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Application and Assessment of Fully-coupled Fuel Performance in VERA

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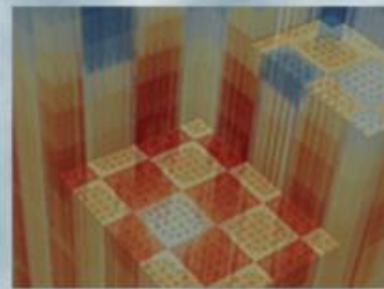

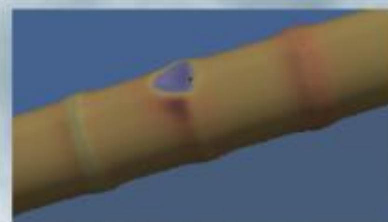

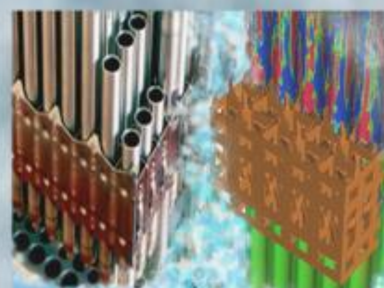

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EXECUTIVE SUMMARY

This report documents demonstrations of the fully coupled multiphysics capability developed in VERA and assesses the agreement between different approaches for integrating fuel performance calculations into VERA. It corresponds to CASL milestone L3:AMA.RX.P15.11 and fulfills the objectives and execution plan set out in that milestone.

A series of calculations were performed combining newly developed and improved coupling approaches in VERA (Tiamat Coupled, Tiamat Inline, and Standalone BISON) with several BISON models available (2D and 1.5D models using solid or tensor mechanics), yielding seven different sets of calculations. Single-pin calculations progressed from a beginning of life (BOL) linear ramp-to-power problem up to simulating multicycle operation of a fuel pin. The BOL ramp calculations showed good general agreement between the approaches, although differences were identified in burnup values calculated by Standalone BISON versus Tiamat. Single pin multicycle results found good agreement among results for some parameters but also identified small but potentially significant differences within the VERA approaches and BISON templates. Those differences will be investigated further to be understood and possibly resolved. Quarter core fully coupled calculations performed for the Watts Bar Nuclear Unit 1 (WBN1) Cycle 1 successfully demonstrated application of VERA multiphysics methods to commercial nuclear power plants for applications in core-follow depletion calculations and eventually core-level fuel performance assessments. Overall, the experience with the VERA approaches and BISON models have been positive in that Tiamat successfully completed fully coupled WBN1 Cycle 1 depletion calculations and results illustrate possible high-impact applications in the future for challenge problems such as PCI. The 1.5D BISON and Tiamat Coupled capabilities were also both delivered on relatively short schedules, and BISON 1.5D appears robust enough to use in Tiamat without causing problems in the overall calculation. Unfortunately, the high computational cost of the current capabilities led to depletion calculations for further cycles being temporarily delayed until speed improvements are implemented. User feedback has been provided to developers on possible improvements to the capabilities and usability of the codes in order to improve future performance and user experiences.

Future work focused on performance improvements will decrease runtimes and improve consistency and accuracy, with the end goal being to deploy this capability for applications at fuel vendors and nuclear utilities. Fully coupled quarter-core depletion calculations are expected to be completed for WBN1 Cycles 1 through 3 in the near future. Assessments will also be needed in the future to investigate the impact of fully coupled calculations compared to one-way coupled calculations for various applications of interest; these assessments would weigh added accuracy against additional computational burden to see which applications would benefit most from increased coupling fidelity.

CONTENTS

FIGURES

TABLES

ACRONYMS

AMA	Advanced Modeling Applications
CASL	Consortium for Advanced Simulation of Light Water Reactors
CTF	COBRA-TF subchannel thermal-hydraulics code
CZP	Cold Zero Power
DOE	US Department of Energy
FA	Focus Area
HFP	Hot Full Power
HZP	Hot Zero Power
INL	Idaho National Laboratory
LWR	Light Water Reactor
ORNL	Oak Ridge National Laboratory
PCI	Pellet-Cladding Interaction
PHI	Physics Integration (Focus Area)
PWR	Pressurized Water Reactor
T/H	Thermal-Hydraulics
TVA	Tennessee Valley Authority
VERA	Virtual Environment for Reactor Applications
WBN1	Watts Bar Nuclear Unit 1
WEC	Westinghouse Electric Company

1. INTRODUCTION

The mission of the Consortium for Advanced Simulation of Light Water Reactors (CASL) is enabling high-fidelity multiphysics simulations of light water reactors (LWRs) that can address significant challenges faced by commercial nuclear power plants. In order to achieve this goal, CASL is developing and deploying the Virtual Environment for Reactor Applications (VERA) [1], which includes coupled multiphysics capabilities. This report documents demonstrations of the fully coupled multiphysics capability developed in VERA and assesses the agreement between different approaches for integrating fuel performance calculations into VERA. The ultimate objective of this work is to demonstrate fully coupled multiphysics simulations for multiple cycles of operation for a pressurized water reactor (PWR), namely Watts Bar Nuclear Unit 1 (WBN1). This work is being led by the Advanced Modeling Applications (AMA) Focus Area (FA) of CASL and is being performed in collaboration with the Physics Integration (PHI) FA, which leads development of the multiphysics integration tools in CASL.

Previous CASL efforts, which described the WBN1 nuclear plant and analyzed it using coupled neutronics and thermal-hydraulics (T/H) codes in VERA, showed good agreement between simulation results and measured plant data including critical boron concentrations and power distributions [2]. Fuel temperature feedback was provided using a BISON-informed temperature lookup table that interpolated on linear heat rate and burnup of the local fuel region in those simulations [2]. Expanding WBN1 analysis to include coupled fuel performance calculations with fuel temperatures fed back to neutronics calculations should provide better accuracy and help determine the impact of fuel temperatures coming from coupled fuel calculations compared to fuel temperature tables. Fuel performance parameters focused on failure probabilities are not compared in any great detail in this work. Instead, efforts focused on demonstrating the use of newly developed capabilities and providing a preliminary assessment of possible neutronics impacts of different approaches. Demonstration and assessment are essential steps along the path to deploying VERA multiphysics tools for use by industrial organizations, including fuel vendors and nuclear power utility companies.

Section 2 of this report provides background information including descriptions of the methods and tools used in subsequent calculations as well as documentation of the selection of a reference plant for this work (WBN1). Within Section 2 is an important description of the various approaches to integrating BISON fuel performance calculations into VERA. Section 3 documents the content and outcomes of a series of discussions between developers and users focused on agreeing upon an approach for fully coupled fuel performance calculations in VERA. Subsequent sections focus on analyses and results from this work. Section 4 describes and summarizes single-pin calculations performed at the beginning of this work to ensure that the problem was simple enough to be adequately understood. In depth analysis of these initial calculations identified differences between alternate approaches and aided tool development and verification. These single-pin calculations build confidence in, and understanding of, the multiphysics tools while exposing any discrepancies that need to be addressed. These activities include providing developers with user feedback by assessing the overall capabilities and usability of each approach to using BISON within VERA. Section 5 describes the current status of quarter core WBN1 analyses. Section 6 then assesses the fuel temperatures calculated during single pin and quarter core calculations. Finally, Section 7 summarizes the results and conclusions of this work and describes likely areas of future work in performing and using fully coupled fuel performance calculations within VERA.

Additional details related to this work may be found elsewhere regarding the goals of this work and single pin results [3], past work describing and comparing these multiphysics tools in VERA [4], PHI-led development of these tools [5], and detailed quarter core analyses led by PHI this year [6].

2. BACKGROUND

2.1Methods

The VERA software environment developed by CASL contains multiple single physics codes that are then coupled together for use in different applications. Figure 1 shows numerous VERA components including single physics codes (e.g., MPACT and BISON) along with tools and libraries used for functions including numerical solvers, geometry, coupling and data transfers, and VERA Input/Output functions. Simulations in this paper used MPACT [7] as a deterministic three-dimensional (3D) neutron transport solver, ORIGEN to calculate isotopic depletion and decay, COBRA-TF (CTF) [8] for subchannel T/H calculations, and BISON [9] for fuel temperature and fuel performance simulations. Specific descriptions of those codes should be found in their source documentation, but useful summaries are also provided in recent documentation of Tiamat development and initial demonstration [6].

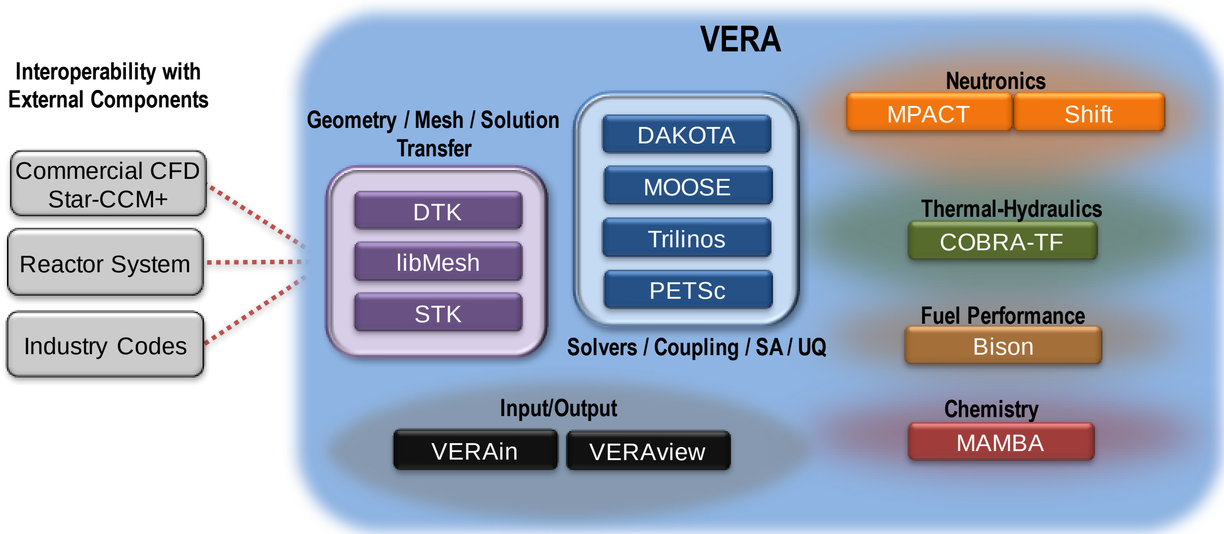

Figure 1. Overview of the VERA software environment, including components grouped by function.

Three approaches exist for using BISON in VERA: Standalone BISON, Tiamat Inline, and Tiamat Coupled. Standalone BISON [10] enables file-based one-way coupling, running BISON fuel performance calculations using existing results from MPACT/CTF neutronics and T/H calculations along with a user-defined VERAIn input file [11]. Tiamat [12,13] is the driver package in VERA coupling MPACT, CTF, and BISON. Tiamat Inline provides a one-way in-memory coupling approach, passing results from coupled MPACT/CTF calculations to BISON calculations for that same statepoint in memory. Tiamat Inline avoids the file-based transfers used in Standalone BISON and allows a user to run all three codes with a single code execution, but it still provides only one-way coupling without feeding results from BISON back to MPACT/CTF. BISON calculations in Tiamat Inline lag behind MPACT/CTF calculations by one state point. Tiamat Coupled fully couples neutronics, T/H, and fuel performance calculations; this approach enforces a converged solution from all three codes at every outer iteration while passing various parameters including power history information from MPACT to BISON, clad surface temperature from CTF to BISON, and fuel temperatures from BISON to MPACT. Core-level screening for fuel performance issues such as pellet-clad interaction (PCI), already demonstrated using Standalone BISON [14], should be significantly enhanced using Tiamat Coupled. Further details about the coupling approaches should be obtained elsewhere [6].

Table 1 summarizes some known benefits and challenges of each approach using data from earlier work [4]. All three approaches support the use of simplified VERAin-based input creation and the use of VERAView for visualizing results. Figure 2 illustrates how neutronics (MPACT), thermal-hydraulics (CTF), and fuel performance (BISON) calculations occur within each of these approaches to using BISON within VERA.

Table 1. Benefits and challenges for Tiamat Coupled, Tiamat Inline, and Standalone BISON.

Approach	Benefits	Challenges
Tiamat Coupled	Highest accuracy physics modeling and results	Computational cost
		Syncing time grid, spatial mesh, and data
		Determination of which parameters to couple / converge on
		Choosing BISON restarts vs. full calculations at each step
Tiamat Inline	More efficient than stand-alone BISON calculations	No feedback during calculations
		Choosing BISON restarts vs. full calculations at each step
Standalone BISON	Lowest computation cost	No feedback during calculations
	Simplest approach	
	No coupling issues	

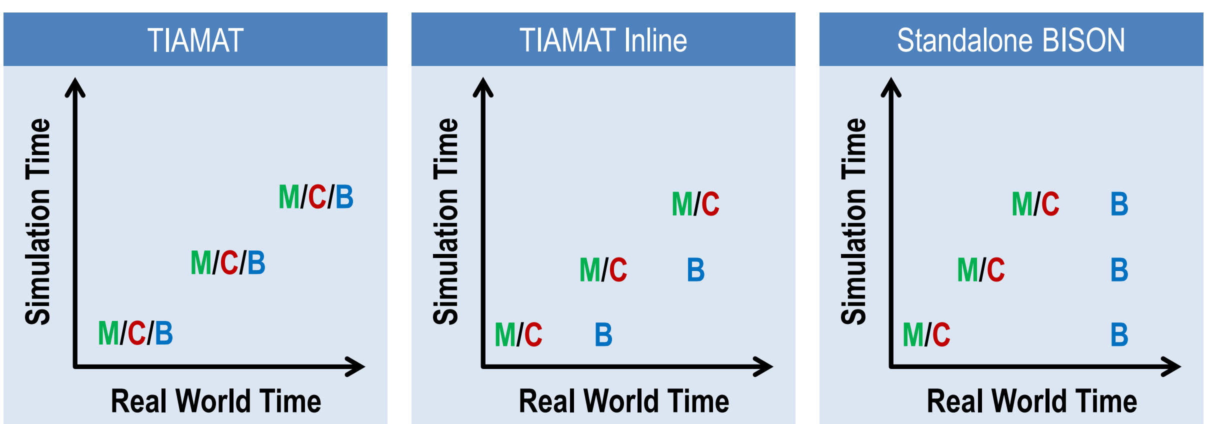

Figure 2. Conceptual illustrations of how MPACT (M), CTF (C), and BISON (B) calculations are performed within real world and simulation time for Tiamat Coupled (labeled "TIAMAT" above), Tiamat Inline, and Standalone BISON in VERA.

BISON calculations may be performed within VERA using three different BISON input templates: 2D solid mechanics (2DSM), 2D tensor mechanics (2DTM), and 1.5D tensor mechanics (1.5D). Previous CASL calculations were generally performed using 2D axisymmetric BISON models with solid mechanics (2DSM), an example of which is shown in Figure 2. However, BISON is in the process of moving away from solid mechanics to a tensor mechanics approach that can be applied within 2D models (2DTM) or a new 1.5D approach in BISON (1.5D) that simulates a PWR fuel pin by approximating it as a series of radial slices linked together axially using gap/plenum conditions between the slices. Reducing the dimensionality from 2D to 1.5D should enable faster BISON calculations and enhance convergence stability in the numerical solver, both of which benefit coupled calculations. It is important to note that fully coupled Tiamat calculations currently fail for the entire problem (e.g., a PWR quarter core model) if a single physics calculation fails for a single pin, so robust convergence in each code is critical to the overall coupling package.

Table 2 summarizes the BISON templates available for use in VERA; Standalone BISON current has all three templates available (2DSM, 2DTM, and 1.5D) while Tiamat calculations can use 2DSM or 1.5D. All three templates are provided for Standalone BISON use to assess single-variable impacts of moving from solid to tensor mechanics in 2D, as well as moving from 2D to 1.5D when using tensor mechanics. The effects and impacts observed using these single-variable control studies in Standalone BISON should hold true for Tiamat calculations as well; therefore, no 2DTM template has yet been generated for use with Tiamat because that use configuration is not expected to be a desired calculation approach in the long term. All BISON calculations in this work use a clad surface temperature calculated by CTF as a thermal boundary condition, rather than using the PWR coolant channel model in BISON; this should improve consistency between the codes as well as overall accuracy.

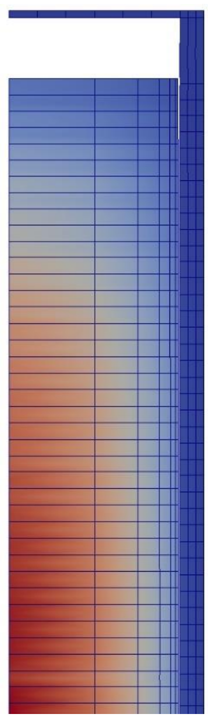

Figure 3. Temperature distribution in a representative 2D axisymmetric (r-z) BISON model.

Table 2. Summary of BISON templates that currently exist in VERA.

<table>
<tr><th rowspan="2">Integration Approach</th><th colspan="3">BISON input templates</th></tr>
<tr><th>2DSM</th><th>2DTM</th><th>1.5D</th></tr>
<tr><td>Standalone BISON</td><td>✓</td><td>✓</td><td>✓</td></tr>
<tr><td>Tiamat Inline</td><td rowspan="2">✓</td><td rowspan="2"></td><td rowspan="2">✓</td></tr>
<tr><td>Tiamat Coupled</td></tr>
</table>

2.2 Plant selection

The calculations performed in this work used WBN1 as the reference nuclear power plant to provide a basis for pin, assembly, and core calculations. The decision to use WBN1 was based on a broad set of existing WBN1 analyses in CASL (e.g., [2]), the availability of core and fuel design and operational data for multiple operating cycles, and the fact that PHI development efforts and initial testing of fully coupled fuel performance calculations will be using WBN1 as a reference plant for analysis. [6]

3. APPROACH FOR COUPLED FUEL PERFORMANCE CALCULATIONS

The addition of fuel performance calculations into VERA, coupled or standalone, introduces additional difficulties into both the computational procedure and the user specifying the desired input and obtaining the desired output. Both developers and users are accustomed to making certain approximations for simulations involving just neutronics or neutronics with thermal-hydraulics, such as step changes in reactor power or temperatures. Adding fuel performance into the workflow adds additional difficulties including not being able to do step changes in power or temperature due to the unstable impact that would have on fuel performance calculations and having to use much smaller time steps for fuel performance calculations than are used for neutronics. In addition, the general approach to analysis may need to change in some instances, such as modeling an operating cycle of a reactor (e.g., Cycle 5 of a given reactor) without explicitly modeling previous operating cycles that contained relevant fuel (e.g., modeling Cycles 3 and 4 to simulate the first and second cycles of operation for twice-burnt assemblies reinserted in Cycle 5 for a third cycle of operation). These differences in time steps, power or temperatures changes via ramps and/or step changes, general modeling approximations or assumptions, and other parameter differences need to be accounted for somehow. In an effort to accomplish this goal, users and developers worked together to try to come to an agreement on specifying user requirements and preferences and determining and documenting a new proposed methodology for running fully-coupled fuel performance in VERA, including the preferred approach to modeling power ramps and outages in a consistent and physically-accurate manner across all computer codes.

Determining consistent time stepping in MPACT, CTF, and BISON would be beneficial for coupled fuel performance calculations. This requires some agreement from PHI developers and AMA expert users. Determining preferred approaches to time stepping should specify what users are required to provide in input files as well as what the codes should be able to do and how they will function. This should, at the very least, handle all power and temperature transitions of interest. Furthermore, it should allow consistency between the different approaches for VERA-CS+BISON; Standalone, Inline, and Fully Coupled should all yield consistent in-sync results and be able to take the same statepoints.

Transition times of interest include (1) cold zero power (CZP) to hot zero power (HZP) ramp at cycle start, (2) HZP to hot full power (HFP) ramp at cycle start, (3) HFP to HZP ramp at cycle end, (4) HZP to CZP ramp at cycle end, (5) refueling outages at CZP conditions, and (6) possible unplanned outages during a cycle (e.g. HFP to HZP/CZP for an unplanned multiday mid-cycle outage).

Discussions involving a set of developers and users explored numerous options for enabling the desired consistent time stepping. These analysis approach options range from users having to explicitly specify all state points and transitions to the codes handling all transitions automatically with default transition times or ramp rates. The consensus of this discussion was that users would likely have to specify some additional information but that the codes could also test for and handle some of the items on their own as well using default values, though defaults could be overridden by explicit user input. In order to minimize the number of MPACT/CTF calculations, radiation transport and T/H calculations for time periods of zero power/flux should be avoided where possible. In addition, it would be beneficial to model something that mimics the evolutions of an actual operating power plant as closely as possible while minimizing the required amount of input and computational runtimes.

The envisioned approach for having consistency in time stepping for VERA-CS+BISON first separates VERA calculations into two main types: depletion calculations and shuffle calculations. Shuffle calculations are envisioned as being the best route to handle all zero power and zero flux time periods, and are likely the best way of handling cold condition calculations for BISON as well. Thus, shuffles would be used to handle all outages, both mid-cycle and between cycles.

Depletion calculations using VERA-CS+BISON can be broken down into 1) calculations that are restarting from an existing statepoint in existing files, or 2) new depletion calculations that are not restarting from anything. Both restart and new depletion calculations have an ending condition specified by the last user-defined power (UDP), which is assumed to be greater than 0% power, but the starting conditions differ substantially between restart and new depletion calculations. Restart calculations use the last UDP in the specified file/statepoint as the starting point for the calculation. And initial all parameters based on information in the restart files. If a user wants to run a restart calculation and change power levels to a new UDP, the user must start from the previous (existing) statepoint/timestep conditions (power, temperature, pressure, etc.) and then ramp to the desired new conditions over a user-specified amount of time. The user cannot specify an instantaneous step change (e.g. changing from 100% power to 110% power without any time elapsing). A new depletion calculation (no restart) could have a 1first STATE point that is 0% power or greater than 0% power. If the first STATE is 0% power in a new depletion calculation, then MPACT/CTF and BISON both start at CZP, ramp CZP to HZP in 100 seconds, and thereafter follow the user-specified STATE points. If the first STATE point is greater than 0% power in a new depletion calculation, then MPACT/CTF start at the UDP but BISON needs to ramp from CZP to HZP using a 100 second time period and then ramp from HZP to HDP at an assumed default power ramp rate of 2% per hour. All depletion calculation approaches (Standalone, Inline, and Fully Coupled) should be modified to ensure that consistent results may be directly obtained by users (i.e. time grids should be synced up so that result profiles line up without offsets in time). Based on the above specifications, the user can start depletion calculations from 0% power or at-power and the code handles ramping to those conditions if/as needed. The user can also end the depletion calculation at any UDP, including 0% power. However, if running a restart calculation, the user cannot change the STATE from the last UDP in the specified restart file; instead, the user must ramp from that last UDP to any new desired state, and should ensure the ramp rates during that transition are reasonable.

Shuffle steps in VERA-CS+BISON will handle outage and ramp modeling as needed. It is important to note that this requires modeling zero power/flux time periods where using effective full-power days (EFPD) as a measure of duration will not work. Thus, durations may need to be specified in hours. Adding the capability to use operational dates (opdates) to specific the beginning and/or end of a period of operation (a STATE in depletion calculations, or for shuffle calculations) would be extremely beneficial. Shuffle calculations use the conditions of the last UDP (assumed to be greater than 0% power) as a starting point. Ideally, this would be followed by MPACT/CTF and BISON both modeling ramps from UDP to HZP and then HZP to CZP, or MPACT/CTF only modeling UDP to HZP and staying at HZP (zero flux) while BISON ramps from HZP to CZP but uses externally provided conditions (temperature, pressure, etc.) to fill in boundary conditions that should be provided by MPACT/CTF in fully coupled calculations. However, these ideal approaches are not deemed likely anytime soon due to the complexities and added runtime of adding CZP statepoints into MPACT/CTF calculations. The best option for now appears to be MPACT/CTF and BISON both ramping from UDP to HZP with a downpower ramp rate of 50% per hour and then MPACT/CTF and BISON both staying at HZP (zero flux) conditions. A comparison to explicit BISON calculations that include a transition from HZP to CZP and an extended outage at CZP could be useful to understand the magnitude of impacts of neglecting CZP conditions, but it is believed that just going to HZP should be sufficient for current thermomechanical fuel performance (BISON) calculations. The end point of shuffle calculations will be that MPACT/CTF and BISON both stay at HZP (zero flux). Based on the above specifications, VERA codes should automatically handle ramping from last UDP to HZP during shuffle calculations without any required user input. However, it would be desired that users could add manual ramp rates to override default values, and furthermore it would be desired that users could specify ramping to (and staying at) CZP conditions during a shuffle if desired for BISON calculations.

One key conclusion at the end of this discussion was that the typical way that neutronics calculations or coupled neutronics/TH calculations have been done in the past will likely change when coupling with BISON. Some of the shorthand conventions or tricks (e.g. instantaneous power changes) that are convenient for neutronics and T/H calculations both in CASL and in industry will fail to work as we move into coupled calculations. While some of these limitations are due to how the fuels codes work or data they require, this problem also stems from the fact that many of these convenient tricks do not match the physical realities of operating a nuclear power plant but they don't impact neutronics and T/H codes in the same way that they affect fuels or other codes.

In addition to this conclusion, several important thoughts and ideas surfaced:

- Handling zero flux state during periods of shutdown or outage (i.e. zero flux time periods) would be easier to handle if the capability to use opdate for STATE blocks were added, allows outage and depletion periods to be set by dates rather than hours/EFPD/etc.
- There is a need to handle isotopic decay during 0% power states. One potential option to do this would be to add zero flux solves at 0% power states.
- There is also a need to handle decay heat production and rate evolution during 0% power states.
- There is still a need to report out data not just at explicit statepoints in Tiamat Inline and Tiamat Coupled, unless the plan is to require users to specify all points in time/burnup that they want results at and thus force extra flux solves. The sparse output results during Tiamat calculations makes understanding results more difficult and makes comparisons especially hard to understand.
- There may still be some questions about how thermal expansion is being handled. MPACT includes its own thermal expansion handling, but BISON needs to explicitly calculate this internally and thus requires starting from CZP at beginning of simulation

4. SINGLE PIN ANALYSES

Using relatively new capabilities in both VERA (Tiamat) and BISON to perform the desired end goal of multicycle quarter core depletion analysis presents substantial challenges and risks. A series of analysis problems was therefore outlined starting with a simple desired simulation and progressing through simulations of increasing complexity. Working through this set of progression problems for coupled fuel performance calculations in VERA provided the opportunity to test code capabilities and usability, identify any deficiencies or desired improvements in the codes, and build confidence in the ability of the user to run calculations that simulate the desired problem and power history and generate useful output data. The set of problems used in this work started simple and progressively added complexity in terms of both the problem geometry and desired power history. The problem geometry in the simulations was designed to start with a single pin and progress through problems with multiple pins and assemblies before running quarter core simulations. The power history used in the simulations initially focused on a simple beginning of life (BOL) ramp to power from CZP to HFP but eventually simulated multicycle operation and depletion.

Seven different sets of calculations were performed to cover the combination of different approaches in VERA to using BISON and different BISON input templates: (1) Standalone 2DSM, (2) Standalone 2DTM, (3) Standalone 1.5D, (4) Inline 2DSM, (5) Inline 1.5D, (6) Coupled 2DSM, and (7) Coupled 1.5D. The set of three Standalone calculations enables an understanding of what happens when switching the BISON model from SM to TM as well as from 2D to 1.5D, allowing independent assessments of the important of the mechanics model and dimensionality in BISON. When possible, results from all seven calculations are shown in each plot in this section to enable direct comparisons; however, Tiamat Coupled results do not appear in some plots due to a current limitation in extracting output data from those calculations. This limitation may be addressed in future work. Standalone BISON simulations include a ramp down from HFP to HZP at the end of the simulation. However, this ramp down in power is not modeled in Tiamat Inline and Coupled simulations. This difference in assumptions may appear in some of the figures in this section but does not indicate a meaningful difference between the approaches.

4.1Linear Ramp to Power

Analyses began by modeling a simplified problem of a single fuel pin linearly ramping from hot zero power (HZP) to hot full power (HFP) over a period of 48 hours. BISON calculations included a 100 second ramp from cold zero power (CZP) conditions to HZP to capture effects of moving from as-manufactured conditions to in-reactor conditions. Thermal expansion is especially important during this ramp from CZP to HZP.

Figure 4 shows the rod total power calculated by each approach for this ramp to power problem, illustrating what the power history used and demonstrating good agreement between the various calculations. Figure 5 shows BISON-calculated fuel burnup results in units of fission per initial metal atom (FIMA), with differences of about 20% appearing between Standalone BISON and Tiamat calculations (both Inline and Coupled). However, there remains good agreement between 2DSM, 2DTM, and 1.5D BISON models within each VERA approach. The 20% difference between Standalone and Tiamat appears to be an artifact of the way the ramp is modeled between the approaches; it is being investigated by PHI developers and may be resolved in the future. Gap thickness (Figure 6) and clad and fuel temperatures (Figure 7) agree well among calculations. Fuel temperature differences are less than 5 K at maximum.

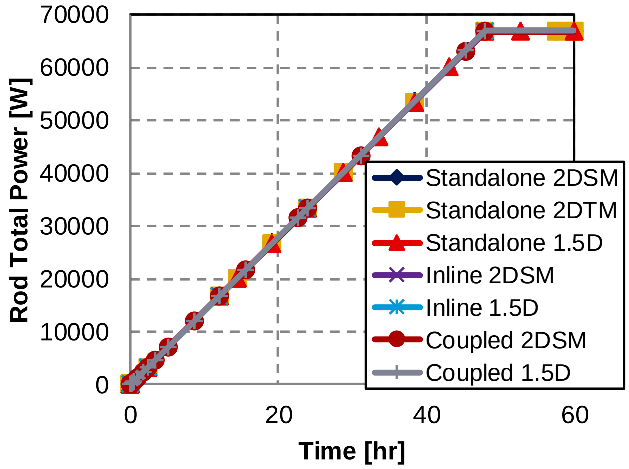

Figure 4. Power history for a linear ramp to power using different VERA coupling approaches and BISON models.

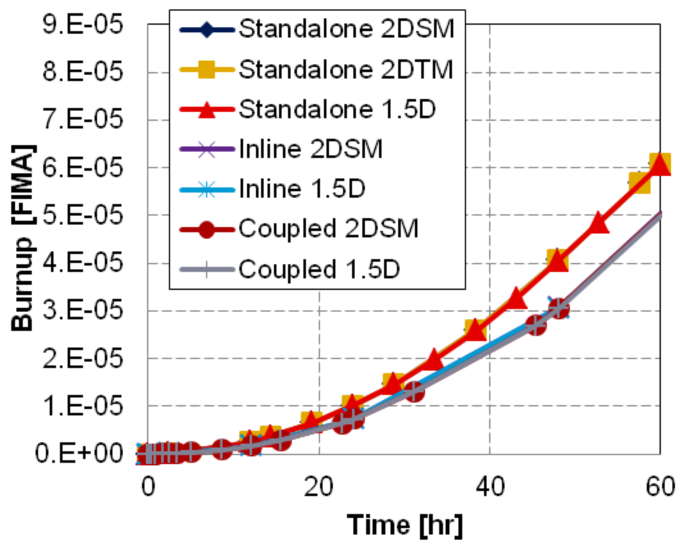

Figure 5. Fuel burnup (in units of FIMA) calculated by BISON during a linear ramp to power using different VERA coupling approaches and BISON models.

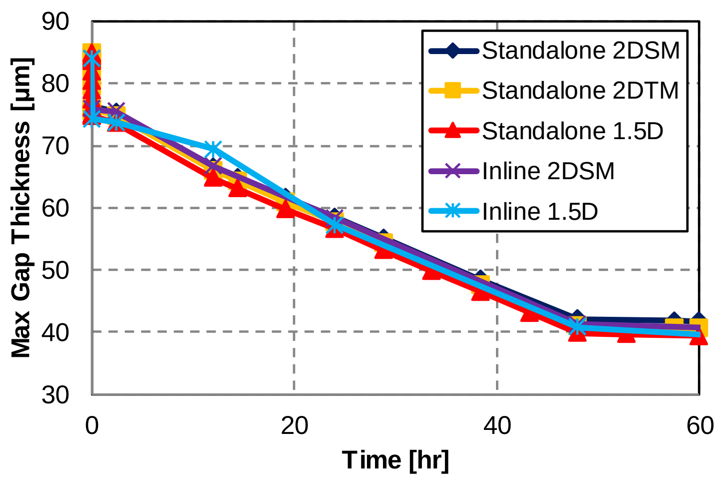

Figure 6. Maximum pellet-clad gap thickness (in units of μm) calculated by BISON during a linear ramp to power using different VERA coupling approaches and BISON models.

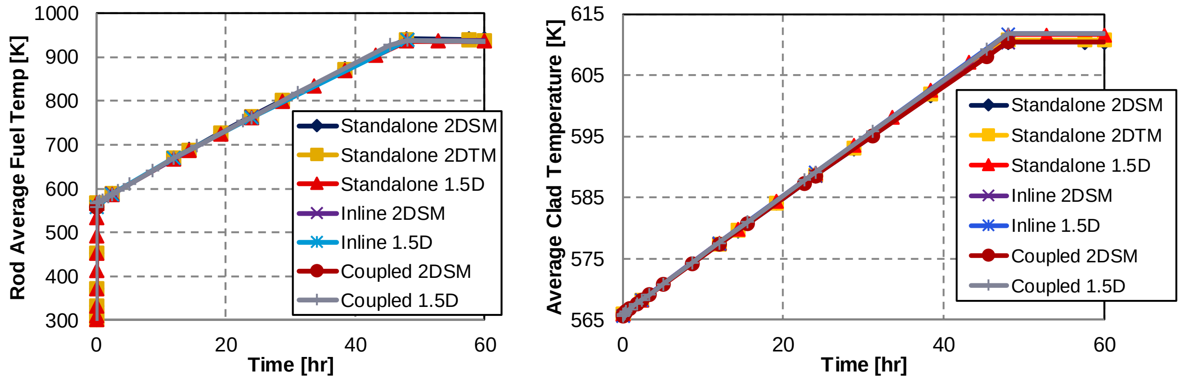

Figure 7. Rod-average fuel temperature (left) and average clad temperature (right) calculated by BISON during a linear ramp to power using different VERA coupling approaches and BISON models.

All of these parameters demonstrate reasonably good agreement between the different VERA approaches and BISON models, indicating there is a sufficient basis to proceed to more complex calculations.

Earlier differences identified during ramp to power calculations, especially differences in rod internal pressure, were corrected when an error in the BISON template being used in VERA was identified and corrected. This error was extremely unfortunate, and difficult to locate, but it illustrated the importance of starting with simple calculations like this before progressing to more complex calculations in which such an error might get lost or be even more difficult to identify.

4.2Single Cycle

After completing the single pin BOL ramp to power calculation and comparisons shown above, the testing and demonstration work progressed to calculations designed to simulate about a single operational cycle in a nuclear power plant. A single fuel pin was simulated as operating at the WBN1 core-average rod power for 475 effective full power days (EFPD), approximating the equivalent of a single operational cycle for a reactor using a fuel management strategy with about 2.5 effective fuel batches. During this simulated operation, the simulated linear heat rate and duration of operation should produce pellet-clad gap closure in most of the axial length of the fuel rod somewhere near the end of the simulation. Results from these calculations are omitted here, for the sake of brevity and because multicycle simulations in the following section will show largely the same trends but have even more details. The results and assessment of these single pin, single cycle simulations may be found elsewhere [3]; however, the results found there do not include subsequent code and input file updates that resolved several small sources of error. These corrections are incorporated into the multicycle analyses shown below, and the reader is therefore encouraged to focus on the trends in the multicycle results instead of these older single cycle results.

4.3Multicycle

Single pin multicycle simulations were performed using the same geometric model from the BOL ramp-to-power and single cycle simulations but operating the pin at WBN1 core-average rod power for about 1000 EFPD. This power history approximates about three cycles of operation for a reactor using the same 2.5 effective fuel batch fuel management strategy described above; in reality, some bundles would be irradiated for two cycles and others for three cycles, yielding discharge endurances of greater than and less than 1000 EFPD, but this simulated power history allows a simplified assessment of an averaged fuel pin.

Figure 8 illustrates the simulated power history by showing the BISON-calculated rod total power during the multicycle simulation, going up to 1000 EFPD. Figure 9 provides the BISON-calculated fuel burnup (in units of FIMA) during the simulation from each set of calculations. Both figures demonstrate excellent agreement between the sets of calculations. The burnup difference between Standalone BISON and Tiamat observed in Figure 5 for the BOL ramp to power simulation no longer appears visible in Figure 9; it is in fact still there, but the absolute difference no longer matters given the scale of the accumulated burnup. This confirms the burnup difference is an artifact of the modeling differences between Standalone and Tiamat during power ramps. This methodological difference is important to note and keep in mind, but likely has minimal impact on steady-state core follow depletion calculations. It could be more significant, however, for transient or load follow calculations.

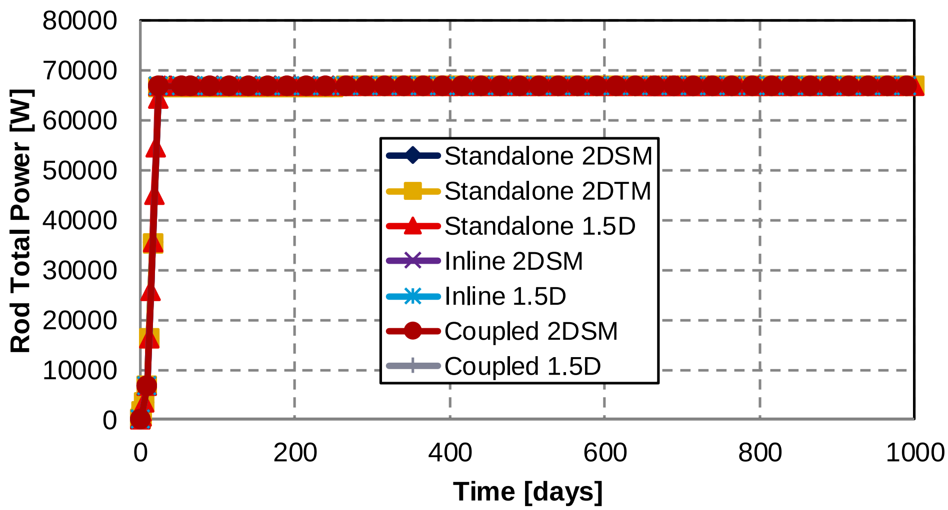

Figure 8. Power history for a single pin multicycle simulation using different VERA coupling approaches and BISON models.

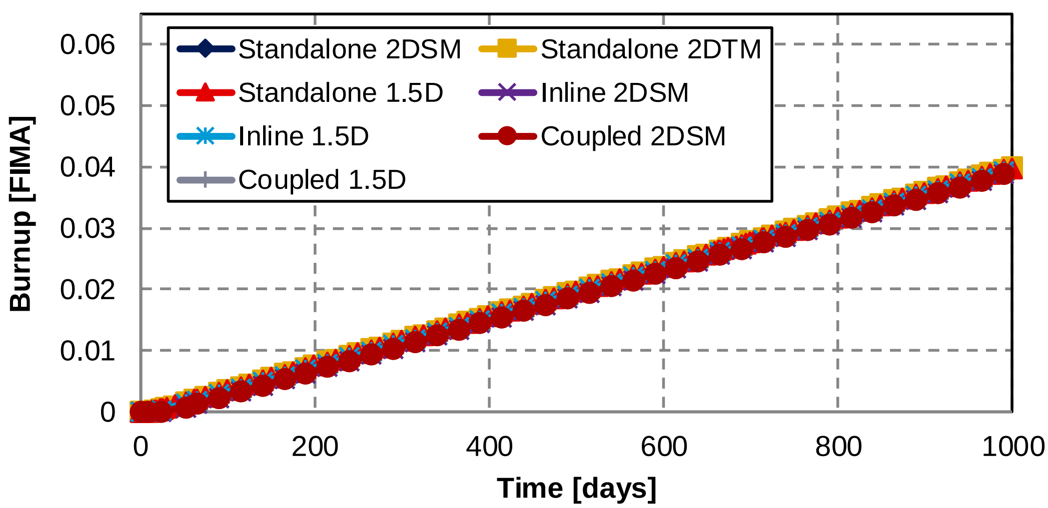

Figure 9. Fuel burnup (in units of FIMA) calculated by BISON for a single pin multicycle simulation using different VERA coupling approaches and BISON models.

The maximum pellet-clad gap thickness calculated by BISON for these multicycle simulations (Figure 10) shows a mixed behavior. Most of the curves agree relatively well, but the Standalone 2DTM results indicate a different behavior than the other calculation. No known reason exists for this deviation; at the present time, it is believed that user input error may be the cause of this difference. Future work will have to investigate and confirm the source of the difference and fix whatever input or model features are responsible for it. Table 3 summarized the estimated time to gap closure for each set of calculations, illustrating that there are small but noticeable differences between Standalone and Tiamat Inline. Note that Tiamat Coupled results are not shown in Figure 10 or Table 3 due to a current limitation in extracting gap thickness data from comma separated variable (CSV) output files generated by BISON during Tiamat Coupled calculations. The gap thickness is available in Exodus output files written by BISON and HDF5 output files written by VERA, but those results have not been parsed out at this time and therefore are not shown.

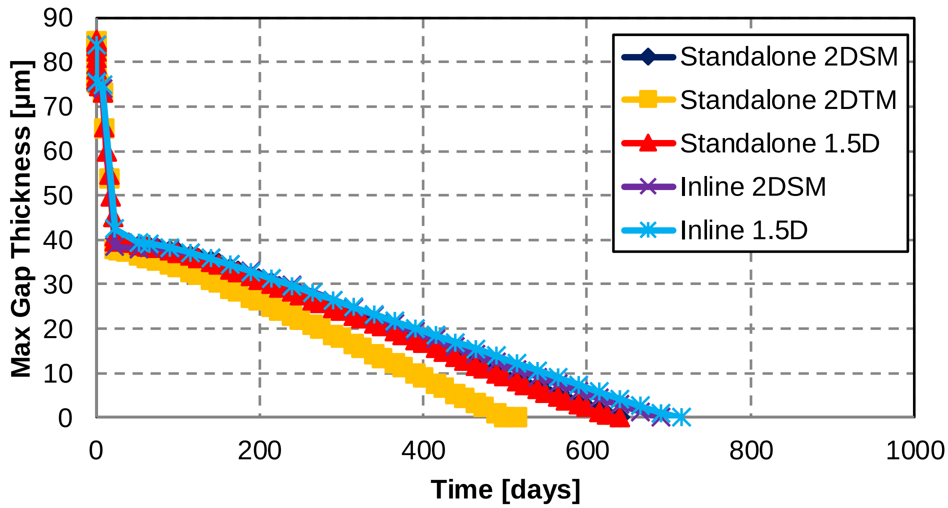

Figure 10. Maximum pellet-clad gap thickness (in units of µm) calculated by BISON for a single pin multicycle simulation using different VERA coupling approaches and BISON models.

Table 3. Estimated time to gap closure for the single pin multicycle simulations using different VERA coupling approaches and BISON models.

VERA+BISON Approach	Estimated Time to Gap Closure [EFPD]
Standalone 2DSM	639.9
Standalone 2DTM	514.9
Standalone 1.5D	639.9
Inline 2DSM	689.9
Inline 1.5D	714.9

The BISON-calculated values for rod-average fuel temperature (Figure 11) and average clad temperature (Figure 12) show very different behaviors during these multicycle simulations. The average clad temperatures (Figure 12) agree extremely well, as was seen for rod total power (Figure 8) and burnup (Figure 9). However, rod-averaged fuel temperatures (Figure 11) tend to be strongly correlated with gap thickness (Figure 10), and indeed exhibit some similar trends. There appears to be a fuel temperature difference of about 20–25K between Standalone and Tiamat approaches in VERA and a difference of about 10K between 2D and 1.5D BISON models. The Standalone 2DSM results again appear to indicate an error in the simulation inputs or models that will have to be resolved during future work.

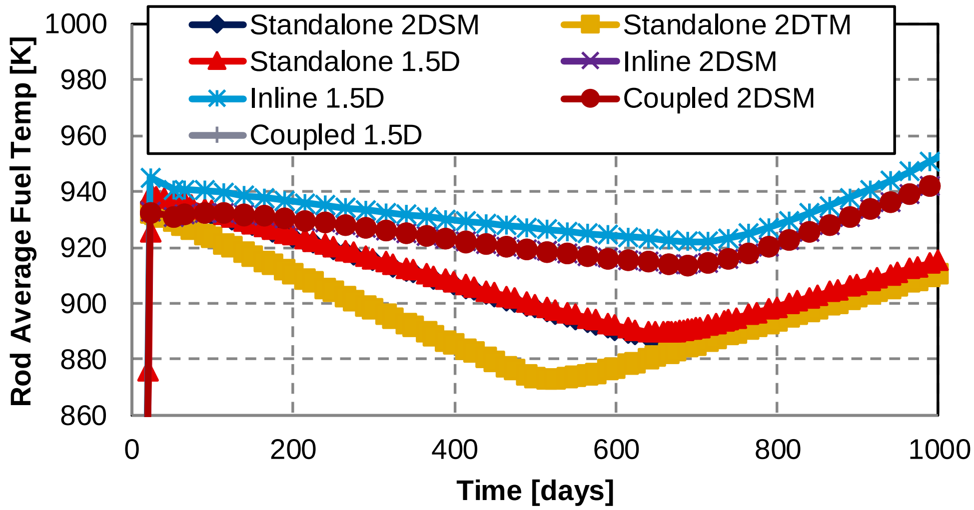

Figure 11. Rod-average fuel temperature calculated by BISON for a single pin multicycle simulation using different VERA coupling approaches and BISON models.

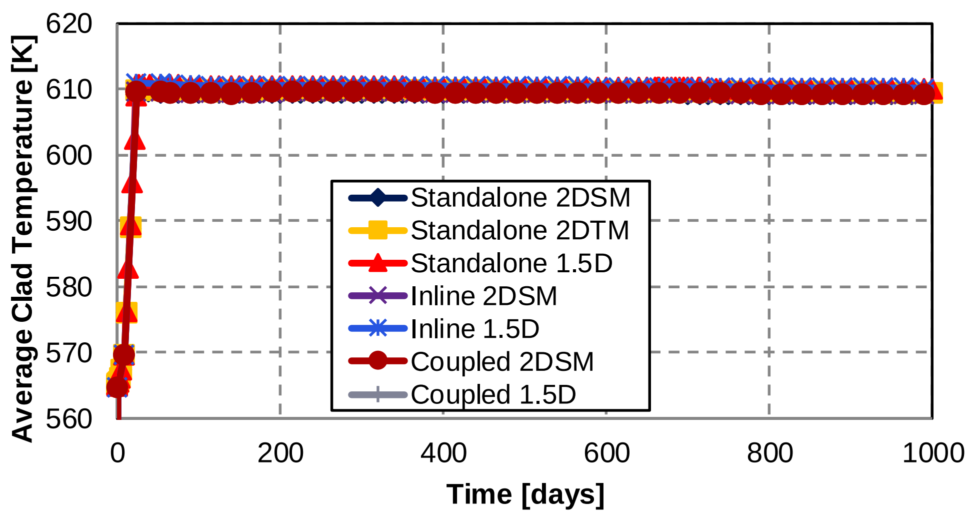

Figure 12. Average clad temperature (right) calculated by BISON for a single pin multicycle simulation using different VERA coupling approaches and BISON models.

5. QUARTER CORE ANALYSES

Initial testing and demonstration of quarter core fully coupled calculations performed by PHI demonstrated that fully coupled calculations successfully completed but required about three days of wall time on about 2000 cores to run depletion calculations for WBN1 Cycle 1 [6]. This effort was extremely successful in that it demonstrated the newly developed Tiamat capabilities successfully completed and the overall computational requirements were less than some developers and users had initially feared they might be. The full detailed results available in that PHI report provide a great deal of information, including power and temperature distributions for the fully coupled calculations.

The computational requirements for this single cycle quarter core depletion were still significantly greater than most industry clusters could likely support, however, so AMA leadership made a decision that follow-on cycle depletion analyses planned to be performed by AMA and documented in this milestone report were put on hold until Fiscal Year 2018 (FY18). This small delay allows time for speed improvements in Tiamat and underlying codes and also delays the calculations to a time of year when there is less demand on high performance computing (HPC) clusters at ORNL and INL. Some discussion of future planned work in this area may be found in Section 7.

6. ASSESSMENT OF FUEL TEMPERATURES

The single pin and quarter core fuel temperature calculation results obtained thus far indicate reasonable agreement between the different approaches from a fuel performance and materials science perspective, but the differences in fuel temperature may cause concern for neutronics applications. Figure 11 showed fuel temperature differences of about 20–25K between Standalone and Tiamat approaches in VERA and about 10K between 2D and 1.5D BISON models. These differences are well within uncertainties for materials models in any fuel performance code, and would likely yield results well within the spread of data points for fuel temperature validation experiments. However, this amount of temperature difference could certainty introduce reactivity differences in neutronics calculations in both total system reactivity and power distributions; therefore, it could have a small but noticeable impact on VERA predictions for critical boron concentrations and local flux maps, both of which are used for code verification and validation efforts to compare simulations against plant data. At this time, no specific error appears to be present in the VERA modeling approaches or BISON models (or underlying materials models) given the overall agreement between calculations and experimental data. Instead, this likely illustrates somewhat of a dilemma that will have to be thought through and addressed as fully coupled calculation proceed forward in CASL and other modeling and simulation efforts: the range covering predicted fuel temperatures using reasonable models and approximations will be well within acceptable levels for fuel performance calculations but may have noticeable impacts on certain neutronics calculations.

In general, moving away from using fuel temperature lookup tables to fully coupled calculations providing real-time fuel temperature predictions with the best physics and input data available should improve accuracy for both neutronics and fuels calculations. Furthermore, it would avoid potential problems where a specific condition doesn't have pretabulated fuel temperatures for certain combinations of linear heat rate, burnup, and fuel type. Simply put, having better physics should yield better answers, but short-term results may suffer when compared to tuned empirical models as physics models are improved.

7. CONCLUSIONS AND FUTURE WORK

A series of calculations were performed combining newly developed and improved coupling approaches in VERA (Tiamat Coupled, Tiamat Inline, and Standalone BISON) with several BISON models available (2D and 1.5D models using solid or tensor mechanics), yielding seven different sets of calculations. The results in this report demonstrate the use of fully coupled multiphysics methods in the VERA software package developed by CASL to simulate the WBN1 core and smaller problems of direct relevance. Single-pin calculations for a linear ramp-to-power problem showed good general agreement between the approaches, although differences were identified in burnup values calculated by Standalone BISON versus Tiamat. Single-pin calculations single cycle and multicycle operational periods, about 475 EFPD and 1000 EFPD at nominal core average power for WBN1, found good agreement among results for some parameters but also identified some small but potentially significant differences between the VERA approaches and BISON templates. Those differences will be investigated further to be understood and possibly resolved. Quarter core fully coupled calculations performed for WBN1 Cycle 1 successfully demonstrated application of VERA multiphysics methods to commercial nuclear power plants for applications in core-follow depletion calculations and eventually core-level fuel performance assessments. Overall, it is extremely positive that Tiamat successfully completed the WBN1 Cycle 1 depletion calculations, and results illustrate possible high-impact applications in the future for challenge problems such as PCI. Another positive outcome was that 1.5D BISON was delivered on a very short schedule, as was the Tiamat Coupled depletion capability, and BISON 1.5D appears robust enough to use in Tiamat without causing problems in the overall calculation. The codes appear reasonably good in their current state, but feedback has been provided to developers on both the capabilities and usability of the codes in order to improve future performance and user experiences. Unfortunately, the high computational cost of the current capabilities led to depletion calculations for further cycles being temporarily delayed until speed improvements are implemented.

Future work will continue to identify improvements to methods and modeling assumptions that will decrease runtimes and improve consistency and accuracy, with the end goal being to deploy this capability for applications at fuel vendors and nuclear utilities. Developers will take feedback provided from this use and make improvements to several underlying codes. Smaller-scale (single-pin and assembly) calculations will continue because of the computational savings and the increased understanding they offer. Fully coupled quarter-core depletion calculations are also expected to be completed for WBN1 Cycles 1 through 3 in the near future. Assessments will also be needed in the future to investigate the impact of fully coupled calculations compared to one-way coupled calculations for various applications of interest (e.g., standard core follow calculations or PCI screening); these assessments would weigh any added accuracy against additional computational burden to see which applications would likely benefit most from increased fidelity in coupling calculations.

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