ORNL/TM-2022/2581

VERAOneWay Coupling for Transients

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August 18, 2022

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Nuclear Energy and Fuel Cycle Division

VERAONEWAY COUPLING FOR TRANSIENTS

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Date Published: August 18, 2022

Prepared by
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, TN 37831-6283
managed by
UT-Battelle, LLC
for the
US DEPARTMENT OF ENERGY
under contract DE-AC05-00OR22725

CONTENTS

LIST OF FIGURES

ABBREVIATIONS

BOC	beginning of cycle
BWR	boiling water reactor
CTF	COBRA-TF
CZP	cold zero power
EOC	end of cycle
FFRD	fuel fragmentation, relocation, and dispersal
GAIN	Gateway for Innovated Acceleration in Nuclear
HDF5	Hierarchical Data Format 5
HFP	hot full power
HZP	hot zero power
MOOSE	Multiphysics Object-Oriented Simulation Environment
NEAMS	Nuclear Energy Advanced Modeling and Simulation
NRC	Nuclear Regulatory Commission
PLR	partial-length rod
PWR	pressurized water reactor
TH	thermal hydraulics
VERA	Virtual Environment for Reactor Applications
VOW	VERAOneWay

ABSTRACT

The VERAOneWay (VOW) package provides one-way coupling between two Nuclear Energy Advanced Modeling and Simulation (NEAMS) codes: the Virtual Environment for Reactor Applications (VERA) and BISON. This package was initially designed and tested on multicycle pressurized water reactor (PWR) problems. Recent work has improved VOW and extended its capability to other problems. VOW was enhanced to simulate fuel performance for reactor transients. Additional fuel types and geometries were added to cover boiling water reactor (BWR) fuels. The BISON version and templates were updated to the most recent version and best practices. The code was refactored to make it easier to add features and to extend VOW to other codes.

1. MOTIVATION FOR VERAONEWAY COUPLING

The Virtual Environment for Reactor Applications (VERA) [2] is a powerful tool for nuclear reactor modeling. Its primary components are MPACT [3, 4], which solves the neutron transport, and COBRA-TF (CTF) [5], which provides thermal hydraulics (TH) feedback. One focus of the NEAMS program is to provide multiphysics coupling and fuel performance in extreme environments; specifically, identifying risk of fuel fragmentation, relocation, and dispersal (FFRD) is of great itnerest to NEAMS, which requires highly accurate coupled calculations to predict. BISON [6, 7] is the NEAMS fuel performance code built on the Multiphysics Object-Oriented Simulation Environment (MOOSE) framework [8]. Coupling VERA to BISON will allow for the creation of very accurate BISON simulations using the power history and TH boundary conditions from VERA. The VOW package was designed to provide this type of coupling using a one-way file-based system. VERA can also simulate reactor transients. Recently, VOW has been updated to take advantage of the VERA transient capability to evaluate fuel performance for reactor accidents with BISON. VOW was initially created to couple VERA to BISON, but it has also been extended to couple VERA to FAST, a fuel performance code used by the Nuclear Regulatory Commission (NRC).

2. CODE OVERVIEW

As its name suggests, VOW is a one-way coupling system from VERA to other codes. This system consists of a preprocessor that takes the fuel materials, geometry, power history, and boundary conditions from the VERA Hierarchical Data Format 5 (HDF5) output files and creates input files for the code it is coupling to (BISON for example). Once the fuel performance code has been executed, a post processor is used to pull the data from the output files and write it to the VERA HDF5 files in a format that can be visualized along with the rest of the VERA data. An overview of the VOW coupling process is shown in Fig. 1.

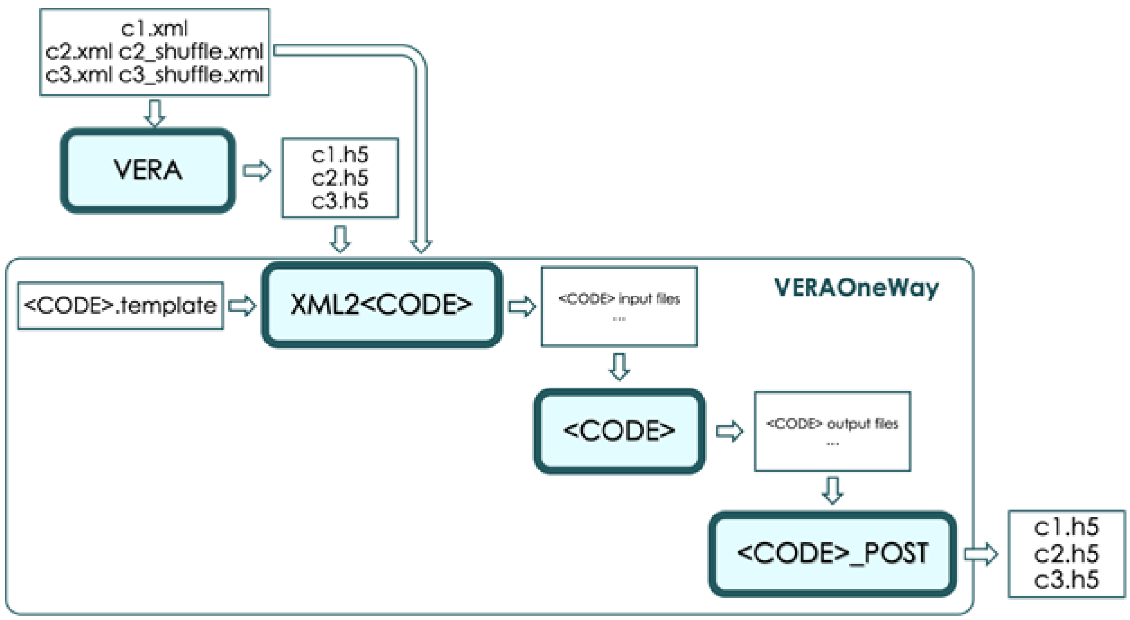


Figure 1. Flow chart of VOW coupling process.

To perform a one-way coupling with VERA, the first step is to run the VERA case to get the output data files. This is technically part of VERA, but it is important to get all the correct input and output files in order for VOW to work properly. The two main parts to the VERA run are *depletion* and *shuffling*. These are often performed together for VERA, but for the sake of VOW, they are kept separate. Figure 2 demonstrates the workflow for a three-cycle case.

Depletion is the primary run that creates the power data that are written to a HDF5 file. The depletion case is run as a standard VERA problem. If multiple cycles are run, then the restart files are used to set up the initial configuration of each cycle after the first. For multicycle cases, a shuffle process is required between all cycles. This shuffle run simply reads in the end of cycle (EOC) data from the previous cycle restart, uses a shuffle map to rearrange the data, and writes the data as beginning of cycle (BOC) conditions in the restart file for the next cycle.

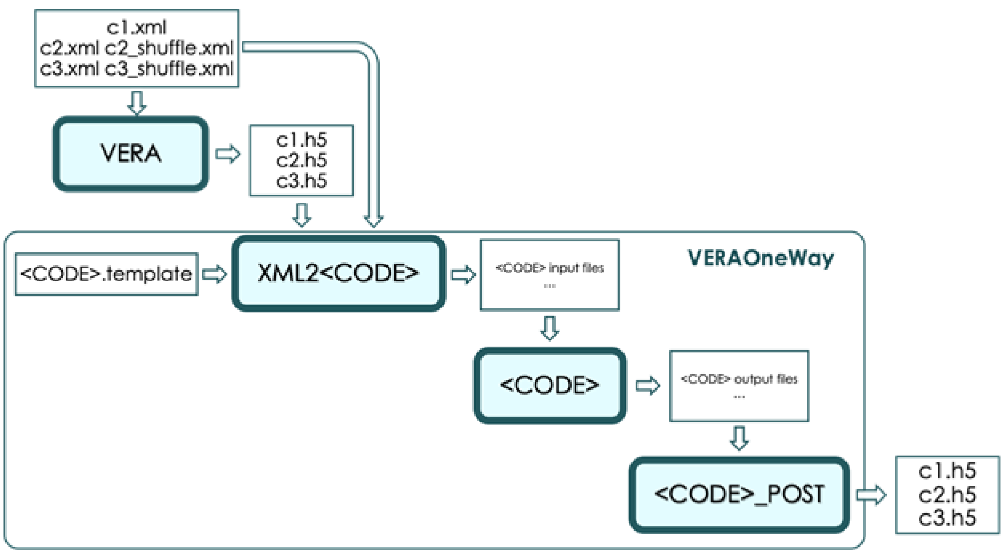


Figure 2. Sequence for running VERA problems.

3. VERAONEWAY ENHANCEMENTS

3.1 TRANSIENT

A driving factor for development of coupling VERA to BISON is to be able to evaluate fuel performance for reactor transients. VOW was initially set up for cycle depletion calculations, so this work required VOW to be modified to read data from VERA transients. VERA writes a state output to the HDF5 file for every transient time step. VOW reads these states as it would a typical depletion state, but it uses the *transient_time* to define the length of the timestep instead of *depletion_efpd* or *depletion_hours* used in a typical depletion state. VERA transient timesteps are usually on the order of milliseconds, whereas depletion steps are usually on the order days. Therefore, the logic in VOW was designed to preserve precision of timesteps and to accurately keep track of depletion and transient timesteps alike. Because BISON intrinsically treats any timestep length in the same manner, there were no modifications needed for BISON to run transient cases. However, there may be some opportunity in the future to optimize the BISON templates to achieve optimum performance for both transient and depletion problems.

Checkpoint capability was added for VERA transients to allow VERA to stop transient simulation at a given time and then to start it up again at that time in a separate VERA simulation. VOW was updated to read the transient timestep data from the two separate resulting files and then reconstruct data for the entire transient. The resulting BISON case would be nearly identical compared to a case in which the entire VERA transient was simulated in a single case; the differences are trivial and likely due to differences in the order of operations or path to solution for the iterative solve.

Analysis of fuel performance during transients late in a fuel cycle can provide very useful information. To model this with VOW, an option was developed to allow for combinations of depletion and transient cases. VERA transient cases always start with a steady-state state-point before the transient timesteps begin. VERA also has a restart capability in which a restart file is dumped on a given state and can then be read back into another VERA case to solve the same state data. By creating a restart file on the last state of a VERA depletion and reading that into the first state of a VERA transient, a transient can be simulated at the end of a depletion cycle. VOW can then be used to create BISON fuel performance input for this case. VOW detects the use of the restart files and avoids writing duplicate data for the restarted state point.

For the depletion problems that VOW was initially created to handle, it imposed default ramp times at BOC and EOC: a 3-hour transition between cold zero power (CZP) and hot zero power (HZP), and a 24-hour transition between HZP and hot full power (HFP). Now that VOW is being used to simulate other types of problems, including transients, the user can specify the ramp times. An optional input was created to specify the ramp times between these states at the beginning and end of each cycle, or it can even skip them. If they are not specified, then default ramp times are used.

3.1.1 TRANSIENT REGRESSION TEST

A single pin regression test was added to the VOW repository to cover testing of the new transient capability. The BISON block for this test is shown below.

```
[BISON]
  solve_type standalone
  bc_type bulk_cool
  fuel_pin_input_file_template = ../bison_2D.template
  mesh_clad_bot_gap_height = 1.52e-3
  power_file = steady.h5 checkpoint.h5 bison.h5
```

```
cycle_xml = steady.xml checkpoint.xml bison.xml
executioner_start_time = 0.0
temp_ramp_times  = 3600.0 0.0 0.0 0.0 0.0 3600.0
power_ramp_times  = 10800.0 0.0 0.0 0.0 0.0 10800.0
```

The *power_file* option defines the sequence of HDF5 files for this case. *steady.h5* is a depletion case with three 1-hour depletion steps. This is followed by a 0.1-second linear material ramp transient with 0.005-second time steps. *checkpoint.h5* is the first two steps of this transient, and *bison.h5* is the remaining state of the transient. *temp_ramp_times* defines the temperature ramp time before and after each of the files in this block. There is a 3,600-second ramp before the data from the first file is read and used. Because the second file is a restart from the first file, there are no temperature ramps before the data from the first file is read and used, so the second and third entries are zero seconds. Because the third file is a checkpoint continuation from the second file, the fourth and fifth entries are also zero seconds. The final down-temperature ramp after the last file has a duration of 3,600 seconds. The *power_ramp_times* are similar, except the power up-ramp and down-ramp at the beginning and end of the first and last files are both 10,800 seconds.

Figures 3–5 show select results from this transient regression test. In Fig. 3, from 0 to 3,600 seconds, the temperature up-ramp can be seen. There is no power in this range, so the fuel and clad both have the same temperature, starting at a cold temperature of 293 K and increasing linearly to a hot temperature of the coolant inlet temperature from VERA, which in this case is about 565 K. From 3,600 to 14,400 seconds, the power-up ramp is shown. As the power increases, the temperature gradient through the fuel and clad increases. Steady-state depletion occurs from 14,400 to 25,200 seconds, and the transient occurs from 25,200 to 25,200.1 seconds, although it is difficult to see in this figure. After the transient, the down-power ramp and down-temperature ramp can be seen. Figures 4 and 5 show that the clad stress and fuel-clad gap are affected by the temperature and power ramp, so it is useful to be able to control these ramp times.

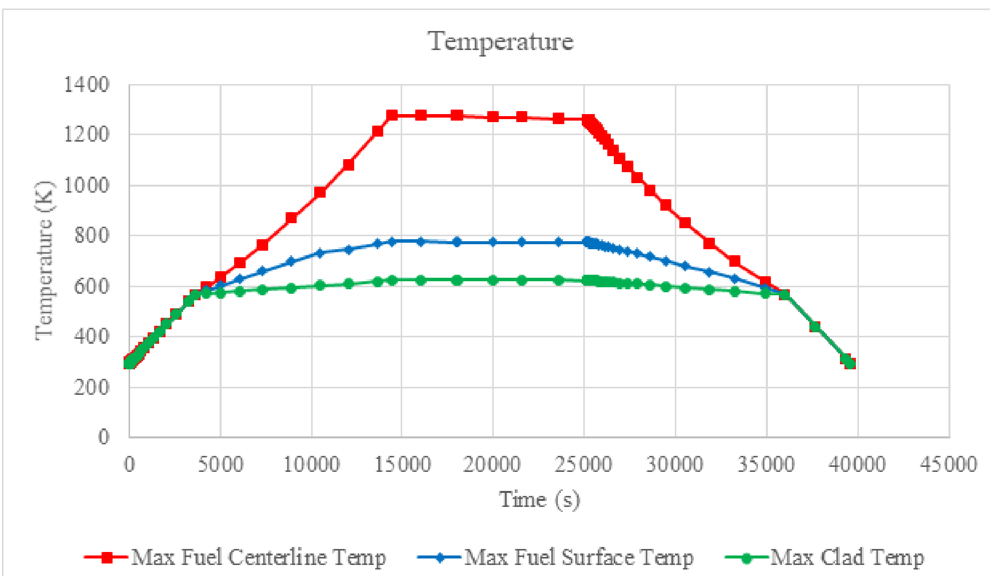


Figure 3. Transient test temperature history.

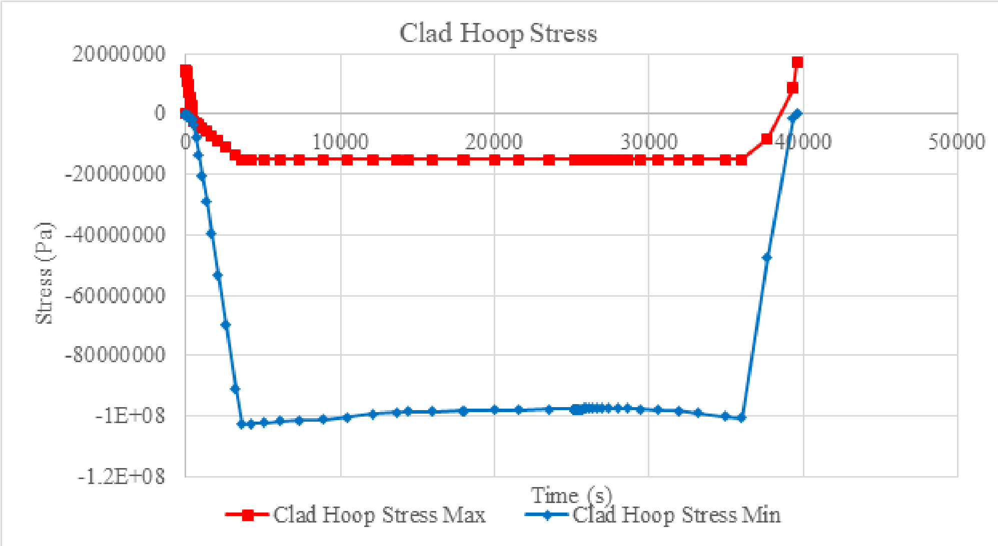


Figure 4. Transient test clad hoop stress history.

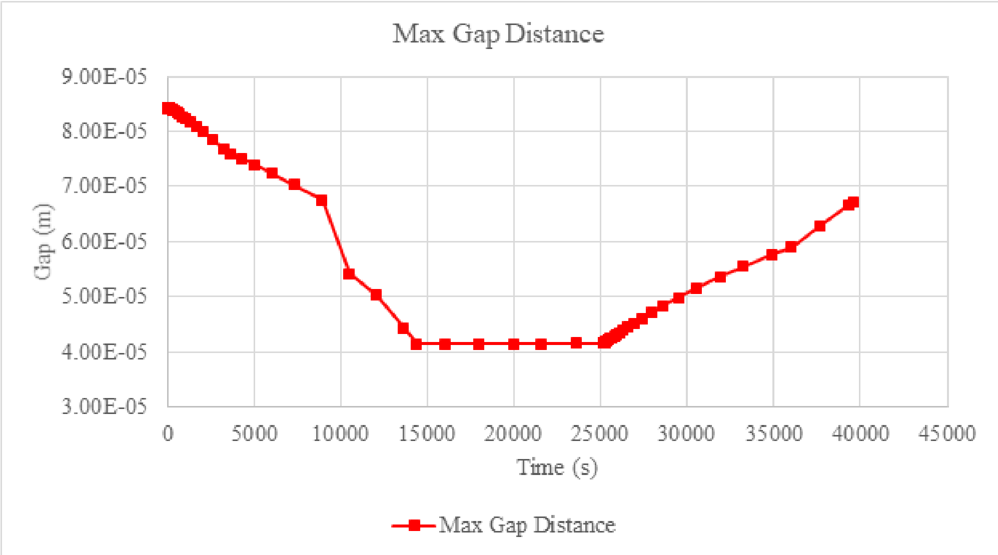


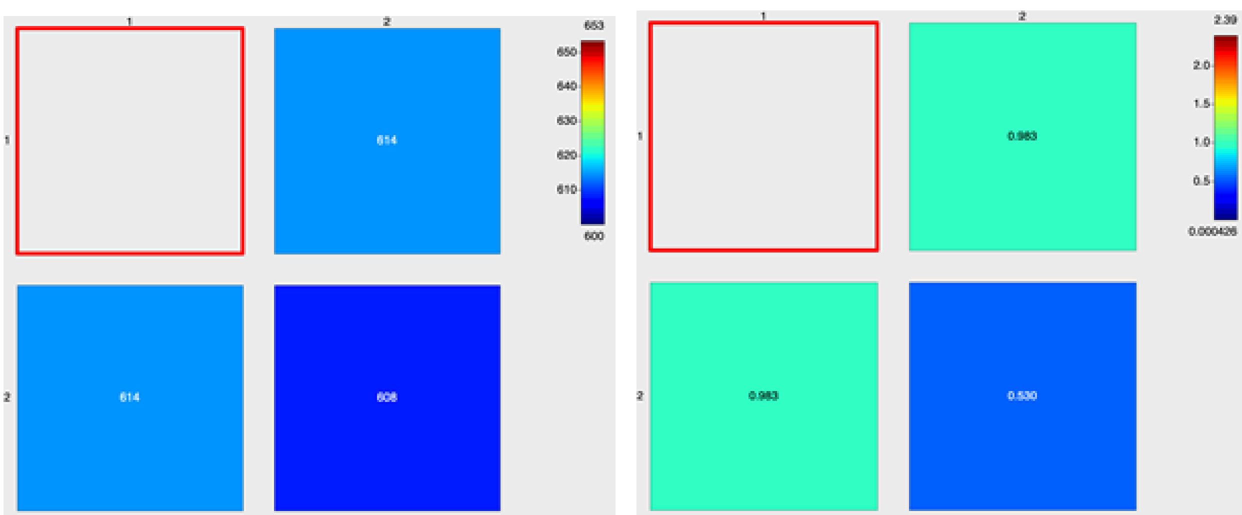
Figure 5. Transient test fuel-clad gap distance history.

3.2 BWR

To make VOW useful for as many cases as possible, BWRs were considered. BWRs often have more complex fuel and geometry than standard PWRs. Some of these fuel rod types include gadolinia-doped fuel, annular fuel, and partial-length rods (PLRs). Many of these features could be handled by VOW, but new capability was needed for the PLRs. The preprocessor was updated to check the length of each rod and the heights of the fuel pellets and to create appropriately sized BISON rods. The post-processor was modified to read the BISON Exodus files from the PLRs and to write them to the HDF5 file in the same format as the VERA data. Note that BWRs can also have fuel rods with different thickness plugs at the tops and bottoms of the fuel rods. BISON currently does not have the capability to input different top and bottom plug thicknesses, so the bottom thickness is used for both.

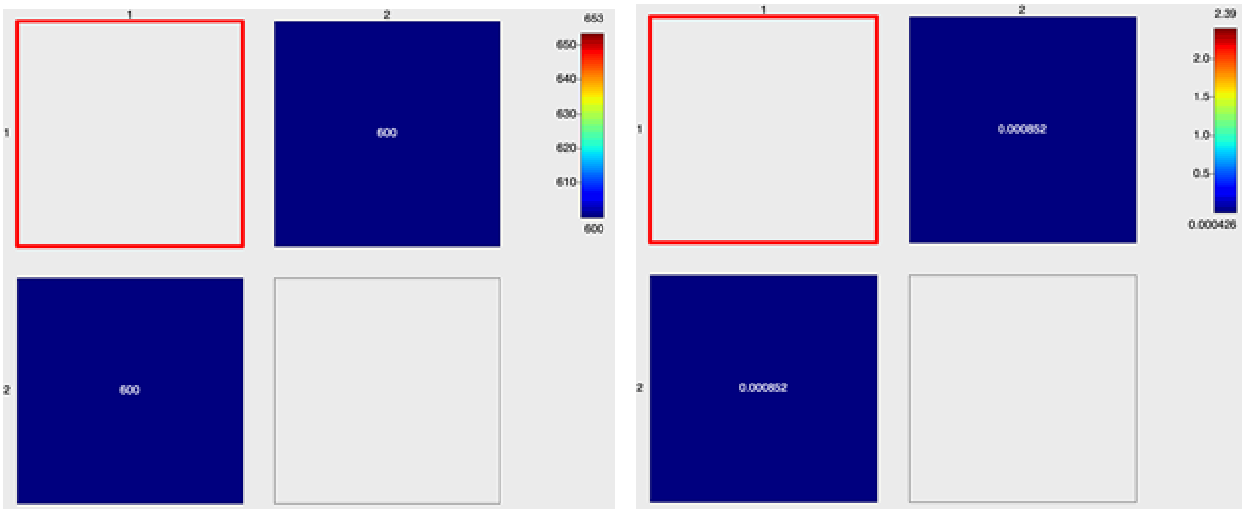
3.2.1 BWR REGRESSION TEST

A BWR regression test was added to the VOW repository to ensure that this newly added capability is working correctly. This test is a 2×2 assembly with two full-length rods and two PLRs of different lengths. Figure 6 shows a plot of the rod data in the HDF5 file at axial level 225.247 cm. These figures show that data for rod (1,1) end on the same level for the max centerline fuel temperature from BISON as the pin powers from VERA. Figure 7 shows the last level for the rod at (2,2) at 366.179 cm. These figures demonstrate that the post-processor is mapping the results from the BISON output to the VERA output with the correct format for the PLRs.



(a) Max centerline fuel temperature **(b) Pin powers**

Figure 6. BWR regression test results at axial location 225.247 cm.



(a) Max centerline fuel temperature **(b) Pin powers**

Figure 7. BWR regression test results at axial location 366.179 cm.

3.3 MODEL UPDATES

3.3.1 BISON VERSION

VOW is an extension of a package that was dependent on a version of MOOSE/BISON that had been included in an older version of VERA. This version of BISON was not updated frequently: the last update was in 2019. To use the most recent version of BISON, the VOW package required updating to resolve incompatibilities with the existing input file templates. A local version of VOW was configured to run successfully with the BISON version dated June 1, 2021 (latest git commit 81a78fa1733e23f3396f9daa9e83f8ed4dd24840). Major VOW modifications include removal of the deprecated solid mechanics objects. Other minor changes to the remaining 1.5D and 2D tensor mechanics templates were made to enhance consistency between the templates, to accommodate changes in input syntax, and to eliminate deprecation warnings. All tests, including the assessment case discussed in the previous section, were rebaselined to reflect these changes.

3.3.2 2D MODEL

The BISON code was initially based on the Solid Mechanics model, which has been deprecated in newer versions of BISON in favor of the tensor mechanics model. Early versions of VOW included templates for both 2D models. With the update of the BISON version, the solid mechanics model was no longer compatible, so that template was removed.

3.3.3 1.5D MODEL

The 1.5D model solves the 2D cylindrical fuel rod as a set of coupled 1D problems. These 1D problems are solved on given axial positions along the rod and are coupled using a generalized plane strain scalar variable. For many problems, this model is sufficient to model most of the fuel performance. The advantage of the 1.5D model is that it can be run faster that the standard 2D model. A 1.5D template was included in the early version of VOW, but the post-processor was not equipped to properly read and process the data from the 1.5D output file. The 1.5D files only have data at discrete axial levels instead of axial elements, so the post-processor was updated to correctly average data over the VERA axial mesh. The 1.5D template was also updated so that BISON would output all the same data as the 2D model. The *bison_from_vera_1.5D* regression test was updated to verify this new capability.

3.3.4 VERAONEWAY/BISON ASSESSMENT CASE

The BISON and FAST input files for each rod are created based on given template files. The template file has input blocks set up for a general rod model. The preprocessor copies the template file and modifies the model parameters for each unique rod. Several template files are provided with VOW. A VOW/BISON assessment case was developed to allow the impact of BISON updates and the VOW input file template modifications to be assessed. Using a case with an accepted solution based on either experimental data or predictions from other codes provides a convenient reference to use to objectively validate changes in VOW/BISON predictions. An existing BISON assessment was selected for this work because (1) documentation, simulation inputs, and comparison data were readily available, reducing the cost and time needed to develop the case; (2) the computational cost associated with running the assessment was low enough to allow the case to be included in the continuous VOW test suite; and (3) the assessment allowed for comparison of integral fuel rod predictions (i.e., peak fuel temperature and rod internal pressure) to capture effects on as many material properties and physics models as possible.

The selected assessment was based on rod TSQ002 from a 16×16 test assembly, which was irradiated in the 1980s to study the effects of extended burnup on light-water reactor fuel. The experiment is described in a report issued by the International Atomic Energy Agency in 2013 [1]. The report also includes results from numerous fuel performance codes that were applied to simulate the test. Additional information related to the fuel rod geometry, composition, and irradiation conditions is available in the BISON documentation [9]. The assessment was reproduced as closely as possible using the 1.5D VOW template.

Minor modifications were made to the assessment to accommodate differences between the assessment input file and the existing 1.5D template, to manage computational cost, and to facilitate running the case within the VOW testing system. VOW and VERAIO infrastructure and documentation were revised to better accommodate using CSV file inputs for power and cladding temperature. VOW and VERAIO input parameters were also defined to allow users to fine tune relative and absolute nonlinear convergence criteria. These code modifications are expected to be useful beyond the current work. Simulation results presented later in this section were analyzed to confirm that these modifications do not introduce inconsistencies between VOW/BISON predictions and the results from the other codes.

As a result of these modifications, the VOW assessment may not reproduce the results of the BISON assessment exactly, but it will provide a convenient baseline with an accepted solution that can be used as a reference to objectively evaluate the effectiveness of future BISON updates or template changes. The case was developed into a continuous test on which diffs are run to check for discrepancies between current and accepted (referred to as *gold*) solutions. Diff failures alert the user that modifications have impacted the VOW/BISON integral fuel performance predictions. Plotting capabilities were developed and included with the test to allow the user to visualize VOW/BISON predictions and to compare them to results obtained the from other codes for the original assessment. The user can inspect these plots to determine whether the results of the assessment are still consistent with those obtained from the other codes and to confirm whether the impact of the modifications is acceptable.

Peak fuel temperature results are compared in Figure 8 [1]. Temperature predictions are impacted by power and cladding temperature inputs, thermal conductivity models, the gap heat transfer model, and more. The results in Fig. 8 show that the codes predictions vary by about 200°C and about 3 MWd/kgU. The VOW/BISON predictions are well within the range defined by the other codes, indicating that the input templates and VOW/BISON setup currently deliver acceptable results.

Rod internal pressure results are compared in Figure 9 [1]. Rod internal pressure predictions are affected by coolant and initial plenum pressure inputs, fission gas release models, and tensor mechanics models such as thermal expansion, elasticity, and creep. The results in Figure 9 show that the code predictions vary by

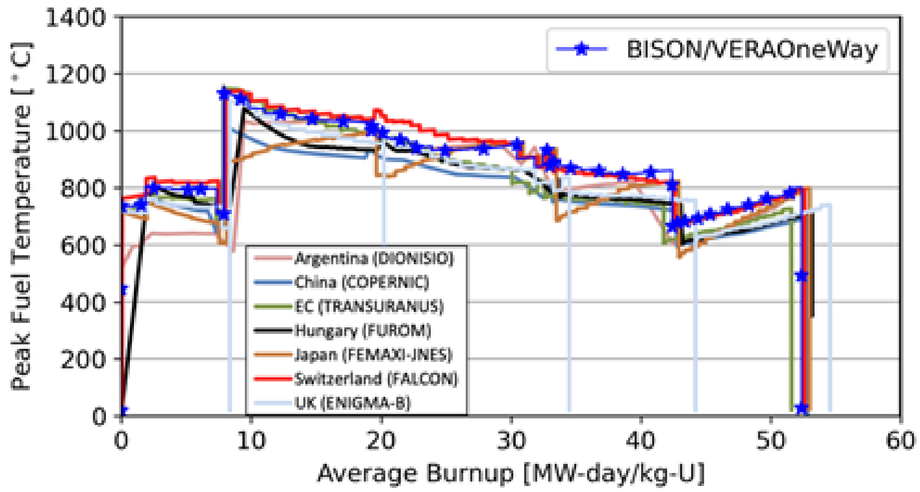


Figure 8. BISON/VERAOneWay peak fuel temperature predictions compared with results from seven other codes [1].

about 2 MPa. The VOW/BISON predictions are once again within the range defined by the other codes. This supports the conclusion that the input templates and VOW/BISON setup currently deliver acceptable results.

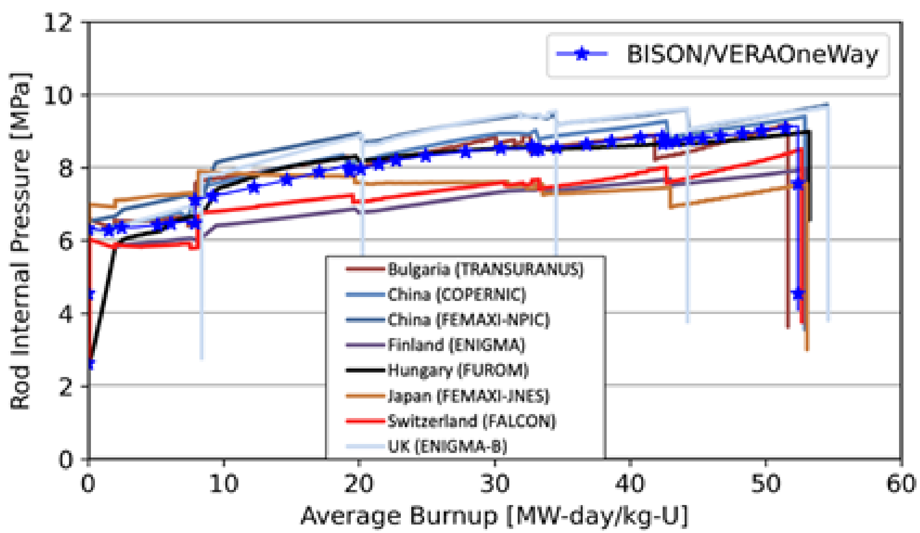


Figure 9. BISON/VERAOneWay rod internal pressure predictions compared with results from eight other codes [1].

3.4 VERAONEWAY STRUCTURE

Efforts were made to improve the structure of the VOW code to make it more user and developer friendly. A number of issues were encountered by users. These mostly consisted of user errors in which VOW did not provide warning or error messages that were useful enough to allow the user to pinpoint the error. A number of error checks were added to address these issues and provide better messages. For example, the HDF5 functions do not provide useful messages about what went wrong or even which file failed, so additional checks were added to avoid errors from HDF5. Other error checks included ensuring that the BISON block inputs were correct, as well as the *.xml* and *.h5* files.

A significant refactor was performed to improve the VOW code structure. The main goal of the refactor was to eliminate duplicates. The VERA-to-FAST capability that was based on the VERA-to-BISON capability has a very similar structure and extensive duplicate code. Additionally, the pre-processors and post-processors for each capability also required a similar setup. The majority of the duplicate code was removed from the *vera2bison* and *vera2fast* source and was condensed into a separate *vera2fuels* library. This simplified the codes structure and reduced the source code by approximately 4,000 lines. Having the majority of the shared code in one place made it easier to add new features and to conduct more complete error checking. This structure will also make it easier to extend VOW to couple to other codes in the future.

4. SYNERGISTIC ACTIVITY

During FY21–22, a project was funded by a Gateway for Innovated Acceleration in Nuclear (GAIN) voucher to model the Holtec SMR-160. As part of that project, fuel performance calculations were performed with BISON for highly burned SMR-160 fuel rods under two different transient scenarios. These BISON calculations were driven by VERA using VOW, which is significant because it constitutes one of the early applications of VOW to a real application unrelated to the NEAMS program. The full details of the project were provided by Graham [10] in a report that is not publicly available because of proprietary design information. Limited versions of the project results which were approved for public release are available in Rader [11] and Sweet [12] and are expected to be more comprehensively published in an upcoming journal article.

Overall, the use of VOW was successful, but several issues were identified during the GAIN project.

- The performance of VOW for a whole core was prohibitive. Generation of the thousands of input files could take many hours or even several days. This indicates much room for improvement in how VOW generates the input files.
- Some issues were encountered when using symmetry. The cycle depletions of the SMR-160 were performed in quarter symmetry; one of the transients was quarter symmetric, but the other was not. The nonsymmetric transient had to be simulated in full core, but some defects were identified in VOW when generating the BISON inputs from a group of files with both quarter symmetry and no symmetry. Although these defects could be worked around for the purposes of the GAIN project, they could be a more significant obstacle for other applications.
- It was found that some unrealistic values could be generated for the power or burn-up histories of certain rods when using VOW. In every case, these were rods which appeared in the early cycles but not the cycle immediately preceding the transient calculation. Because the rods were discharged before the transient, they were not of interest for the GAIN project analysis, but this could be an issue for other analyses.

It should also be noted that although this was one of the first applications of VOW to an external application, the full VOW capability was not used as illustrated in Fig. 1. VOW was used only to generate inputs; a screening process was then applied manually to select only a few rods of interest for analysis. This was accomplished primarily because of limitations on computational resources and time that disallowed running thousands of BISON calculations. Therefore, even though the full VOW workflow was not skipped because of a known issue with VOW, the capabilities to drive the BISON calculations and map the results back to the VERA HDF5 file were not exercised as part of this project.

5. CONCLUSIONS AND FUTURE WORK

The VOW package has been shown to be an effective tool for coupling VERA to fuel performance codes like BISON and FAST. Recent work has been focused on extending the capability of VERA to BISON coupling. VOW is now able to perform BISON simulations for reactor accidents based on VERA transients. PLRs were considered so that VOW could be used for BWRs. The BISON version and templates were updated to obtain better results and performance, and an assessment case was added to compare to other codes. The VOW source code was refactored to simplify the structure and make testing and maintenance easier. This refactor was also designed to make it easier to add new features and to extend VOW to couple to other codes in the future. Application of VOW for an external non-NEAMS project was successful, and it also identified some areas for improvement.

Next steps in supporting FFRD simulation and analysis will focus on improving the robustness of VERA and VOW. Several issues with VOW that need to be addressed were stated in the previous section. VERA also has several improvements that will be made. An initial capability to calculate decay heat has been implemented in VERA, but this capability has not been integrated with the transient calculations in VERA. This is crucial to modeling certain transients which are driven by decay heat rather than prompt power generation. The other major improvement needed for VERA is to reduce the computational burden of transient calculations.

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