cycle methodology, which is the shuffle operator. To allow LWROpt to determine equilibrium loading patterns a new constraint was added, the maximum end of cycle node exposure difference between an equilibrium cycle and the initial equilibrium cycle of the same kind. Testing of the equilibrium cycle methodology and determination of which of the LP generation operators should be used is ongoing. Equilibrium cycle functionality has been implemented in LWROpt along with an exposure distribution difference constraint to get the optimization to move toward actual equilibrium cycles.

Two methods for generating equilibrium cycles have been implemented. The first of these methods is duplicating the loading pattern operator which consists of the new fuel loading pattern and a rank for each reload fuel location that specifies the assembly from the previous cycle to load in that location based on the assembly order when sorted based on either k-infinity or exposure. The loading pattern operator method was implemented because LWROpt already used loading pattern operators to specify the loading pattern so it was relatively easy to implement. The second method, which is what is typically used for and referred to as equilibrium cycles, is to use the same new fuel loading pattern and the same shuffle moves for the reload locations.

Testing of both methods is under way, but a series of minor bugs and the fact that calculations are somewhat slow because 5 cycles are being optimized in the test cases (2 transition cycles and 3 equilibrium cycles) has thus far prevented getting results for an evaluation of their effectiveness. The first issue encountered with the equilibrium cycle cases was that the cross section library for the Watts Bar model initially only had data for burnups up to 55 GWD/MTU, which was fine for the
single cycle calculations that had been performed previously, but during the optimization LWROpt often considers many candidate "solutions" that don't make any sense and some such solutions for the equilibrium cycle test cases had node burnups exceeding 90 GWD/MTU. Obviously such solutions should be rejected by the optimization but in order for this to happen accurate (i.e. not extrapolated) cross sections are needed so a new cross section library with burnups up to 100 GWD/MTU was created.

The other significant issue encountered was an unusually high number of non-converging and also some failing NESTLE calculations, which is largely caused by the poor quality of the early solutions (so far none of the test cases have progressed far enough that the solution quality has started to improve). The current method of dealing with this or at least reducing its effect on the option was to compile a special optimized NESTLE executable with Floating Point Exception (FPE) checking to catch failing NESTLE calculation as soon as a NaN or other FPE error is encountered. Work is also being done to try to improve the reliability of NESTLE in general including the fuel temperature model, which often produces incorrect results for the failing cases either causing or as a result of other issues.

Manual Generation of Equilibrium Patterns with CASMO/SIMULATE

In an effort to most accurately compare alternate claddings with the standard, Zirconium cladding, an equilibrium core was developed manually using Watts Bar Unit 1 Cycle 1 as the initial core. Given that none of the Watts Bar cycles are open source like the 1st cycle, several approximations and assumptions were made concerning the 2nd through N (equilibrium) cycles. One of the assumptions included using a 2-batch loading scheme, with 84 total feed assemblies, 40 assemblies with 4.2% enriched $^{235}\text{U}$ and 44 with 4.6% enriched $^{235}\text{U}$. The burnable absorber used was an Integral Fuel Burnable Absorber (IFBA), which adds a thin ZrB$_2$ coating to the outside of the fuel pellet. The fuel has 6 in. axial blankets at 3% $^{235}\text{U}$ enrichment. The cycle length is 510 EFPD, or 18 months. The core loading pattern is shown in Figure 5-17, where ‘TYPE11’ and ‘TYPE12’ are the new fuel and the others are core map positions.

![Figure 5-17. Equilibrium Core Loading Pattern (Obtained Manually)](image)
In order to have an equilibrium core, the End-of-Cycle (EOC) burnup values must not change from Cycle N to any cycle following. Additionally, the power shape of the reactor must also be constant after the Nth cycle; the F-Delta-H values are often used to check for any power peaking. Figure 5-18 and Figure 5-19 show the core exposure values and F-Delta-H for Cycles 1 through 6.

![Figure 5-18. Multicycle EOC Core Exposure versus Cycle Number](image)

![Figure 5-19. Multicycle EOC F-Delta-h Values versus Cycle](image)

Although the exposure and peaking values are acceptable values and constant after just 4 cycles, a plot of the soluble boron concentration (see Figure 5-20) during any given cycle indicates that the burnable absorbers in the fuel were not of a sufficient quantity. Further development will need to be done
increasing the number of IFBA rods or $^{10}$B enrichment in order to decrease the soluble boron concentration in the early depletion steps of the cycle. This will, most likely, cause the $F$-delta-$H$ values to rise, meaning an updated shuffle plan will be required. Though not a ‘true’ equilibrium cycle given the aforementioned issue, such a model could still be useful in comparing different cladding concepts.

![Figure 5-20. Soluble boron concentration for Cycle 6](image)

### 5.3 Task 3: Analysis of SMR with standard fuels and operating regime

#### 5.3.a Stated Objective of Task 3

Data available for current designs will be used to define and establish representative analysis for an SMR (e.g. mPower), using UO2-Zircaloy fuels. The more heterogeneous fuel and core in an SMR, the higher burnable poison loading and use of control rods to reduce excess reactivity, all contribute to a very different fuel pin power history compared with the standard large PWR cases in Tasks 1 and 2. Neutronics and fuel performance calculations will be completed, consistent with the earlier tasks, such that results from this task can then be compared with the previous tasks, hence the phasing.

#### 5.3.b Report on Task 3

Task 3 was completed ahead of schedule and reported early within Year 2. A journal article was completed, submitted, and accepted outlining the neutronics characteristics of an optimized SMR that was obtained with the LWROpt optimization code.


The thermal mechanical fuel performance aspects of this design have been preliminary reported as part of this DOE NEUP project in the form of progress reports. Ongoing work continues to verify and ensure the validity of these results so that they may also be released to the public in the form of conference and/or journal articles within the near term. Highlights of the journal article and development of the SMR model are provided below.
Update on SMR Model Development

Recent updates made upon the LWROpt code enabled us to develop additional optimized SMR fuel cycles that can provide better representations for their use in this project. The new features included Optimized New Fuel Inventory, Loading Pattern, and Control Rod Pattern using Separate Searches.

The (fuel cycle cost) FCC and constraint values for the baseline design and the best solution found during the LP search are given in Table 5.4. LWROpt was able to eliminate the insufficient reactivity and node RPF constraint violations present in the baseline design. It should be noted that these values are for ARO and that the RPF values are therefore not necessarily what would be seen in actual operation. The FCC values presented are very approximate and therefore mostly useful for comparing the various LPs. The best overall LP found during the LP and CRP searches is shown in Figure 5-21. The distribution of the fuel types is somewhat similar to the baseline design with the least reactive fuel in the center and the most reactive on the outside. However, there is much more type A fuel leading to no variation in the fuel in the outer ring and higher FCC. This increase in type A fuel was likely driven by the insufficient reactivity of the baseline design. If ShutDown Margin (SDM) was considered (there is currently not a quick method of calculating this in NESTLE or LWROpt) the outer ring would likely have to be more diverse because the two corner assemblies do not have CRs. The run time for the standalone LP optimization was a little less than 4 days.

<table>
<thead>
<tr>
<th>Constraint</th>
<th>Limit</th>
<th>Baseline</th>
<th>Best</th>
<th>Best CRP</th>
<th>Best Coupled</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minimum k_{eff}</td>
<td>1.000</td>
<td>0.9983</td>
<td>1.0037</td>
<td>0.9956</td>
<td>1.0000</td>
</tr>
<tr>
<td>Maximum k_{eff}</td>
<td>1.001</td>
<td>-</td>
<td>-</td>
<td>1.0061</td>
<td>1.0016</td>
</tr>
<tr>
<td>Maximum 2D RPF</td>
<td>1.6</td>
<td>1.53</td>
<td>1.40</td>
<td>1.61</td>
<td>1.50</td>
</tr>
<tr>
<td>Maximum 3D RPF</td>
<td>2.0</td>
<td>2.400</td>
<td>1.998</td>
<td>2.1884</td>
<td>2.0858</td>
</tr>
<tr>
<td>FCC ($/kwh)</td>
<td>-</td>
<td>0.01170</td>
<td>0.01175</td>
<td>0.01175</td>
<td>0.01165</td>
</tr>
</tbody>
</table>

Figure 5-21. Best SMR loading pattern found by LWROpt using only the loading pattern optimization

Constraint values for the depletion of the best LP with the CRP found during the CRP search are plotted for each of the depletion steps in Figure 5-22. As can be seen there were constraint violations for all of the constraints though only a very minor violation for assembly RPF. The value of k_{eff} oscillates between high (+500 pcm) and low (-450 pcm) values early in the cycle then settles...
into a smaller range a little above critical. The node RPF was less than 120% of the limit for the first half of the cycle and roughly equal to or less than the limit afterwards. The run time for generating the CRP was about 40 minutes.

The CRPs generated at each depletion step are shown in Figure 5-23. Early in the cycle bank two required most of the CRs to be fully inserted and still was not able to meet the keff limits while bank one had excess worth. Comparing the constraint violation plots and the CRPs reveals that two of the three highest keff values coincided with bank two being fully or nearly fully inserted. The highest assembly and node RPF values coincided with the second highest keff value indicating the peaking would be worse for a critical core. The inability of bank two to meet the keff limit indicates the LP will need to be adjusted because bank two does not have enough worth in the outer region to suppress the reactivity of the ring of type A fuel. This data also points to the need for the ability to use alternate banks when the primary bank is not capable of meeting constraints which is a possible future improvement to LWROpt (this will also help with power shaping). Also the core keff is slightly more than 1.0 at EOC and there are still CRs inserted which was also seen in the EOC keff from the LP optimization and indicates that there is excess reactivity in the new fuel. This could be caused by the small number of assemblies in the eighth core shuffle and the gap in the reactivity of the available assembly types or it could also indicate the need for feedback between the LP and CRP searches.
Figure 5-22. Constraint values vs burnup for the best LP/CRP for the individual searches case
Figure 5-23. Control rod patterns generated for the best LP/CRP for the individual searches case (notches withdrawn, 40 total notches).
**Optimized New Fuel Inventory, Loading Pattern, and Control Rod Pattern using the Coupled Optimization**

The coupled LP and CRP optimization was not able to find a solution that met all of the constraints but the best solution found was much closer to the meeting the constraints than the LP/CRP combination from the separate searches case. The best LP found during the coupled search is shown in . This LP is much more diverse than the best LP found with the standalone LP search because it takes into account the realities of reactivity control with CRs throughout the cycle. The run time for the coupled optimization was approximately 19 days at which point the calculation was manually terminated because further improvement if any was expected to be minimal. This run time is roughly 4.75 times longer than the separate searches case, but the improved results are generally going to be worth the extra time as long as the time is available. Also, the best LP/CRP combination was found after only 12 days so the optimization could have been terminated significantly earlier without affecting the results or at least the best result if desired.

![Figure 5-24. Best SMR loading pattern found by LWROpt using the coupled LP/CRP optimization](image)

A summary of the constraint values for the coupled search is given in Table 5.4. Constraint values for the baseline design and each of the SMR optimizations along with the values for the other cases for comparison. The constraint values as a function of burnup for $k_{eff}$, maximum assembly RPF, and maximum node RPF are given in Figure 5-25. As can be seen from the table and the figure the constraint violations for this case were much smaller than for the separate search case. The $k_{eff}$ values vary from just above the lower limit to 60 pcm above the upper limit (the acceptable range is 100 pcm wide from 1 to 1.001). There are no constraint violations for the assembly RPF and the node RPF constraint violations are all less than 5% with only two violations greater than 2%. Because the algorithm left several small constraint violations it may be necessary to change the OF so that the constraint violation portion is a step function or at least add this as an option so that any constraint violation has a significant impact on the OF making it much harder for decreases in the FCC to offset small constraint violations.

The CRPs generated for each depletion step for the best solution found in the coupled LP/CRP search are shown in Figure 5-26. Like the CRPs for the separate search case these CRPs are not eighth core symmetric. The CRP search is capable of making symmetric CRPs but the results are
typically worse than non-symmetric CRPs possibly due to the larger moves and lack of the functionality to introduce small asymmetries for refinement. Improving the CRP search so symmetric or near symmetric CRPs can be generated is another area of possible future development for LWROpt. The coupled optimization long term CRP requires significantly less control early in the cycle than the separate search CRP due to the lower average reactivity of the assemblies and the improved distribution of the assemblies.

Figure 5-25. Constraint values as a function of burnup for best LP/CRP for the coupled searches.
Figure 5-26. Control rod patterns generated for the coupled LP/CRP search (notches withdrawn, 40 total notches).
The LP optimization in LWROpt was able to find an eighth symmetric LP for the SMR model that met all of the constraints specified. However, the CRP search was not able to find a satisfactory CRP for the optimized LP. The failure of the CRP search was at least partially the result of the LP optimization, which was performed using a stepped ARO depletion, not taking into account the limitations of reactivity control with the CR banks. The results of the coupled LP and CRP search were significantly better than the results obtained by performing a LP optimization and then performing CRP searches on the best several LPs found. This improvement was not unexpected because increasing the number of pertinent variables considered by an optimization should generally improve the overall results, but this result does confirm this expectation and shows that it is possible to perform the coupled optimization in a reasonable amount of time (though significantly longer than using separate searches). In spite of the improvement the coupled search was not able to find a solution that met all of the constraints. To try to remedy this different form of the constraint OF (including using a step function) will be evaluated to make small constraint violations more significant so the optimization will be more likely to completely eliminate all constraint violations.

The best-found design was provided to the fuel performance team for initial evaluation of thermal mechanical and other constraints, described in the section that follows.

**Results of SMR analysis with Zircaloy-4 (1400 EFPD)**

These results were completed ahead of schedule, because the standard PWR results had been delayed. Thus, were reported in early quarterly reports. However, for completeness, highlights are being summarized below to capture the deliverables. The reactor physics calculations developed an optimized SMR core that closely met the requirements specified for the mPower reactor. Control rod patterns were developed and the cycle length of 48 months was achieved. The power histories from this model were provided to our fuel performance BISON experts. The case studied was for a small modular reactor using Zircaloy-4 cladded fuel rods. Similar to the analysis for standard PWRs, select parameters were monitored over the fuel simulation. This is a rather short analysis as there is no complementary data to compare to. Figure 5-27 shows the average and maximum fuel centerline temperatures. These are different because of the changing shape of the axial power profiles used.

![Figure 5-27. Peak and Average Fuel Centerline for SMR with Zirc-4 (1400 EFPD)](image)

Figure 5-28 shows the axial and radial displacements of the fuel cladding. Axial displacement is driven by thermal expansion initially and subsequent irradiation growth. While contact does occur,
the cladding does not protrude further than the end caps. This is because of the large amount of thermal and irradiation creep that zircaloy experiences.

Figure 5-28. Cladding Axial (left) and Radial (right) Displacements for SMR with Zirc-4 (1400 EFPD)

Figure 5-29 shows the cladding hoop stress. It is initially compressive due to the pressure differential across the cladding. This is from the reactor coolant pressure and the rod plenum pressure. There is no fission gas release in this rod, and the plenum pressure increases ~1MPa. This is presumably because of the cladding creep and fuel swelling. As the average rod temperature does not change much over this simulation.

Figure 5-29. Maximum Cladding Hoop Stress for SMR with Zirc-4 (1400 EFPD)

5.4 Task 4: MOOSE/BISON evaluation and development for ATFs
5.4.a Stated Objective of Task 4
This task will evaluate the existing capabilities of the Moose/Bison and Peregrine fuel performance codes to identify changes that will be needed for modeling ATF concepts with these tools. Some differences between baseline UO2/Zirc and ATF concepts will be relatively straight-forward to accommodate, such as changes in material properties (e.g., temperature-dependent thermal conductivity of the cladding material) or geometry (e.g., cladding thickness). More fundamental phenomenological differences, such as switching from a constant-volume irradiation growth model
in the cladding material to a volumetric swelling model in iron-based alloys, will require much more extensive modifications to the existing Moose/Bison and Peregrine codes and possibly development of new models or modules for analyzing ATF concepts with these codes. The linking of the neutronics pin power history to MOOSE/BISON will be developed here, including data needs, automation and format.

5.4.b Report on Task 4

Background on BISON-CASL

As previously reported, but for completeness, BISON-CASL (formerly PEREGRINE) is a finite-element simulation tool for nuclear fuel elements that is based on the MOOSE (Multiphysics Object Oriented Simulation Environment) framework and utilizes capabilities from the BISON fuel-modeling tool developed by Idaho National Laboratory. It utilizes Jacobian-Free Newton-Krylov method to solve fully coupled, fully implicit partial differential equations while leveraging the scalability of parallel computing. Because of the expandability of the MOOSE framework, BISON-CASL can incorporate a host of materials as well as behavioral models for fuel and fuel cladding. It has the capability to model complex thermo-mechanical behavior of discrete and smeared fuels, the fuel rod gap and plenum, and various cladding materials over time [14-16].

Though primarily used for LWR applications, BISON-CASL has the ability to analyze TRISO fuel designs as well as metal fuel in rod and plate form [17]. Models have been implemented in BISON-CASL to analyze thermal and irradiation creep and growth of Zircaloy as a cladding material [18]. However the code can model specified compositions of alternate cladding candidates by creating fuel performance material libraries [19]. Obviously, a goal of this project is to push the developments and applications further into the area of ATFs, for ferritic steel cladding and/or FCM fuel forms.

Update of Modifications to BISON-CASL

The modification of the fuel degradation models for the different material properties and behavior of TRISO FCM fuel and FeCrAl clad, is being closely coordinated with the efforts to integrate whole-core neutronics. Preliminary Moose/Bison results to be published are already being generated at this time for ATF models such as FCM fuel. Research that focused upon LWRs was presented at the 2015 Winter ANS meeting in Washington, DC [20].

Fuel performance assessment and modeling efforts in this project is intended to help identify knowledge and capability gaps, develop new capabilities or models as needed using initial estimates for any unknown material properties, and demonstrate the application of existing tools to new problems. In addition, sensitivity studies performed during fuel performance assessment could help establish needs and priorities for new experimental data for ATF concepts by identifying and ranking which phenomena and material properties are most influential. Note that this activity will help identify gaps in fuel performance modeling and analysis of ATF concepts because there will remain gaps in the data and knowledge of phenomena that will eventually have to be addressed via experimental irradiation programs.
Current status is awaiting the power history data (limiting kW/ft as a function of burnup) from the Watts Bar Unit 1 Cycle 1 analysis. Once that information is available for the initial cycle and also for an equilibrium cycle, these data will be analyzed with BISON-CASL as it was done for reference [20]. Our fuel performance team is well underway and equipped to handle analyses with zircaloy, so their recent focus has shifted toward developments needed in BISON to handle FeCrAl, FCM, and other ATFs. Preliminary results from these model upgrades are presented here for FeCrAl in a modern PWR. These results are shown in the next section under Task 5.

**Brittle Fatigue Crack Propagation in FCM fuel**

Fatigue was added as a failure mode for the NITE-SiC for load following performance with FCM fuel. The model assumes an intact material with initial flaws distributed throughout the material. The flaws are assumed to be spherical in shape with the “flaw size” being the average diameter. The model assumes that there is at least one flaw on average per element, and the flaw diameters have a normal distribution.

Flaw growth is thought to occur when the material is repeatedly placed in tension but not in compression. Hence the signed von Mises or max principal stresses are used. Signed von Mises has the same magnitude as the von Mises or effective stress but takes the sign of the greatest principal stress. This formulation has the advantage in a bi or triaxial stress condition because it accounts for all principal and shear stresses. However, in the case of a compressive max principal followed closely by a tensile principal stress, the model would not predict any crack growth. The max principal uses the largest tensile principal stress for crack growth. However, it does not account for the other principal or shear stresses which may be tensile. The assumption is that largest principal stress will dominate crack growth rate.

The crack growth per cycle, da/dn, is calculated using Eq 1.

\[
\frac{da}{dn} = C \Delta K^n K_{max}^p
\]  

Where C, p, and n are material constants. K is the stress intensity as shown in Eq 2.

\[
K = \sigma \sqrt{2\pi a} EXP[C'(a - a_0)]
\]

Where \(\sigma\) is the signed von Mises or max principal stress, \(a\) is the current crack size, \(a_0\) is the initial flaw diameter, and \(C'\) is a constant currently set to 0.08/mm to help account for increasing stress in the mesh element as the crack grows.

Using data and recommendations from Chen et. al. for ABC (Al, B, and C additives) SiC, the material constant C was modeled as temperature dependent. The constant p was modeled as temperature and load ratio dependent, while n was set to a constant 75.3 as shown in Table 5.5. The load ratio (R) is the ratio of the min over the max load.
Table 5.5 Material constants used to calculate the crack growth per cycle

<table>
<thead>
<tr>
<th></th>
<th>C</th>
<th>N</th>
<th>P</th>
</tr>
</thead>
<tbody>
<tr>
<td>25C</td>
<td>5.9e-73</td>
<td>75.3</td>
<td>8.6</td>
</tr>
<tr>
<td>1300C</td>
<td>3.3e-61</td>
<td>13.2</td>
<td></td>
</tr>
<tr>
<td>25C R=0.5</td>
<td></td>
<td>12.73</td>
<td></td>
</tr>
<tr>
<td>1300C R=0.5</td>
<td></td>
<td>20.26</td>
<td></td>
</tr>
</tbody>
</table>

The model linearly interpolates between the values during the simulation. Figure 5-30 plots the resulting crack growth rates $da/dn$ versus max stress intensity $K_{max}$ for 25-1300C. Figure 5-31 plots crack growth rate for load ratio.

**Figure 5-30. Crack growth rate for various temperatures total**

**Figure 5-31. Crack growth rate for load ratio 0.1 and 0.5 at 25 and 300C**
Mesh element size stability was done by scaling the crack growth rate by Eq 3.

\[
Scale = \left( \frac{V_e^{1/3} - a_0}{\frac{4}{3} \pi \left( \frac{a_0}{2} \right)^3} \right)^{1/3} \frac{\rho - \rho_{th}}{\rho_{th}} a_o
\]

(3)

Where \( V_e \) is the mesh element volume, \( a_0 \) is the initial flaw diameter, \( \rho \) is the current density, and \( \rho_{th} \) is the theoretical density.

A simulated bar measuring 5x5x50mm was modeled with a pressure applied on the end cycling at 25°C and a load ratio (R) of 0.1 and initial flaw size of 25µm. \textit{Figure 5-32} shows the results for the same bar with different sized meshes. It should be noted that the initial flaw size of 25µm was taken from data for B4C and NITE-SiC may be quite different.

\textit{Figure 5-32. Crack length for the 5x5x50mm bar with 1250 and 1800 mesh elements}

In \textit{Figure 5-33} the two on the left used signed von Mises for 1250 and 1800 mesh elements respectively. The two on the right used max principal for 1250 and 1800 respectively. The 1800 element mesh using max principal had some difficulty cracking the last row of elements. Currently signed von Mises is recommended for future simulations.
Figure 5-33. Failure profile for the bar using signed von Mises and max principal criterion

**Modeling FeCrAl clad in Watts Bar Unit 1**

In order to begin modeling of FeCrAl cladded fuel and comparing it against Zircaloy cladding, reactor operating conditions and geometric models were created and implemented into the BISON fuel performance code.

For this study, fuel performance is simulated using conditions based on available data from the Watts Bar I PWR. Geometric models of the various cladding thicknesses have been made (366µm, 500µm, and 570µm). These fuel rod models use the same outer diameter but vary the fuel and cladding radii; the gap thickness is held constant. Data from the thermal hydraulic system has also been implemented from design documents.

Fuel rod power history and axial power profile data from the NESTLE 3D full-core simulator have been input into BISON. This data analyzes the highest-power and average-power fuel rods as the reactor is in load-following operation.
Material models for the FeCrAl alloy (Kanthal APMT and Alkroth 720) have been made during a previous study and behavioral models are informed by ongoing experiments aimed at identifying alloy behavior under load and during irradiation. Material models for Zircaloy cladding, UO2 fuel, and plenum gas behavior have been developed and implemented previously using the MATPRO database.

With the input data nearly complete, these simulations will be run and completed during the next quarter. After the initial simulations are complete, modeling activities will focus on compiling more operational data to compare fuel performance effects from power history features.

Fuel performance simulations during this quarter were performed using data provided from neutronics calculations for 3 fuel rods. These simulations were performed using the finite-element based fuel performance code BISON and included the following 3 cases:

1. Maximum power operation in an AP1000 PWR for 441 EFPD – FeCrAl Cladding
2. Average power operation in an AP1000 PWR for 441 EFPD – FeCrAl Cladding
3. Average power operation in a SMR for 1400 EFPD – Zry-4 cladding

Fuel rod parameters for each case are shown in Table 5.6 below:

<table>
<thead>
<tr>
<th>Case</th>
<th>Fuel (µm)</th>
<th>Radius (µm)</th>
<th>Gap Thickness (µm)</th>
<th>Cladding Thickness (µm)</th>
<th>Rod Length (m)</th>
<th>Enrichment (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4300</td>
<td>84</td>
<td>366</td>
<td>3.85</td>
<td>4.4</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>4300</td>
<td>84</td>
<td>366</td>
<td>3.85</td>
<td>4.4</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>4096</td>
<td>84</td>
<td>570</td>
<td>2.413</td>
<td>4.95</td>
<td></td>
</tr>
</tbody>
</table>

*Table 5.6. Fuel rod parameters for power histories studied with BISON*
**Cases 1 & 2 for the WB1C1 AP1000 PWR with FeCrAl**

Cases 1 and 2 used FeCrAl cladding rods based on the AP1000 PWR design and were operated for nearly 1.2 years. The difference between these cases was the operation power (max operation is ~1.5x power output of the average operation). Figure 5-35 shows the peak and average fuel centerline temperature for both simulations. This shows a substantially larger peak temperature for the maximum operation; approaching 2/3 the melting temperature of UO$_2$ fuel. The temperature histories between the average and peak centerlines differ because of changes in the axial power profiles of the fuel rods. The maximum operation shows a significantly larger average fuel centerline temperature than the average operation. This will impact the fission gas release and fuel swelling as they will be greater in fuel operated at higher temperatures.

![Figure 5-35. Average vs Peak Fuel Centerline Temperature](image)

Because these rods are only operated for about a single cycle, they are not expected to show many of the effects that currently limit fuel operation such as fuel-cladding mechanical interaction or high plenum pressures. Figure 5-36 shows the maximum radial displacement and the maximum hoop stress in the cladding. These show that the maximum power operation is in the early stages of PCMI. The cladding hoop stress shows the cladding initially in a compressive state due to the 15.5 MPa coolant pressure in the reactor pressure vessel. The cladding for the average operation remains in this state for the entire cycle; the maximum operation does not. As the fuel comes into contact with the cladding, it gradually begins to push on the cladding and changes from compressive to tensile hoop stress as the pressure-induced stress is overcome. The radial displacement also shows a small blip in the maximum operation corresponding to this mechanical interaction.
Measuring the plenum volume is an indicator of the amount of swelling occurring in the fuel in FeCrAl cladded rods before gap closure. This is true because of the small amounts of creep deformation occurring in FeCrAl cladding. Figure 5-37 shows the plenum volume from these simulations. The plenum volume is immediately decreased by the thermal expansion of the fuel and cladding (greater for the fuel – higher temperatures). Immediately after the simulation begins, the fuel begins densification and subsequent swelling. As shown in the figure, the average operation shows an extended densification phase because of the lower temperatures in the fuel and swells very little. The maximum operation undergoes densification much faster and begins swelling much more.

Because the temperatures in the fuel are higher for the maximum operation, the expectation is that there will be more swelling and more thermally activated fission gas release. Both of these processes will contribute to an increase in plenum pressure. Figure 5-38 shows the fission gas release and plenum pressure for these simulations. As shown in the figure, the fission gas release corresponds well to the increase in plenum pressure for the maximum operation case, and seems to obscure any contribution to plenum pressure form fuel swelling. The average operation case doesn’t achieve temperatures high enough (or enough fission gas production) to initiate release, and the plenum pressure remains relatively constant.
While fission gas can reduce the thermal conductivity of the fuel, it can cause more detrimental effects during a loss of coolant accident scenarios. This is because large plenum pressures induce a tensile stress state in the cladding. This can contribute to clad bursting in a reactor if coolant pressure is lost along with core cooling capabilities.

Figure 5-38. Fission Gas Release (left) and Plenum Pressure (right)

**Cases 3 for the SMR with Zircaloy-4 (1400 EFPD)**

The final case that was simulated was for a small modular reactor using Zircaloy-4 cladded fuel rods. Similar to the analysis above, select parameters were monitored over the fuel simulation. This is a rather short analysis as there is no complementary data to compare to. Figure 1 shows the average and maximum fuel centerline temperatures. These are different because of the changing shape of the axial power profiles used.

Figure 5-39. Peak and Average Fuel Centerline for SMR with Zirc-4 (1400 EFPD)

Figure 5-40 shows the axial and radial displacements of the fuel cladding. Axial displacement is driven by thermal expansion initially and subsequent irradiation growth. While contact does occur, the cladding does not protrude further than the end caps. This is because of the large amount of thermal and irradiation creep that zircaloy experiences.
Figure 5-40. Cladding Axial (left) and Radial (right) Displacements for SMR with Zirc-4 (1400 EFPD)

Figure 5-41 shows the cladding hoop stress. It is initially compressive due to the pressure differential across the cladding. This is from the reactor coolant pressure and the rod plenum pressure. There is no fission gas release in this rod, and the plenum pressure increases ~1MPa. This is presumably because of the cladding creep and fuel swelling. As the average rod temperature does not change much over this simulation.

Figure 5-41. Maximum Cladding Hoop Stress for SMR with Zirc-4 (1400 EFPD)

**Conclusion for Fuel Performance Studies**

Three separate fuel performance simulations have been performed and analyzed. These highlight several complex effects inherent in integral nuclear fuel rod analysis. This shows a good framework for performing these analyses with material and geometric models that have been implemented into the BISON fuel performance code. Future work is a continuation of these analyses as more data becomes available for simulation.
5.5 Task 5: Analysis of large PWR with leading ATF concepts

5.5.a Stated Objective of Task 5

This task will involve looking at the same large PWR design examined during Tasks 1 and 2 but shifting from a baseline UO2/Zirc fuel/cladding system to analysis of leading ATF concepts in a large PWR being operated with the current (baseline) operating regime or an aggressive (e.g., load-following) regime. The analysis activities in this task will be similar to those performed during Tasks 1 and 2, focusing on full-core 3-D neutronics analysis with accompanying fuel performance analysis using pin power histories generated by neutronics results; however, the shift from a baseline existing fuel/cladding system to innovative ATF concepts will require extensive parametric design studies to evaluate the available design space and establish appropriate reference core designs and values for some fuel design parameters (e.g., cladding thickness). At the present time, UO2/FeCrAl and FCM/FeCrAl have been identified as representative leading ATF concepts to serve as analysis examples; however, the project could change this to other ATF fuel/cladding concepts if the Advanced Fuels Campaign ATF program identifies more attractive concepts in the meantime.

5.5.b Report on Task 5

Selection of Power Histories

While analyzing the performance of enhanced accident tolerant claddings, it is important to consider each alternative cladding’s performance when subjected to the ‘most limiting’ conditions. One reactor physics parameter by which to gauge ‘limiting’ is end-of-life burnup; rods that produce the most power the longest tend to be closer to mechanical failure than rods that don’t reach such burnups. It is for this reason that the assembly with the highest burnup after 3 operating cycles, with the first cycle being at equilibrium, was used to produce the linear heat rates that are subsequently fed into the fuel mechanics code, BISON. Figure 5-42 below shows the core map with purple and blue indicating once and twice burnt fuel, respectively. Included in the figure are the locations for the assembly chosen for analysis, which has a discharge burnup of 61 GWd/MT. The cycle length is 500 EFPD and has an end-of-cycle core average burnup of 33 GWd/MT.
With the full-core neutronic analysis performed using NESTLE, it was necessary to translate the nodal powers given by NESTLE into more realistic pin powers. This was done using CASMO, which was also used to generate cross sections for NESTLE, by weighting the nodal powers by the relative pin power of the “hottest” rod from a CASMO branch that had the operating parameters closest to that of the full-core cycle. The plot of power vs. burnup for the pin chosen is shown in Figure 5-43 below. A high order fit was made for the curve and was factored into the linear heat rate calculation:

\[
Axial\ assembly\ nodal\ power\ (NESTLE) \times \text{pin power (CASMO)} \times \frac{\text{core power (W)}}{\#\ assemblies \times \#\ pins\ assembly \times \#\ nodes\ pin \times \text{meters} \text{node}}
\]
**Power History Profiles Generated**

The method detailed above was used for the analysis of both the standard, zircaloy claddings, as well as with SiC and FeCrAl cladding types. The cases were operated at normal conditions (100% power, no rods). The base, zircaloy case used 4.4 % U-235 enrichment with a cladding thickness of 570 µm. Three cases were run for the FeCrAl cladding: 570 µm thickness at 4.4% U-235, 570 µm thickness at 5.6% U-235, and 350 µm thickness at 5.2% U-235. The latter two were neutronically equivalent to the zircaloy case. Similarly, the two SiC case were at 4.4% and 4.2% U-235, with both at 570 µm thickness; because of its neutronic superiority to zircaloy, no thinner cladding case was tested. The two sets of figures below show the comparisons of the alternate claddings vs. zircaloy, looking both as a function of axial length and multi-cycle length. A middle-of-cycle exposure point was chosen for the axial comparison, and a middle axial slice was chosen for the comparison versus time.

![Figure 5-44. Axial Linear Power Density for FeCrAl Claddings at Varying Enrichments/Thicknesses](image1)

![Figure 5-45. Multi-Cycle Linear Power Density for FeCrAl Claddings at Varying Enrichments/Thicknesses](image2)
For both the axial and time comparisons, the FeCrAl and SiC 570 μm 4.4% enrichment cases differed the most from zircaloy, which is because of the reactivity difference. However, the shapes were largely similar for the cases with equal reactivities.

**BISON Fuel Performance Studies of Most Recent Core Designs**

Using power histories and axial power profiles generated from neutronics calculations, the BISON fuel performance code was used to simulate FeCrAl and Zircaloy cladding for power maneuvering during normal operation in an AP1000-like PWR. The power data used for these fuel rods are generated from neutronics simulations using the core simulation tool NESTLE. The geometry for the fuel rods is shown in the following table:
Table 5.7. Rod Geometry and Characteristics for BISON Calculations

<table>
<thead>
<tr>
<th>Material</th>
<th>Fuel Radius (µm)</th>
<th>Gap Thickness (µm)</th>
<th>Cladding Thickness (µm)</th>
<th>Fuel (Rod) Height (m)</th>
<th>Enrichment (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>FeCrAl</td>
<td>4096</td>
<td>84</td>
<td>570</td>
<td>3.65 (3.92)</td>
<td>4.4</td>
</tr>
<tr>
<td>Zircaloy</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

This study highlights the differences in performance of the cladding materials for identical fuel rod geometries. While the average rod power is the same for both rods, there is a large difference between axial power distributions between rods. This is a result of the optimization method used when generating the power data. Because of limited data, only a short scoping analysis was performed.

Figure 5-48 shows the average fuel centerline temperature for both fuel cladding materials. Because FeCrAl alloys exhibit significantly less thermal and irradiation creep deformation than Zircaloy, they remain much more rigid. This reduces the amount of cladding creep-down, in comparison with Zircaloy, leading to significantly increased fuel temperatures before the onset of gap closure. Because the gap remains open, the temperature of the FeCrAl-cladded rod remains greater through the entire simulation. Not only are these temperatures greater, but they are also slowly converging toward the Zircaloy temperatures as the gap conductivity improves from closure.

Because the fuel temperatures in the FeCrAl clad fuel are greater, fuel thermal expansion and gaseous fission product swelling are greater. Figure 5-49 shows the maximum radial displacement for both fuel rods over the simulation. They initially increase as they are heated to operating temperatures. Next, the claddings begin to creep down. Because Zircaloy creeps down more, the...
fuel radial displacement begins to decrease. Meanwhile, FeCrAl undergoes isotropic irradiation swelling which increases its diameter offsetting the minuscule amount of creep-down that it undergoes. Gap closure in the FeCrAl rod begins at 1.5 years, while for Zircaloy it begins at .5 years.

![Graph showing the maximum radial displacement of Zirc and FeCrAl cladding materials](image)

*Figure 5-49. The maximum radial displacement of Zirc and FeCrAl cladding materials*

This short scoping analysis confirms that under similar conditions FeCrAl and Zircaloy cladding behave quite differently, and more work is being done to provide greater detail to these discrepancies and their understanding.

**Parametric Study of Single Test Rod and Assembly Substitutions**

Given the lack of experimental data and uncertainty associated with how both of these materials might perform in nuclear power reactors, extensive research and experimentation needs to be done to ensure that they can hold up to anticipated and unanticipated operational reactor conditions. One such initial experiment performed to demonstrate viability may be what is commonly carried out in the commercial nuclear industry when a new fuel type is introduced, which is to insert lead test rods or assemblies in an existing power reactor. So, for example, placing a limited number of FeCrAl or SiC rods in a single assembly and operating it to a typical burnup would provide crucial information for utilities and regulators to have before making the major decision to switch to an alternate cladding. Before experimentation, however, research should be done on how single test rods affect power peaking, and perhaps inform some of the experimental decisions on where to place such test rods. Further analyses, in fact, could provide expectations of the actual fuel performance expected.

**Core/Assembly/Test Rod Simulation Description**

This work examined the impact of substituting FeCrAl and SiC cladding on both single rod and single assembly test cases. The goal was to provide insight on a pin-by-pin level of the peaking effect caused by heterogeneity in the lattice. All analyses herein reported were performed using CASMO/SIMULATE on a representative PWR using an equilibrium core. The base case used Westinghouse 17x17 assemblies with 4.2% and 4.6% enriched U-235, with 104 IFBA rods. Figure 5-50 and Figure 5-51 show the lattice and core maps used.
Whether a single rod or whole assembly, substitutions were only made to the 4.6% enriched assembly, noted by orange and an asterisk in Figure 5-50. The assembly was chosen because it was the assembly that had the highest FΔH value, given by SIMULATE, over the cycle length. The hottest non-IFBA rod from CASMO and an average power non-IFBA rod, noted by A and B in Figure 5-51, were chosen to be the single rod test cases, herein labeled as the “hot” and “cold” test rods, respectively.

Description of Alternate Claddings

The FeCrAl composition split used was 75-20-5 for Iron, Chromium, and Aluminum, respectively. The density was 7.1 g/cc. Given the higher absorption cross section (2.4 barns vs. 0.2 barns for Zircaloy [25]), cases were run with higher U-235 enrichment in addition to the 4.6%, since a hypothetical wholesale cladding change would require an increase in U-235 loading. The cladding thicknesses were also varied from the standard 570 µm to 366 µm in order to increase fissile loading. The outer clad radius and gap thickness were held constant when changing the clad thickness. When changing the enrichment, the following equation was used for the UO2 nuclides [11]:

\[
\begin{align*}
U-234 &= 0.007731 \cdot w^{1.0837} \\
U-235 &= w \\
U-236 &= 0.0046 \cdot w \\
U-238 &= \text{balance}
\end{align*}
\]

The SiC composition was 70-30 for Silicon and Carbon, respectively, with a density of 2.58 g/cc. Each SiC case used the same cladding thickness and enrichment since SiC outperforms Zirconium neutronically (thermal cross-section of around 0.09 barns).

Results for Neutronics and Power Distribution Analysis

This work evaluated several parameters while comparing each test case against the standard, Zircaloy case: hot channel factor (FΔH), 2-D pin power and burnup, and 2-D assembly average relative power.
fraction. Table 5.8 shows the case where a single FeCrAl and SiC rod was inserted in the hottest rod (‘A’ from Figure 5-51) and assembly location. The cladding thicknesses were 570 µm for each. Due to there being only one test rod, the soluble boron concentration is unchanged from case to case.

**Table 5.8.** \( F_{\Delta H} \) values for 570 µm, 4.6% U-235 case

<table>
<thead>
<tr>
<th>Burnup (EFPD)</th>
<th>Zirc</th>
<th>FeCrAl rod</th>
<th>SiC rod</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>1.462</td>
<td>1.461</td>
<td>1.462</td>
</tr>
<tr>
<td>26.0</td>
<td>1.463</td>
<td>1.462</td>
<td>1.462</td>
</tr>
<tr>
<td>52.1</td>
<td>1.475</td>
<td>1.474</td>
<td>1.475</td>
</tr>
<tr>
<td>104.1</td>
<td>1.474</td>
<td>1.474</td>
<td>1.474</td>
</tr>
<tr>
<td>156.2</td>
<td>1.465</td>
<td>1.465</td>
<td>1.465</td>
</tr>
<tr>
<td>208.3</td>
<td>1.448</td>
<td>1.448</td>
<td>1.45</td>
</tr>
<tr>
<td>260.4</td>
<td>1.428</td>
<td>1.428</td>
<td>1.429</td>
</tr>
<tr>
<td>312.4</td>
<td>1.406</td>
<td>1.406</td>
<td>1.406</td>
</tr>
<tr>
<td>364.5</td>
<td>1.383</td>
<td>1.383</td>
<td>1.383</td>
</tr>
<tr>
<td>416.6</td>
<td>1.36</td>
<td>1.36</td>
<td>1.36</td>
</tr>
<tr>
<td>468.7</td>
<td>1.339</td>
<td>1.339</td>
<td>1.339</td>
</tr>
<tr>
<td>484.7</td>
<td>1.335</td>
<td>1.335</td>
<td>1.335</td>
</tr>
</tbody>
</table>

Table 5.8 shows virtually no significant difference in \( F_{\Delta H} \) values for a single rod substitution where the cladding and enrichments are unchanged. Table 5.9 shows how the \( F_{\Delta H} \) values change for a FeCrAl case with 570 µm thick cladding and 4.8% U-235, as well as 366 µm cases with 4.6% and 4.2% U-235 test rod enrichments.

**Table 5.9.** \( F_{\Delta H} \) values for select FeCrAl cases – hot location ‘A’

<table>
<thead>
<tr>
<th>Burnup (EFPD)</th>
<th>Zirc</th>
<th>570 µm – 4.8% rod</th>
<th>366 µm – 4.6% rod</th>
<th>366 µm – 4.2% rod</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>1.462</td>
<td>1.517</td>
<td>1.461</td>
<td></td>
</tr>
<tr>
<td>26.0</td>
<td>1.463</td>
<td>1.546</td>
<td>1.462</td>
<td></td>
</tr>
<tr>
<td>52.1</td>
<td>1.475</td>
<td>1.564</td>
<td>1.481</td>
<td></td>
</tr>
<tr>
<td>104.1</td>
<td>1.474</td>
<td>1.568</td>
<td>1.491</td>
<td></td>
</tr>
<tr>
<td>156.2</td>
<td>1.465</td>
<td>1.554</td>
<td>1.482</td>
<td></td>
</tr>
<tr>
<td>208.3</td>
<td>1.448</td>
<td>1.530</td>
<td>1.463</td>
<td></td>
</tr>
<tr>
<td>260.4</td>
<td>1.428</td>
<td>1.505</td>
<td>1.441</td>
<td></td>
</tr>
<tr>
<td>312.4</td>
<td>1.406</td>
<td>1.480</td>
<td>1.419</td>
<td></td>
</tr>
<tr>
<td>364.5</td>
<td>1.383</td>
<td>1.455</td>
<td>1.398</td>
<td></td>
</tr>
<tr>
<td>416.6</td>
<td>1.360</td>
<td>1.432</td>
<td>1.378</td>
<td></td>
</tr>
<tr>
<td>468.7</td>
<td>1.339</td>
<td>1.410</td>
<td>1.358</td>
<td></td>
</tr>
<tr>
<td>484.7</td>
<td>1.335</td>
<td>1.403</td>
<td>1.352</td>
<td></td>
</tr>
</tbody>
</table>

As Table 5.9 shows, the power peaking limits can be affected significantly by changing a single rod. Even with the same enrichment as the rest of the rods in the assembly, the increased fuel volume caused by thinning the clad pushes \( F_{\Delta H} \) beyond the accepted limit. Unlike with the cases from Table 5.8, these cases result in significant differences in pin powers and end-of-life burnups. The 570 µm, 4.8% case only has a 1.5% higher pin power over the cycle and the same percent increase in burnup, but the 4.6% and 4.2% 366 µm cases have 8% and 4% longer burnups, respectively, compared to the standard pin.
Table 5.10 shows the same results as Table 5.9, except the pin location is ‘B’ from Figure 2 instead of ‘A’.

Table 5.10. \( F_{\Delta H} \) values for select FeCrAl cases - cold location ‘B’

<table>
<thead>
<tr>
<th>Burnup (EFPD)</th>
<th>Zirc 570 µm – 4.8% rod</th>
<th>366 µm – 4.6% rod</th>
<th>366 µm – 4.2% rod</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>1.462</td>
<td>1.495</td>
<td>1.462</td>
</tr>
<tr>
<td>26.0</td>
<td>1.463</td>
<td>1.489</td>
<td>1.462</td>
</tr>
<tr>
<td>52.1</td>
<td>1.475</td>
<td>1.485</td>
<td>1.474</td>
</tr>
<tr>
<td>104.1</td>
<td>1.474</td>
<td>1.474</td>
<td>1.474</td>
</tr>
<tr>
<td>156.2</td>
<td>1.465</td>
<td>1.465</td>
<td>1.465</td>
</tr>
<tr>
<td>208.3</td>
<td>1.448</td>
<td>1.448</td>
<td>1.448</td>
</tr>
<tr>
<td>260.4</td>
<td>1.428</td>
<td>1.428</td>
<td>1.428</td>
</tr>
<tr>
<td>312.4</td>
<td>1.406</td>
<td>1.406</td>
<td>1.406</td>
</tr>
<tr>
<td>364.5</td>
<td>1.383</td>
<td>1.383</td>
<td>1.383</td>
</tr>
<tr>
<td>416.6</td>
<td>1.360</td>
<td>1.360</td>
<td>1.360</td>
</tr>
<tr>
<td>468.7</td>
<td>1.339</td>
<td>1.339</td>
<td>1.339</td>
</tr>
<tr>
<td>484.7</td>
<td>1.335</td>
<td>1.335</td>
<td>1.335</td>
</tr>
</tbody>
</table>

The rod location clearly has a significant impact on the peaking, as the 4.6% case was the only one of the three test cases that showed an elevated \( F_{\Delta H} \) value. For all three cases, the percent differences in pin power and end-of-life burnup were the same as when compared to the same pin location from the standard case.

For a comparison to the 366 µm 4.6% case, replacing all fuel rods with FeCrAl cladding instead of just the hottest rod gives much different \( F_{\Delta H} \) values. Since the entire assembly is less reactive because of the quantity of FeCrAl, an extra, 5.0% enriched assembly case was added; the soluble boron concentration of the 5.0% FeCrAl assembly matched that of the standard, Zirconium case. Figure 5-52 shows the 2-D average relative power fraction of the test assembly vs. the standard assembly. Table IV lists this comparison and shows a much lower peaking for the 4.6% assembly, whereas the 5.0% assembly is only slightly below that of the 4.6% rod. The 5.0% assembly did, however, stay below the 1.55 \( F_{\Delta H} \) limit.

![Figure 5-52. Average 2D relative power of standard assembly vs. 5.0% U-235 FeCrAl assembly](image)
Table 5.11. \(F_{\text{th}}\) values for 366 \(\mu\text{m}\) 4.6\% FeCrAl single rod and whole assembly

<table>
<thead>
<tr>
<th>Burnup (EFPD)</th>
<th>4.6% Single rod</th>
<th>4.6% Assembly</th>
<th>5.0% Assembly</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>1.517</td>
<td>1.471</td>
<td>1.545</td>
</tr>
<tr>
<td>26.0</td>
<td>1.546</td>
<td>1.475</td>
<td>1.528</td>
</tr>
<tr>
<td>52.1</td>
<td>1.564</td>
<td>1.487</td>
<td>1.530</td>
</tr>
<tr>
<td>104.1</td>
<td>1.568</td>
<td>1.483</td>
<td>1.517</td>
</tr>
<tr>
<td>156.2</td>
<td>1.554</td>
<td>1.469</td>
<td>1.498</td>
</tr>
<tr>
<td>208.3</td>
<td>1.530</td>
<td>1.450</td>
<td>1.480</td>
</tr>
<tr>
<td>260.4</td>
<td>1.505</td>
<td>1.428</td>
<td>1.460</td>
</tr>
<tr>
<td>312.4</td>
<td>1.480</td>
<td>1.405</td>
<td>1.439</td>
</tr>
<tr>
<td>364.5</td>
<td>1.455</td>
<td>1.381</td>
<td>1.420</td>
</tr>
<tr>
<td>416.6</td>
<td>1.432</td>
<td>1.359</td>
<td>1.400</td>
</tr>
<tr>
<td>468.7</td>
<td>1.410</td>
<td>1.342</td>
<td>1.381</td>
</tr>
<tr>
<td>484.7</td>
<td>1.403</td>
<td>1.338</td>
<td>1.374</td>
</tr>
</tbody>
</table>

The results from this analysis show how the power peaking is affected by the test rod location and make a case for using test assemblies instead of rods, as the power shifts can be smoother for the former. Given that the burnups of the higher enriched test rods can be significantly higher than the other rods in the lattice is also something to be considered with these mixed-rod assemblies.

**BISON Analysis of Parametric Single Rod/Assembly Studies**

The BISON fuel performance code was used to provide detailed behavior for fuel rods to augment a parametric analysis conducted with the code SIMULATE. This analysis targeted the effects of using FeCrAl cladding as a replacement for Zircaloy cladding, as well as the effects of varying the cladding thickness, fuel enrichment, fuel rod position, and the cladding material of other fuel rods in the assembly. Neutronics data provided from the SIMULATE simulations was implemented into BISON in the form of operating conditions. These are generally a series of individual power histories and axial power profiles.

Fuel rod geometries, shown in Table 5.12, were provided from the neutronics simulations to resemble a typical PWR; the fuel rod outer radius in all nine simulations is 0.475 cm. Simulations using the FeCrAl cladding are just a single FeCrAl-cladded rod in a full core of Zircaloy-cladded rods. All operating conditions are selected from either a hot or cold position in the same fuel assembly. This fuel assembly was chosen because it highest hot channel factor over the cycle length. Simulation cases 2, 5, and 9 use conditions from the rods in the cooler position in the fuel assembly, and simulation 4 uses conditions where the full assembly containing this rod is FeCrAl cladding.

Table 5.12. Summary of Simulations for BISON Parametric Analysis

<table>
<thead>
<tr>
<th>Case</th>
<th>Clad</th>
<th>Fuel Radius</th>
<th>Gap Size</th>
<th>Clad Thickness</th>
<th>Fuel Stack Height</th>
<th>Cladding Length</th>
<th>Fuel Enrichment</th>
<th>Single Rod/Assembly</th>
<th>Position</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>FeCrAl</td>
<td>4300 (\mu\text{m})</td>
<td>84(\mu\text{m})</td>
<td>366 (\mu\text{m})</td>
<td>3.66 m</td>
<td>3.90 m</td>
<td>4.2%</td>
<td>Assembly</td>
<td>Cold</td>
</tr>
<tr>
<td>2</td>
<td>FeCrAl</td>
<td>4300 (\mu\text{m})</td>
<td>84(\mu\text{m})</td>
<td>366 (\mu\text{m})</td>
<td>3.66 m</td>
<td>3.90 m</td>
<td>4.2%</td>
<td>Assembly</td>
<td>Cold</td>
</tr>
<tr>
<td>3</td>
<td>FeCrAl</td>
<td>4300 (\mu\text{m})</td>
<td>84(\mu\text{m})</td>
<td>366 (\mu\text{m})</td>
<td>3.66 m</td>
<td>3.90 m</td>
<td>4.6%</td>
<td>Assembly</td>
<td>Cold</td>
</tr>
<tr>
<td>4</td>
<td>FeCrAl</td>
<td>4300 (\mu\text{m})</td>
<td>84(\mu\text{m})</td>
<td>366 (\mu\text{m})</td>
<td>3.66 m</td>
<td>3.90 m</td>
<td>4.6%</td>
<td>Assembly</td>
<td>Cold</td>
</tr>
<tr>
<td>5</td>
<td>FeCrAl</td>
<td>4300 (\mu\text{m})</td>
<td>84(\mu\text{m})</td>
<td>366 (\mu\text{m})</td>
<td>3.66 m</td>
<td>3.90 m</td>
<td>4.6%</td>
<td>Assembly</td>
<td>Cold</td>
</tr>
</tbody>
</table>
Figure 5-53 shows the power histories used in each of these simulations. The rod average linear heat rate of the fuel rods varies over time as the operating conditions generated by SIMULATE are different for each case. There are three distance reactor cycles, each covering slightly more than a year, with a decreasing average power. Because the linear heat rates vary for each simulation, the expected thermal behavior of each of the fuel rods is expected to vary. Over the lifetime of these fuel rods, the pronounced differences in the fuel linear heat rates (2-4 kW/m) will lead to a wide range of expected outcomes among simulations. This makes deriving conclusions based on fuel geometry and cladding mechanical behavior difficult, nevertheless, it does provide some insight on general behavioral trends.

Similar to previous update, these simulations are performed using previously developed models for Zircaloy cladding and using best-estimate material models for the APMT FeCrAl cladding. Previously implemented models are also used for the UO2 fuel, however, there was uncertainty in the fuel creep response and it was not included. This will present large increases in the cladding hoop stress and radial deformation for the FeCrAl cladding after mechanical contact with the fuel has occurred.

<table>
<thead>
<tr>
<th></th>
<th>Rod Diameter</th>
<th>Rod Average Power (kW/m)</th>
<th>Time (years)</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>Zirc 4096 µm</td>
<td>4.6%</td>
<td>570 µm</td>
</tr>
<tr>
<td>8</td>
<td>4096 µm</td>
<td>4.6%</td>
<td>570 µm</td>
</tr>
<tr>
<td>9</td>
<td>4096 µm</td>
<td>4.6%</td>
<td>Cold</td>
</tr>
</tbody>
</table>

Figure 5-53. The rod average linear heat rate of the fuel rods as a function of time.

Figure 5-54 and Figure 5-55 show the peak and average fuel centerline temperatures, respectively, for the simulations. The peak fuel centerline temperatures are different among simulations arising from the differences in fuel radius, cladding creep down behavior, and the shape of the axial power profile over the fuel lifetime. The average fuel centerline temperatures over time more closely resemble the linear heat generation rates than the peak centerline temperatures, but show consistently higher temperatures for the FeCrAl cladded fuel rods. The peak fuel centerline shows more variation than the average, due to continuous changes to the axial power profile shape. This causes local hot spots along the fuel, even though the axial profile averages to unity. The average fuel centerline temperatures more closely resemble the average linear heat generation rates. In these simulations, the Zircaloy cladded fuel rods exhibit noticeably lower fuel temperatures, even though the linear heat rates are, for some time, larger than the corresponding FeCrAl cladded fuel rods. This is a result of the difference in creep down behavior between the Zircaloy and FeCrAl alloys. Because Zircaloy cladding is expected to exhibit more thermal and irradiation creep under equivalent conditions and a reduction in the cladding radius from anisotropic (axially-oriented) irradiation growth, the gap is expected to close much faster than FeCrAl cladded fuel rods. As the gap is closed, heat transfer between the fuel and cladding is improved, and fuel temperatures are decreased.
Both the axial elongation and radial deformation, shown in Figure 5-56 and Figure 5-57, respectively, initially increase due to thermal expansion as the cladding temperature reaches operating temperature. The cladding axial elongation is initially dominated by thermal expansion. Steady-state irradiation-induced deformation begins to elongate the cladding until radial expansion from mechanical contact begins to counteract the elongation. Because the FeCrAl cladding possesses a slightly higher thermal expansion coefficient, the axial and radial expansion is slightly greater. After this point, steady-state irradiation-induced deformation and creep begin to influence the cladding dimensional changes. Thermal expansion initially increases the cladding radius. Steady-state isotropic swelling in the FeCrAl begins to slowly increase the cladding radius, while creep down and anisotropic irradiation growth quickly reduce the cladding radius for Zircaloy. Mechanical contact with the fuel quickly expands the cladding radius.

The Zircaloy cladding elongates axially and shrinks radially as volume-conservative anisotropic irradiation growth begins. Due to the coolant system pressure, the Zircaloy also immediately begins to
creep down radially, further reducing the cladding radius. This causes the Zircaloy cladding to undergo mechanical interaction much quicker than the FeCrAl cladded fuel rods. After mechanical contact occurs, the fuel pushes the cladding radially, offsetting the axial elongation of the cladding. This causes the cladding to shrink axially, which the fuel radially pushes the cladding outward.

The FeCrAl alloy cladding behaves much differently because it only exhibits isotropic irradiation growth and orders of magnitude less thermal and irradiation creep than the Zircaloy cladding. Instead of creeping down, like the Zircaloy cladding, the cladding is actually slightly expanded, as shown in Figure 5-57. The cladding expands both axially and radially due to isotropic irradiation swelling, until mechanical contact occurs. Here, much like the Zircaloy cladding, as the fuel expands into the cladding radially, the axial elongation is offset.

![Figure 5-56. The cladding axial elongation.](image)

![Figure 5-57. Thermal expansion versus time.](image)
Figure 5-58 shows the maximum hoop stress generated in the cladding over time. The maximum cladding hoop stress is initially compressive due to the pressure differential across the cladding. This arises from the large differences between the rod internal pressure and the coolant system pressure. This generally remains compressive until mechanical contact occurs. As the fuel pushes the cladding radially, the hoop stress rapidly increases. Hoop stress in the Zircaloy cladding begins to saturate near 100 MPa, as creep deformation acts to relieve the stress during expansion. Hoop stress in the FeCrAl cladding, however, continually increases as the cladding is expanded. The maximum cladding hoop stress is initially compressive because of the pressure differential between the rod internal pressure and the coolant system pressure. After the onset of mechanical contact occurs, the hoop stress quickly becomes tensile and rapidly increases. For the Zircaloy, the hoop stress remains less than 200 MPa, while for the FeCrAl, the simulations end with hoop stresses between 300-600 MPa. Note: these simulations do not include fuel creep, which will significantly diminish the large hoop stresses that for in the FeCrAl cladding.

![Graph showing maximum cladding hoop stress versus time.](image)

The percentage of fission gas released to the fuel rod plenum is shown in Figure 5-59. The percentage initially increases as a large portion of the fission gas produced early in the first cycle is released. This is motivated primarily by the high operating power and consequent fuel temperatures in the first cycle of operation, as seen in Figures 1-3. Because the linear heat rates are all different for each of the simulations, the amount of fission gas that is produced varies between fuel rods. This shows that because the FeCrAl cladded fuel rods exhibit greater fuel temperatures for much of the simulated time, the proportion of fission gas that is released will be greater than the Zircaloy-cladded fuel rods. The percentage of fission gas released to the fuel rod plenum increases quickly during the first cycle, as the fuel temperatures are greatest. As the simulations proceed into the second and third cycles, the lower fuel temperatures facilitate greater fission gas retention.
As a standalone analysis, these results show general performance differences between the FeCrAl and Zircaloy cladding materials, such differences in creep down behavior and stress development after mechanical contact, and differences in fuel temperature and gap closure arising from the geometric models used for these fuel rods. However, when taken in the context of the neutronics analysis, these results show that the FeCrAl-cladded fuel rods can be engineered to perform similarly, both neutronically and thermo-mechanically, to Zircaloy cladded fuel rods in many ways.

**Cartesian Pin Power Reconstruction in NESTLE**

NESTLE pin power reconstruction has been shown to work in hexagonal lattice geometries, like those found in a VVER. NESTLE’s ability to produce pin power peaking factors for nodes of Cartesian geometry has largely been unexplored after being added by Dr. Keith Ottinger in the summer of 2016. Dr. Ottinger’s departure from UT left some commented code and version control commit messages, with limited documentation on the pin power reconstruction (PPR) features. Recent exploration of these routines has identified some confirmed some code bugs in the Cartesian pin power reconstruction routine that hinder full-core PPR. Thus, code development is underway to find and address these bugs.

Recent research efforts are aimed at reinstating continuous integration (CI) practices in NESTLE involving nightly builds. CI practices enable sustainable code development through checking that legacy code functionality remains intact as the code evolves. If one of NESTLE’s thirty-nine regression tests fails, an email gets sent to alert developers containing diagnostic information.

Some example functionality of pin power reconstruction is shown in the table below for a simple vintage 7x7 problem. Also, visualization in ParaView/VisIt has been demonstrated, which primarily allows a developer to check for reasonable results regarding pin power but allow future code users to investigate core design metrics. An example of the ParaView-compatible NESTLE output for linear power density (kW/ft) can also be found in Figure 5-60.
Aggressive Operation via Load-Follow

As part of the process of evaluating some of the ATFs, it is necessary to study how these react within “normal,” full-power operation, and also within more “aggressive” operations, such as those dictated by a typical load-follow operational scheme. Consequently, a representative aggressive operation cycle has been developed using our Watts Bar Unit 1 core model with standard Westinghouse 17x17 assemblies. Where the normal operation was run completely unrodded (all-rods-out), the aggressive load-follow operation was performed using rod movement (using only Bank D, consistent with reference [11]); whereby the step insertions were performed linearly using two endpoints given by two known power levels from Cycle 1 [11]. The insertion steps are shown below in Figure 5-61. The scheme used in the study was modeled after a typical French load-following maneuver, where the power level is at 100% for 12 hours, then decreased to 50% over a 3-hour span, then held at 50% for 6 hours, to finally ramping back to 100% over the last 3 hours of the day [13]. Although a plant that is licensed for load following would probably operate in such a condition for a large portion of its cycle, there were computer limitations in
running that many state-points. Thus, the approach employed was to run three separate cases, where a 5-day load following scheme as described above is performed at the beginning, middle, or end of cycle. Performing load-following at these three different points in the cycle should provide representative information as to what happens to the nodal powers during the transients.

**Base Case**

The base case is the same case as the standard normal operation cases reported previously. Namely, 570 μm thick zirconium cladding, 4.4% U-235 enriched fuel with 104 IFBA rods per lattice. The number of axial nodes used in NESTLE was 48, all equidistant. As with the normal operation cases, the aggressive cases were run for 3 18-month cycles, with the first starting at equilibrium. Figure 5-62 through Figure 5-64 below show the linear heat rates for the base case for BOC, MOC, and EOC; the figures show just one axial slice approximately 1/3 from the bottom of the rod. As mentioned, the load following is a very small fraction of the cycle (5 days). By inspection, it can be determined that the spread in LHRs is greater in the 1st cycles as opposed to the 2nd and 3rd, and also greater in the EOC case that in the MOC and BOC cases. Figure 5-65 through Figure 5-67 provide a closer picture of these differences, showing only the load following portion of the cycle. The LHR from the BOC case has almost the exact shape as the power, but this is not true for the MOC and EOC cases, where the shape of the LHR exhibits a ‘sawtooth’ shape; this is due to the greater difference in flux levels between 100% and 50% power at the EOC than BOC, which increases the effects from xenon buildup.
Figure 5-63. Base case: Linear heat rate with load following at MOC

Figure 5-64. Base case: Linear heat rate with load following at EOC

Figure 5-65. Base case linear heat rate with load following at BOC
Figure 5-66. Base case linear heat rate with load following at MOC

Figure 5-67. Base case linear heat rate with load following at EOC

**ATF cases**

For the ATF testing, FeCrAl and SiC were used. The three cases evaluated were FeCrAl at 570 \( \mu \)m and 350 \( \mu \)m, and SiC at 570 \( \mu \)m. In order to match the EOC reactivity of the base case, the U-235 enrichment was changed to 5.6% and 5.2% for the two FeCrAl thicknesses, and 4.2% for the SiC case – less than the base enrichment because of SiC’s lower absorption cross section. In a similar fashion to the normal operation analysis, the same equilibrium core was used for the ATFs as for the base case, as opposed to finding the equilibrium core for each separate ATF; doing so gives each case the same starting point. The results for the three ATF cases were very similar to that of the base case, however there were some differences observed during the EOC load following, albeit fairly minor. Figure 5-68 shows how the thicker FeCrAl has a slightly more ‘constant’ LHR during the transient than its thinner counter part; for example, the thicker case was about 4 kW/m hotter after the first 50-100% ramp, but was approximately 4 kW/m colder just before the 2nd 100-50% power maneuver. The SiC tends to behave similarly to the zircaloy base case.

Figure 5-68. Base vs ATF cases linear heat rate with load following at EOC

The figures above, which show only 1 axial slice of 48, are just a sample of the data that is to be used in the fuel performance (BISON) analysis. Though there hardly seems to be a difference in the effect on the heat rates, the data generated will, at the very least, provide to BISON an accurate representation of the magnitude and shape of the linear power heat rates expected from operation with ATFs.

**Aggressive Operation via Load-Follow**

The previous quarterly report presented the neutronics calculations that have been performed assuming aggressive load-follow operations for a large PWR with zircaloy and FeCrAl claddings, both. The fuel
performance group is currently finalizing the BISON calculations for these conditions. This quarter, some additional focus was placed upon the FCM fuel performance models in BISON, which are described in a section that follows.

**Pin-based Linear Power Density in NESTLE**

While our fuel performance group finalizes the BISON calculations, we decided to revisit the topic of pin power reconstruction in the NESTLE code, which exists within the Hexagonal geometry version of the code and has been recently validated for a separate VVER modeling and simulation application [26]. Thus, for completeness, and so that we may report thermal limits more accurately from our neutronic calculations in NESTLE, some effort is being invested into finalizing this option within the code.

In fact, in order to perform a more accurate analysis of the effects of substituting enhanced accident tolerant fuels into reactors, as well as other pertinent reactor analyses, Cartesian pin power reconstruction has been implemented into NESTLE but still requires validation. The method used is the same as that which was originally developed for SIMULATE-3 by Rempe et al. [21]. For the interior of the assembly, the method assumes that the intranodal flux shapes can be approximated by non-separable polynomial expansions. At interfaces, heterogeneous form functions are defined by performing colorset calculations, which adequately correct any inaccuracies in the intranodal flux shapes at said interfaces. The method uses the following 13 known (or calculated) quantities: average node flux, average side fluxes (4), average side currents (4), and corner point fluxes (4); to determine 13 unknown coefficients for the fast and thermal flux fits; there are 25 coefficients needed for the flux fits, however, the additional 12 coefficients can be disregarded by assuming the flux to be quadratic on each surface. The method requires depletion calculations to use homogenous flux in order to get surface average quantities.

A single assembly test case based on a BWR assembly has been modeled and the aforementioned pin power reconstruction method performed. Figure 5-69 below shows a slice of the lattice and the results are given in kW/ft. An example of the fast flux fit is shown in Figure 5-70. The assembly is a 14x14 type, modeled as a quarter lattice and completely surrounded by water reflectors. The current efforts are placing focus upon the PWR and SMR type assemblies, which are more applicable to this project.

![Energy production in kW/ft for all of the pins in a node for test case.](image-url)
Additional benchmarking is required in order to verify the accuracy of the method’s implementation into NESTLE. This includes using the TRITON lattice code to verify that the form factors produced are consistent with the pin powers from NESTLE, for cases such as the test case above as well as others that include assemblies on the periphery.

Update on FCM as a Potential ATF Concept

The use of FCM in this project as possible accident tolerant fuel has not been ruled out, thus, studies continue to be carried out by our fuel performance group led by Dr. Brian Wirth. An update on this was provided in our previous report, which is work being carried out by Mr. Danny Schappel. Since then, Mr. Shappel has completed his PhD thesis, thus, some of the latest results from his thesis are herein summarized and provided, specifically highlighting Chapter 6 from his dissertation.

FCM SIMULATIONS IN AN LWR ENVIRONMENT (Ref. Ch.6 D. Schappel’s PhD Dissertation)

LWR Simulation Setup

This chapter of Dr. Schappel’s dissertation focuses on simulating FCM pellets in a light water reactor environment. The same methods and models that were used for the HTGR simulations are likewise implemented in these simulations. Figure 5-71 shows the mesh used for the FCM pellet with the matrix removed for visibility. These simulations were likewise performed on the FALCON cluster at INL. The mesh used for the LWR simulations has 2.3 million degrees of freedom. The DOF allocated for the variables and aux-variables was 9.2 and 115.4 million respectively. In these simulations, 256 processors with 1.9 TB of ram were used and the resulting run time was about one day.

The modeled FCM pellet is 8.2 mm in diameter, 13.5 mm long, and contains 41.5 vol% TRISO particles. However, the dishes and chamfers commonly used in UO2 pellets were not included in the FCM matrix. The dishes and chamfers can be neglected in this case because the NITE-SiC only swells about 2% under
Irradiation. The embedded TRISO particles are 1130 µm in diameter with 780 µm diameter kernels. Minimum particle separation was 35.2 µm, minimum radial pellet cover was 31.1 µm, and the minimum axial cover was 36.4 µm and 38.8 µm for the bottom and top surfaces respectively.

![Image](image.png)

Figure 5-71. This is a representation of the mesh used for the FCM pellet in a LWR environment.

Table 5.14 lists the dimensions of the FCM pellet. Note that dishes and chamfers were not used in the model, and a smear power of 35 kW m\(^{-1}\) or 1.2 W per TRISO particle with a 41.5 vol% packing fraction was used in this model. A steady state simulation was run with a power level of 1.2 W per particle that corresponds to an average power of 662 W cm\(^{-3}\) averaged over the pellet, and a linear power of 350 W per cm. The coolant temperature was modeled to be 290 °C and 15.5 MPa.

The outer surfaces of the pellet were constrained using a penalty Dirichlet boundary condition. This allows for displacement at the perimeter but provides sufficient constraint so that the simulation is able to converge. The power history was an initial ramp up to full power over 2.78 hours, then remaining at a constant power for 671 days, and reaching an average burnup of about 290 MWd per kg of UN. Figure 5-72 shows the results of these simulations, in which: a) This is a plot comparing the maximum, 95%, and 50% matrix hoop stress levels using LLNL dimensional change correlations. b) This plot shows the maximum, 95%, and 50% matrix hoop stress levels using FZJ dimensional change correlation. c) This is a plot showing the maximum temperature in the matrix. d) This representation shows the temperature profile across the matrix and cladding at 33x10^25 n m\(^{-2}\). The TRISO particles have been removed for visualization purposes. e) This figure compares the fission gas pressure for the LLNL and FZJ simulations.

Table 5.14. The geometry for a TRISO-III fuel pellet intended for use in LWRs

<table>
<thead>
<tr>
<th>Layer</th>
<th>[mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outer clad radius</td>
<td>4.720</td>
</tr>
<tr>
<td>Inner clad radius</td>
<td>4.150</td>
</tr>
<tr>
<td>Outer fuel pellet radius</td>
<td>4.100</td>
</tr>
<tr>
<td>Fuel pellet length</td>
<td>13.50</td>
</tr>
<tr>
<td>Gap diametral</td>
<td>0.100</td>
</tr>
</tbody>
</table>
Figure 5-72. This figure illustrates the effects of constant volume growth versus large volumetric swelling in the PyC irradiation induced dimensional change.

5-72a plots the maximum, 95%, and 50% matrix hoop stress. This figure displays the results using the LLNL pyrolytic carbon dimensional change correlations. The global maximum matrix hoop stress will occur where particles are in close proximity to each other or other pellet surfaces and have very limited symmetry.

5-72b plots maximum, 95%, and 50% matrix hoop stresses using the German FZJ correlation. The primary difference is in the base assumptions of constant volume dimensional change for the FZJ and volumetric swelling in the LLNL correlations. Using the LLNL correlation results in the large stress increase at a fluence of about 13x10^{25} n m^{-2} due to a modeled PyC volume increase. The FZJ correlation results in partial interface contact, which produces scatter in the maximum matrix, hoop stresses. It is also important to note that for both the LLNL and FZJ simulations the maximum matrix hoop stresses are considerably larger than the 95% hoop stresses. This indicates that the maximum stresses are occurring in a few elements and that very large maximum stresses will be experienced before long range cracking occurs in the matrix.
5-72c compares the maximum temperature in the matrix between the LLNL and FZJ correlations. When using the LLNL dimensional change the buffer/IPyC gaps were predicted to close at a fluence of about \(11-14 \times 10^{25} \text{ n m}^{-2}\). As a result, the maximum temperature decreased.

5-72d shows a representation of the temperature profile across the matrix and cladding. A considerable amount of heat passes through additional particles on its way to the matrix surface. As a result, the thermal resistance caused by interface gaps has an impact on the temperature of the matrix and interior particles. This is an additional reason for homogenous particles being insufficient for use in FCM fuel performance modeling.

5-72e plots the global maximum fission gas pressure as a function of burnup. Initially the temperatures for the FZJ and LLNL pellets are almost identical at low burnup, and as a result so are the fission gas pressures. However, the different gas pressure trend occurs once the buffer/IPyC gaps close in the pellet using the LLNL dimensional change correlation and the temperature decreases.

Figure 5-73 shows vertical slices of the hoop stress through the pellet at 0.02, 3.5, 13.0, and \(33 \times 10^{25} \text{ n m}^{-2}\) respectively. Early in life, the matrix stresses are dominated by the differential thermal expansion of the NITE-SiC matrix. This produces a stress state that is tensile in the perimeter and compressive in the interior. At a fluence of about \(1 \times 10^{25} \text{ n m}^{-2}\) the matrix stress is dominated by the matrix swelling gradient. This produces a stress state that is compressive at the perimeter and tensile in the interior. This is due to the fact that SiC swells more at low then high temperature. At \(13.1 \times 10^{25} \text{ n m}^{-2}\) the LLNL IIDC correlation predicts very large volumetric swelling. This large volume expansion in combination with the geometry produces the profile seen in 5-73c. After the IIDC has saturated, the 0.4 Poisson ratio in creep allows the OPyC to reduce its volume and relax the PyC swelling stresses. In Figure 5-73d, the stress state is now dominated by the saturated perimeter, kernel swelling, and gas pressure.
The color scale shows the magnitude of the hoop stress. Tension is positive while compression is negative. **a)** The hoop stress profile at a fluence of $0.02 \times 10^{25}$ n m$^{-2}$. **b)** The hoop stress profile at a neutron fluence of $3.2 \times 10^{25}$ n m$^{-2}$. **c)** The hoop stress profile at a neutron fluence of $13.1 \times 10^{25}$ n m$^{-2}$. **d)** The hoop stress profile at a neutron fluence of $33 \times 10^{25}$ n m$^{-2}$.

An additional simulation was performed to examine and compare the potential effect of hydrostatic stress on the PyC dimensional change and the resulting stresses in the matrix. The dimensional change was modeled with a linear dependence on hydrostatic stress. Additionally, the effect of hydrostatic stress was modeled as being capable of accelerating or inhibiting the dimensional change depending on the direction of the hydrostatic stress and volumetric change. Figure 5-74 shows the effects of using a stress limited PyC IIDC. In the simulation, an elemental hydrostatic stress value of 50 MPa was considered a sufficient stress to prevent further volumetric increase in that element. The limiting of the IIDC prevented the characteristic peak in matrix hoop stress and maintained the compressive perimeter and tensile interior as shown in 5-36c. Figure 5-36e and f show that the predicted matrix hoop stresses can be significantly reduced when a stress limiting term is used for the PyC IIDC. It also shows the 95% stress when using a stress limited behavior remains about half of the maximum stress. This produces a lower probability of nucleating and propagating cracks through the matrix.
Figure 5-74. Effects of using a stress limited PyC IIDC

The color scale shows the magnitude of the hoop stress. a) The hoop stress profile at a fluence of $0.02 \times 10^{25}$ n m$^{-2}$. b) The hoop stress profile at a neutron fluence of $3.2 \times 10^{25}$ n m$^{-2}$. c) The hoop stress profile at a neutron fluence of $13.1 \times 10^{25}$ n m$^{-2}$. d) The hoop stress profile at a neutron fluence of $33 \times 10^{25}$ n m$^{-2}$. e) Plot comparing the global maximum hoop stress in the matrix for stress independent and stress limited IIDC. f) A plot of the 95% hoop stress which refers to the level that 95% of the matrix elements are less than.

Due to each element being assigned a random value for the fracture threshold criterion, it was necessary to consider the uncertainty from using this method. It proved difficult to establish random seed that would provide a unique distribution for each simulation. As a result, four simulations were conducted that called the threshold distribution function different number of times. This was successful in generating four unique distributions to provide a comparison of the results. The FZJ dimensional change correlations were selected for these FCM simulations due to the predictions of partial debonding and re-contact. The remaining parameters are the same as the previous LWR FCM simulations, which include 8.2 mm diameter by 13.5 mm long pellet operating at 35 kW m$^{-1}$. Figure 5-75 shows the results. The different distributions do have an impact on the maximum matrix hoop stress. However, the trends are the same and the values are similar with the characteristic scatter for fluences above $10 \times 10^{25}$ n m$^{-2}$. This gives confidence to continue moving forward with the FCM model.
Figure 5-75. A comparison of the maximum matrix hoop stress using four different distributions for the debonding threshold values.

Summary of FCM Modeling in LWR Environment

The transition from 2D to 3D was completed. Methods to mesh and simulate a large random arrangement of discrete TRISO particles were developed. This provides the ability to determine stresses, temperatures, and gas pressures for FCM fuel in both LWR and HTGR environments. Due to meshing limitations, tetrahedral and pyramid elements were used for the fuel kernels. As a result, the model can predict temperatures but not stresses within the UN kernels. This is not expected to be significant limitation for the current applications.

The effect of IIDC was considered and as before, the volume change is the important parameter. Stress limited dimensional change was also included and found to significantly reduce the predicted stresses in the matrix.

A range of linear powers was examined, and the model predicts the FCM fuel would perform well for linear powers less than about 40 kW m\(^{-1}\). This limitation is due to the mixed SiC swelling. Thus, it is possible for the FCM fuel to operate at higher linear powers for short durations.

The model indicates that the use of BISO particles in a NITE-SiC matrix should also perform well. However, it is expected that the BISO particles will be more susceptible to manufacturing defects than a TRISO particle.
5.6  Task 6 Analysis of SMR with leading ATF concepts

5.6.a  Stated Objective of Task 6

Using the SMR design data from Task 3, and the lessons learned from the ATF analysis in Task 2, plus the development work on fuel performance in Task 4, the use of ATFs in SMRs will be analyzed. As indicated above, this will be most onerous cases evaluated and the most challenging for the fuel performance. A direct comparison with the large PWR and SMR analyses will be made.

5.6.b  Report on Task 6

The neutronics portion of this task was completed and power history data was provided to our fuel performance analysts. Results were ultimately deemed rather inconclusive due to a number of reasons, primarily due to the large number of freedoms involved. Namely, the fuel design dimensions; clad thickness, gap width, pellet diameter. We modeled most representative SMR core design documented in the journal publication shown below:

Some updates to the NESTLE SMR model were made on the basis of cross-section generation, namely, being generated with CASMO-4 instead of TRITON, as well as fuel bundle hydraulic data updates provided with RELAP5. A description of these updates follows.

**Lattice Relative Power Peaking Comparisons**

The lattice relative peaking factors (RPFs) are examined. for both the CASMO and TRITON codes at the beginning and the end of cycle (BOC and EOC, respectively). The power peaking at beginning and end of cycle for CASMO-4 and TRITON are tabulated in Figure 5-76. Because the TRITON and CASMO cycles do not end on the same step (TRITON ends at BU 31000, CASMO-4 has steps at BU 30,000 and BU 32,500), a linear interpolation was used to obtain the power peaking of the CASMO-4 model at the end of cycle. The absolute difference between the two maps are calculated and color coded based on severity in the same figure.

As indicated by the BOC ⅛ lattice map, the absolute differences between the CASMO-4 and TRITON lattices are largely insignificant due to the similarity of the isotopic compositions. However, there is a
notable difference between the power drop as a result of the gadolinium pins in the CASMO-4 model compared to the TRITON model. This has little effect on burnup characteristics near BOC, but becomes more much more pronounced due to propagating errors at EOC. Large differences also arise from the B4C which alters burnup but has little difference to start due to the isotopic similarities. However, both codes provide excellent peaking factors less than 1.2 in all locations, regardless of difference between codes.

![Image](image_url)

*Figure 5-76. Comparison of SMR lattice power peaking between CASMO-4 and TRITON.*

**Lattice Infinite Multiplication Factor Comparisons**

Due to the marginal divergence of burnup characteristics from BOC to EOC, there is a corresponding divergence of $k_{\text{inf}}$. At BOC the PCM difference is 381.8 and at EOC the PCM difference is -1738.5 (using the second to last data points). There is excellent agreement through around 17.5 MWd/kg, at which point the models diverge significantly. $k_{\text{inf}}$ versus burnup is shown in Figure 5-77. Ultimately, these differences continued to be evaluated so they are better understood, however, it is believed that this difference is due largely to the different libraries employed by these codes, and also due to the how the codes treat burnable poison depletion, such as the gadolinium fuel rods.
**Thermal-Hydraulics with RELAP5**

Development of a reliable thermal-hydraulics is necessary for accurate core physics, so since NESTLE does not have integrated functionality for the formulation of an explicit fuel dependent thermal-hydraulic model. NESTLE employs polynomial expressions for thermal-hydraulic relationships in order to improve model the fuel specifics to couple to its one or two phase drift flux model. The model for RELAP5 was developed for an average assembly of the core, and thus provides a reasonable model for bundle specific relationships.

A coarse evaluation for the temperature distribution in the assembly was used as shown in Figure 5-78. This coarse evaluation divides the temperatures into five distinct and discrete regions, the outermost of which ensures that there are no discontinuity effects due to a large jump between wall temperature and coolant temperature, though it does have the effect of making the average wall temperature in the NESTLE output appear slightly closer to the coolant temperature than it actually is due to its weighting.
In order to perform a proper temperature correction in NESTLE using Thermal Hydraulics, it is necessary to find four thermal-hydraulic relationships and can be achieved solely through power perturbation. The power perturbations used to obtain these relationships were approximately 500 kW in magnitude. The thermal-hydraulic parameters are obtained from the core model and scaled to assembly level (6376811.5 MW/Assembly power output and 54.7504 kg/s-assembly mass flow rate). The relationships that must be obtained are Heat Transfer Coefficient versus Fuel Rod Surface Temperature, Average Fuel Temperature versus Linear Power Density, Average Surface Temperature versus Linear Power Density, and Heat Capacity versus Temperature. These relationships are then fit with polynomial approximations, and those polynomials coefficients are read by NESTLE to determine the thermal-hydraulic properties of the fuel bundles based on channel flow. These relationships are seen in Figure 5-79.

**Figure 5-79. Thermal Hydraulic relationships obtained by RELAP5.**

**Updated SMR Core Analysis with NESTLE**

Based on the updated thermal hydraulic models and employing CASMO4, the newly designed SMR core has a total burnup of 31,000 MWd/MTM with a maximum assembly burnup of 46,080 MWd/MTM. This relatively low maximum assembly burnup makes it possible to extend the total core burnup near 40,000 MWd/MTM without compromising safety margins. Because the control rods removed from the top, the core experiences a power shift towards the top of the core as burnup progresses. Important parameters which undergo this phenomenon are relative peaking factors, temperature, and to a lesser extent burnup though the assemblies will always have the greatest amount of burnup towards the bottom and very low burnup assemblies towards the top of the core. At all points during burnup, the core is viable with a k-
effective that is within 52 pcm of critical. A checkerboard control rod pattern was developed manually for this SMR core because there was no functional way to develop a control rod pattern algorithmically. The updated k-effective profile versus burnup is provided below in Figure 5-80.

![Figure 5-80. Updated k-effective behavior for SMR core.](image)

Ultimately, the conclusions from the SMR analyses effectively confirmed the same trends as those observed in the standard LWR analyses, but depended greatly on the many assumptions used to define the SMR model.

5.7 Task 7 Integration and Conclusions

5.7.a Stated Objective of Task 7

With several distinctly different tasks being undertaken by different students, and across a number of years and topic areas, it is important to draw together the work in an integrated manner to support the ATF development programs. The final activity will focus on identifying lessons learnt, highlighting the tools and methodologies developed, and identifying key gaps/needs in terms of material properties, changes in phenomena related to ATFs and high demand fuel pin power histories, and potential experimental programs required.

5.7.b Report on Task 7

Due to some issues with technical personnel departing the project midway through it, this project requested a no cost extension of the original end date. Therefore, the completion of the project shifted into the first quarter of FY18.

The key results for BWRs, PWRs, and SMRs that emerged from this research have been documented in peer-reviewed publications which included 6 journal articles and 9 professional conference articles that were presented, primarily by students. These are listed in Section 8 and summarize the body of work.
6. References


7. Students and Personnel

The following students have supported this project:

- Troy Eckleberry, US Citizen, completed MS degree in Nuclear Engineering in 2016 and continued in this project through August 2017. He recently left the university to pursue employment due to personal/family reasons, now works as a reactor operator in PA.
- Ryan Sweet, US Citizen, seeking PhD in Nuclear Engineering expected graduation in 2018. Focusing on development of BISON-CASL models for Zirc-4 and other ATFs.
- Daniel P. Schappel, US Citizen, seeking PhD in Nuclear Engineering, graduated in early fall 2017. Focusing on development of BISON-CASL models for ATFs, particularly FCM. Currently working as a postdoctoral researcher for Drs. Wirth and Terrani.
- Parker Olson, US Citizen, entered the UT MS program in the fall of 2016 and joined this project initially under a US NRC fellowship, but subsequently supported by this project. Supporting SMR neutronics developments. Completed degree on December 2017, then joined the US Nuclear NAVY.
- Gavin Ridley, US Citizen, undergraduate seeking BS in Nuclear Engineering, graduated May 2018. Supported as a part-time research assistant.
- David Dixon, US Citizen, PhD student expected to graduate by December 2018. Added to this project after Mr. Eckleberry decided to leave the university.
- Nathan George, US Citizen, PhD graduated in 2015. Began ATF related work with application to BWRs. Currently a staff member at the Defense Nuclear Facilities Safety Board in Washington, DC.

Additional post-doctoral researchers included Dr. Keith Ottinger and Dr. Ondrej Chvala, currently a research assistant professor at the University of Tennessee, Department of Nuclear Engineering.
8. Publication Legacy

The list below summarizes the peer-reviewed articles contributed that were inspired by this NEUP project.

8.1.a List of Journal Publications Inspired by NEUP Project


8.1.b List of Conference Publications Inspired by NEUP Project


