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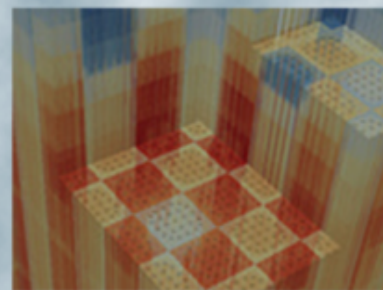

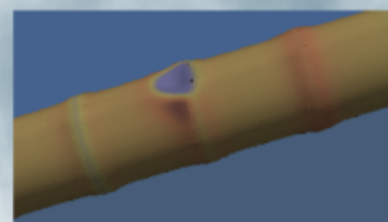

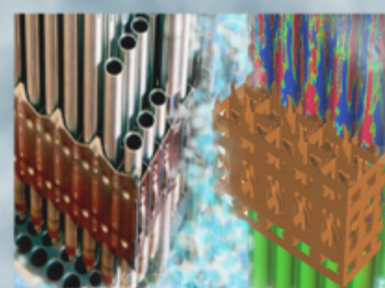

Verify and Validate 1.5D Capability L3:FMC.FUEL.P15.04

S. A. Pitts, INL
S. R. Novascone, INL
H. Chen, INL
B. W. Spencer, INL
S. Satpathy, INL
R. J. Gardner, INL
J. D. Hales, INL

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Initial 1.5D BISON Simulation Verification and Validation
CASL FY17 Letter Report

S. A. Pitts, S. R. Novascone, H. Chen, B. W. Spencer, S. Satpathy, R. J. Gardner, J. D. Hales

Fuels Modeling and Simulation
Idaho National Laboratory
P.O. Box 1625
Idaho Falls, ID 83415-3840

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Introduction

This milestone report describes the current efforts to improve the usability of the recently developed 1.5 dimensional (1.5D) capability in BISON, the initial verification of this 1.5D capability, an initial validation of the 1.5D models against existing 2D axisymmetric full length light water reactor (LWR) fuel rods, and a convergence study on the number of 1.5D axial fuel slices used in the model geometry. The 1.5 dimensional (1.5D) capability in BISON was developed to enable the simulation of LWR fuel rods in a less computationally demanding simulation formulation while retaining key physics of interest. BISON was originally developed to solve 2D axisymmetric and 3D models, and this original development focus allows BISON to examine a wider range of fuel types and geometrically complexity than can be solved with lower dimensional frameworks [1].

Coupling physics in a higher dimensional geometry is not always required to resolve the physics of interest, such as the modeling of radial heat transfer and radial displacement. BISON, built on the dimension-agnostic MOOSE framework [2], is able to solve problems in 3D, 2D, and 1D with only minor modifications to the thermomechanical material behavior definition code so that the appropriate geometrical representation can be applied in different problems of interest. The motivation for the development and validation of the BISON 1.5D capability is the CASL program's need for a simplified and computationally efficient version of BISON for use in the large multi-physics VERA simulations. These VERA simulations include hundreds of individual fuel rods.

The original development of the BISON 1.5D simulation capability is described in the CASL FY17 Letter Report from January 2017, and this report documents the continuing work identified in the previous report. The improvements to the usability of the 1.5D capability through input file simplifications, a description of the verification simulations, the results of the initial validation against the 2D assessment cases in BISON [3], and the future development needs are included within this report.

1 1.5D Model Overview

The term 1.5D is used in BISON to describe a model of a cylindrical fuel geometry that is a collection of coupled 1D simulations; the individual 1D simulations are used to represent the behavior of the fuel at specific given axial positions along the rod. The fuel rod is divided into several axial slices, and a 1D model of the physics (energy conservation, stress divergence, thermal and mechanical contact) is solved on each slice. A schematic of these 1D axial slices is shown in Figure 1.

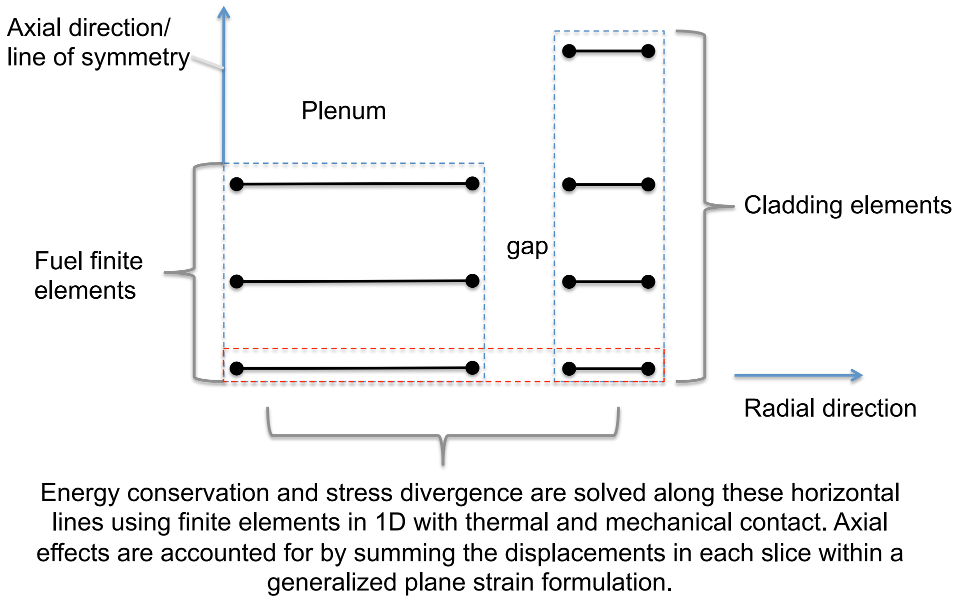


Figure 1: Schematic of a representative 1.5D problem and mesh

The individual 1D simulations are coupled through the use of a generalized plane strain scalar variable; these scalar plane strain variables enforce the mechanical effects of volume change, such as changes due to thermal expansion and swelling, in the axial direction. In the 1.5D simulations, an individual generalized plane strain scalar variable is applied to each axial slice, separately, for each fuel slice and each clad slice.

2 Usability Improvements

The use of individual scalar generalized plane strain variables is necessary to represent the axial variations within a fuel rod at each slice elevation. For a 10 slice 1.5D model, 21 total generalized plane strain variables are required, which must be correctly applied to the corresponding slices: 10 slices in the fuel and 11 slices in the clad. The main goal in the usability improvements to the 1.5D BISON capability is to mitigate the potential for error in the construction of the 1.5D input files, particularly in regards to the scalar generalized plane strain variables.

These improvements have been implemented in the form of specialized 1.5D actions, which automate the creation of the scalar generalized plane strain variables and the connection of those scalar variables to the appropriate slices. The MOOSE tensor mechanics module master action has also been extended to the 1.5D capability. The MOOSE tensor mechanics master action automates the settings for the stress divergence kernel and the strain calculator; this automation ensures the correct correspondence among these elements of the input file. Additional 1.5D specific settings have been added to the contact module to ensure that contact is allowed only across adjoining fuel-clad slices at the same elevation. Finally the output of the individual scalar variables have been combined into a single axial strain variable to increase the ease of data visualization and post processing. The combination of these three automation improvements reduce the length of a nominal 1.5D input file by nearly 25% in addition to reducing the potential for error in the use of the scalar generalized plane strain variables.

3 Initial Verification

A set of the verification problems were designed and added to the BISON code repository during the development of the 1.5D BISON capability. This set of verification problems can be divided into four subsets, ranging from material behavior verification to the post processing capabilities which must correctly handle the reduced geometry of the 1.5D BISON simulations.

The first subset of verification problems are designed to verify that the generalized plane strain variables, which act between the axial slices as shown in Figure 1, correctly represent the non zero axial strains due to axial loading and interaction between adjoining slices. The interaction among slices is often due to axial expansion from volumetric swelling and thermal expansion. We developed verification problems with both a constant generalized plane strain variable value and a variable value which changed in response to thermal expansion. The simulation results of these verification problems compare well against the analytical solutions.

The second subset of 1.5D capability verification problems is concerned with ensuring the correct calculation of material properties with the existing material classes within BISON in a 1.5D capability simulation. This verification problem subset specifically tests the cladding creep materials and the fuel volumetric swelling materials. The creep simulation result is compared against 2D axisymmetric and 3D simulation results, and the volumetric swelling 1.5D capability simulation result is compared against an analytical calculation.

The third verification problem subset focuses on establishing that the fuel rod specific boundary conditions are applied correctly to the reduced geometry problem. These verification problems include radial heat transfer between two blocks, axial pressure due to external conditions such as the coolant, and application of the axial power profile. The radial heat transfer and axial pressure problem simulation results are compared against analytical solutions while the power profile test compares the power profile calculated by the 1.5D BISON capability to the input power profile.

The final set of 1.5D capability verification problems is focused on ensuring that the post processors used to calculate average side and total internal volume values, such as average pellet-clad interior temperature and plenum pressure, correctly account for the geometrical assumptions made in the 1.5D meshes. These post processors, which compute integral type quantities, have been specialized for the 1.5D capability to perform the required integrals in a domain-aware manner to correctly account for the heights represented by each axial slice. Simulation results from the verification problems for the side average and the internal volume post processors are compared against analytical solutions.

The complete set of these verification problems is included in the BISON source code repository, which is available at `hpcgitlab.inl.gov`. In particular these verification problems are stored in the source code repository folder `bison/tests/layered_1D` and the analytical solutions are included at the top of each input file.

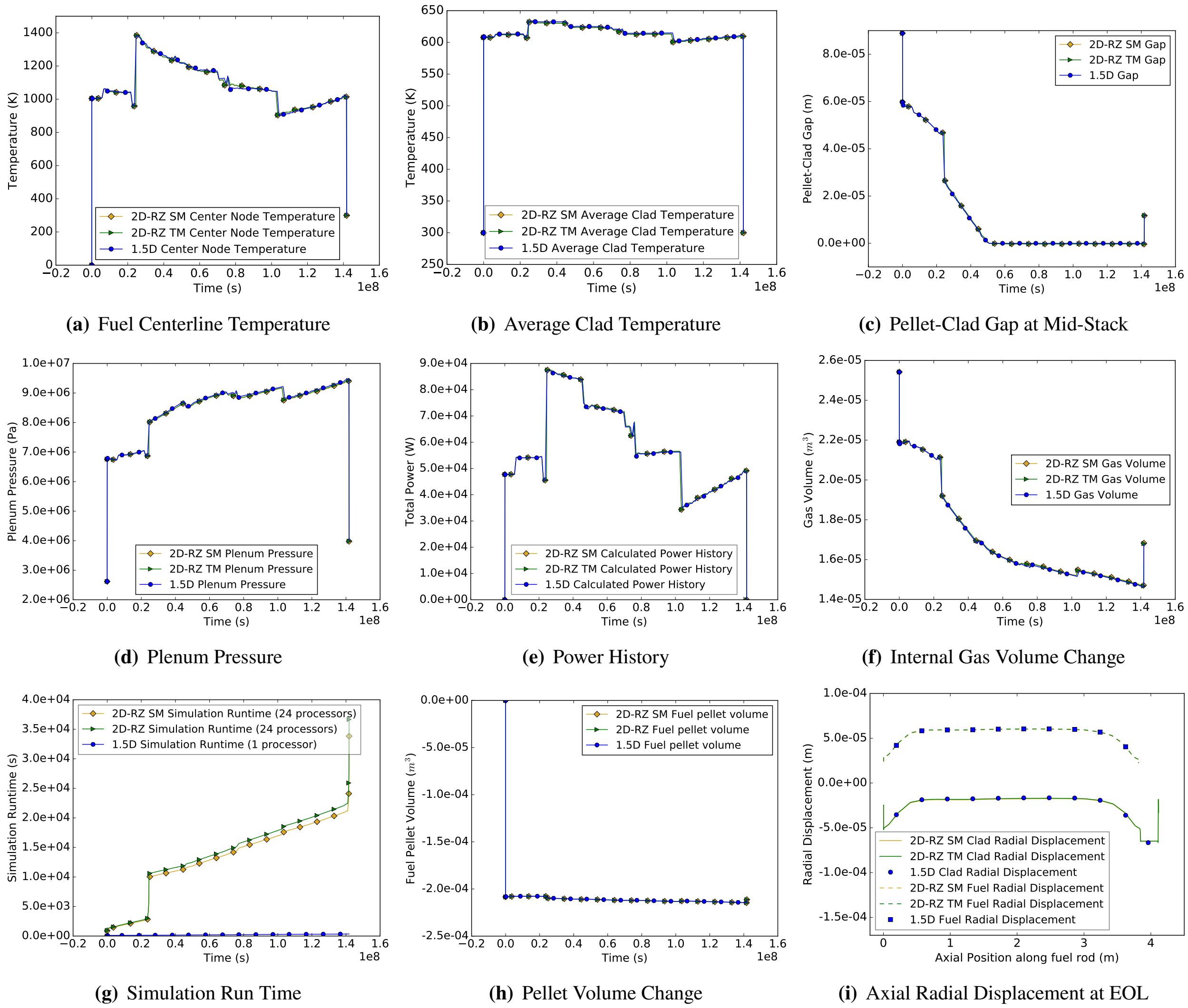
4 Initial Validation

The 1.5D BISON capability is intended for the modeling of several hundred full length fuel rods. Ensuring that the 1.5D capability gives reasonable results for a full length full rod is a key consideration in this stage of the 1.5D BISON capability development. In this initial validation effort, a few of the full length 2D axisymmetric assessment cases [3] were selected for duplication as 1.5D simulations. The engineering scale results, including fuel centerline temperature, gap, and simulation run time, were compared for the 1.5D simulation results against the original 2D axisymmetric assessment cases. The set of comparison plots for the assessment case simulations are presented below.

The BISON source code repository at `hpcgitlab.inl.gov` contains a set of input files corresponding to the original 2D axisymmetric assessment case and the 1.5D version. In the process of converting the selected assessment cases to the 1.5D simulation formulation, these assessment cases were also converted to the newer, more general, tensor mechanics 2D axisymmetric system. The 1.5D capability is built on the tensor mechanics system, and the conversion to tensor mechanics within the 2D axisymmetric geometry is an important step in the implementation of these assessment cases in the 1.5D BISON capability. The input file for all three versions of the selected assessment cases presented below have been added to the BISON source code repository.

4.1 US PWR 16x16 solid pellets, full length fuel rod

The US PWR 16x16 lead test assembly (LTA) extended burnup demonstration was conducted during the 1980's in a US commercial pressurized water reactor (PWR) [4] to increase final discharge burnup. The TSQ002 rod was discharged at a burnup of approximately 58 MWd/kgU; TSQ002 is a full length fuel rod with standard (solid) fuel pellets. This rod was selected for 1.5D validation for the higher burnup value, moderately complex power history, relatively simple fuel pin geometry. In the graphs shown in Figure 2, the results of the comparison among the original 2D axisymmetric solid mechanics formulation, the new 2D axisymmetric tensor mechanics formulation, and the 1.5D capability are presented. The input files used to generate these comparison plots are available in the folder `bison/assessment/US_PWR_16_x_16/analysis/TSQ002` of the BISON development code repository. Ten axial pellet slices were used in the 1.5D simulation.



(a) Fuel Centerline Temperature
(b) Average Clad Temperature
(c) Pellet-Clad Gap at Mid-Stack
(d) Plenum Pressure
(e) Power History
(f) Internal Gas Volume Change
(g) Simulation Run Time
(h) Pellet Volume Change
(i) Axial Radial Displacement at EOL

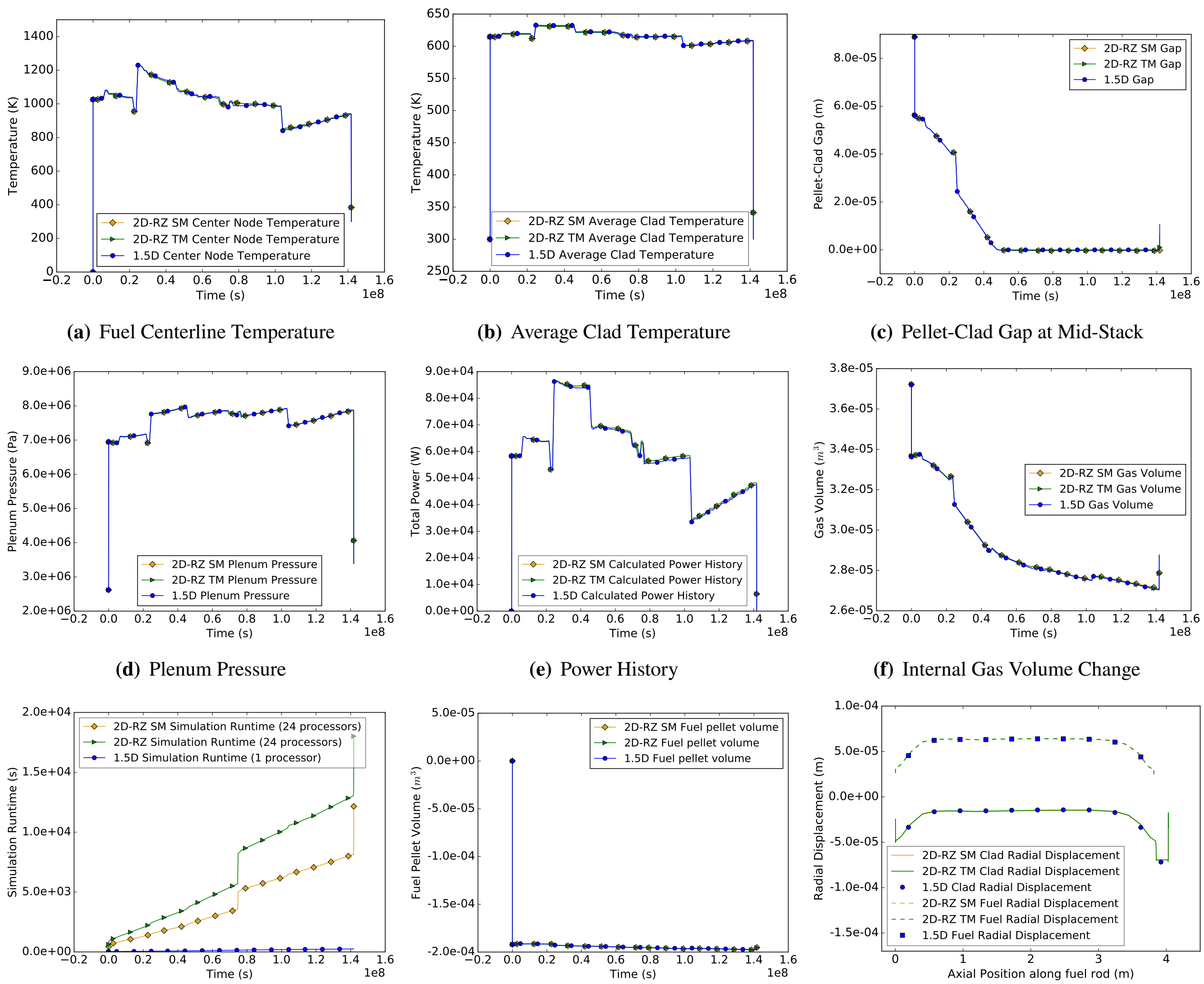
Figure 2: US PWR 16x16 Solid Pellets: Comparison of the 1.5D BISON capability against the 2D axisymmetric simulation results for the TSQ002 assessment case shows alignment among the different simulation results with a significant reduction in simulation time for the 1.5D simulation

The simulation comparison results demonstrate promising agreement between the 2D axisymmetric and the 1.5D cases for the temperatures, plenum pressure, and volume change quantities. The slight discrepancies in the end of life (EOL) radial displacements are expected consequences of the axial slice approach of the 1.5D capability: the ten axial positions of the 1.5D simulation cannot fully capture the axial radial displacement profile of the 2D axisymmetric simulations.

Similarly, the minimal discrepancy in the pellet-clad gap size is an anticipated result of the limited number of axial positions in the 1.5D simulation. The simulation run time is significantly reduced by a factor of 140 in the 1.5D simulation compared to the full 2D axisymmetric simulations.

4.2 US PWR 16x16 annular pellets, full length fuel rod

The US PWR 16x16 lead test assembly (LTA) extended burnup experiment also included a full length fuel rod with annular pellets [4]: the TSQ022 rod. The TSQ022 rod was selected for the 1.5D validation as an natural accompaniment to the TSQ002 rod to ensure the functionality of the 1.5D BISON capabilty with annular pellets. As in the TSQ002 solid pellets rod validation comparison, ten axial pellet slices were used in the 1.5D simulation of the TSQ022 annular pellets rod.



(a) Fuel Centerline Temperature **(b)** Average Clad Temperature **(c)** Pellet-Clad Gap at Mid-Stack

(d) Plenum Pressure **(e)** Power History **(f)** Internal Gas Volume Change

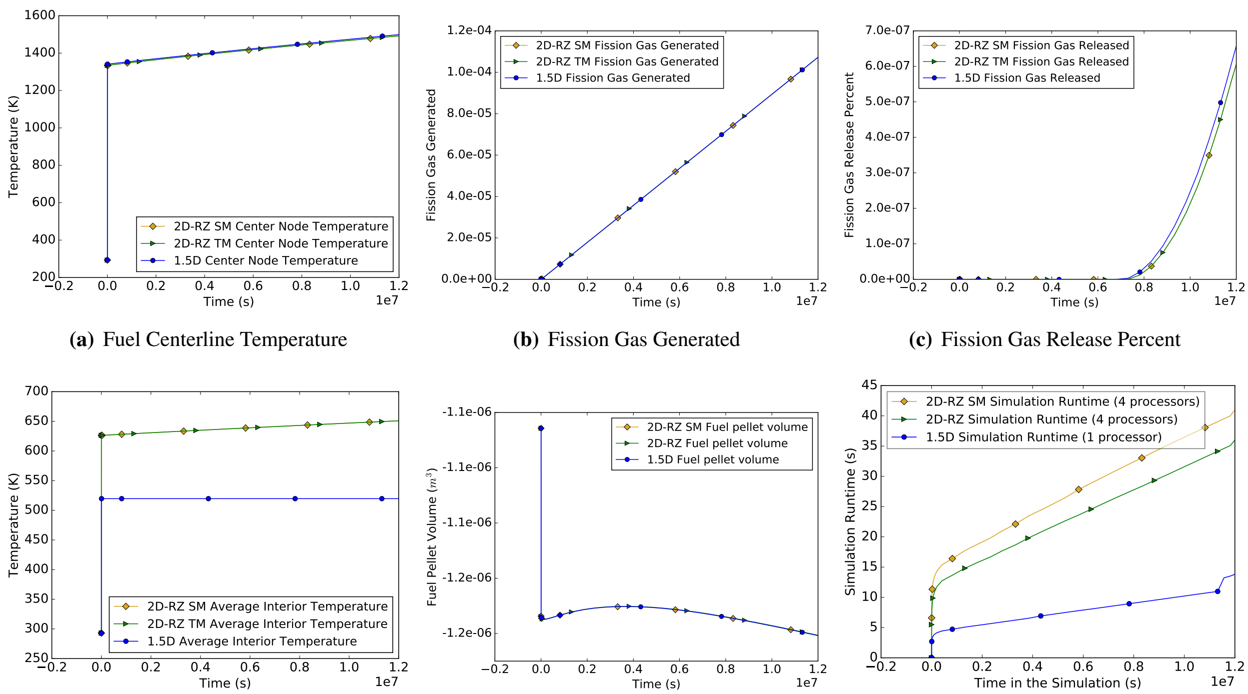
(g) Simulation Run Time **(h)** Pellet Volume Change **(i)** Axial Radial Displacement at EOL

Figure 3: US PWR 16x16 Annular Pellets: Comparison of the 1.5D BISON capability against the 2D axisymmetric simulation results for the TSQ022 assessment case shows alignment among the different simulation results with a significant reduction in simulation time for the 1.5D simulation

Similar to the solid pellet TSQ assessment case, the comparison results of the TQS annular pellet 2D axisymmetric and 1.5D cases demonstrate agreement in temperature, volume change, and plenum pressure with comparable deviations in the pellet-clad gap and the EOF radial displacement. The 1.5D simulation represents a factor of nearly 50 reduction in computation time compared to the 2D axisymmetric simulations. The input files used in the comparison simulations and the matplotlib script used to generate the plots shown in Figure 3 are available in the BISON development code repository folder `bison/assessment/US_PWR_16_x_16/analysis/TSQ022`.

4.3 FUMEXII simplified fuel pellet rod

The Fuel Modeling at Extended Burnup (FUMEXII) program, conducted from 1999-2007, outlined relevant collections of analytical exercises and appropriate experiments to increase comparison among fuel performance codes and experimental data [5]. In particular the FUMEX experiments focused on the collection of fission gas release data [5]. The simplified FUMEX assessment case, based on the Vitanza criterion [6], was selected for the 1.5D validation exercise in recognition of the role played by fission gas generation and release in the calculation of the fuel rod temperature distribution. The simplified case 27_1 case selected for the comparison shown in Figures 4 and 5 consists only of a short fuel stack and is subject to a constant power profile of 45 kW/m.

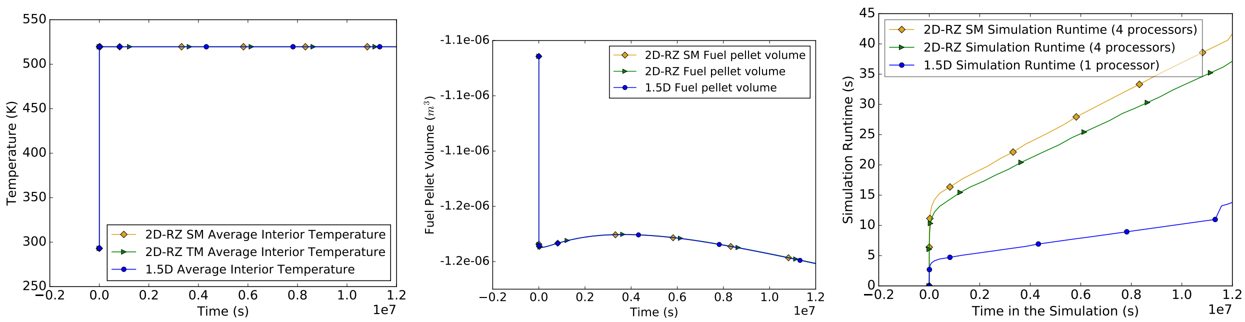


(a) Fuel Centerline Temperature **(b)** Fission Gas Generated **(c)** Fission Gas Release Percent

(d) Average Pellet Exterior Temperature **(e)** Fuel Pellet Volume Change **(f)** Simulation Run Time

Figure 4: FUMEXII Simplified Pellet Only Simulation: Comparison of the 1.5D BISON capability against the the 2D axisymmetric simulation results for the FUMEXII Simplified 27(1) pellet only assessment case demonstrates alignment among the simulations for the fuel center node temperature and fuel pellet volume change. The results for average exterior pellet temperature demonstrate significant disparity among the simulation results because the top and bottom of the fuel pellets is included in the average pellet exterior temperature only in the 2D axisymmetric simulation.

The geometry of the FUMEXII simplified 27_1 assessment case highlights a difference in the calculation of the average fuel pellet exterior temperature between the 2D axisymmetric and the 1.5D capability simulations with the shorter and wider fuel pellets. Figure 4 demonstrates a significant difference in the average fuel pellet exterior temperature values among the 2D axisymmetric and the 1.5D simulations. We note that in this simplified assessment case problem the plenum pressure is affected significantly by the average pellet exterior temperature. In the 2D axisymmetric simulation, the average fuel pellet exterior temperature is calculated by averaging the radial exterior, top, and bottom of the fuel pellet while the 1.5D simulation only the radial exterior of the pellet is used to calculate the pellet exterior temperature. The short and wide geometry of this FUMEXII simplified assessment case fuel pellet results in a significant contribution of the top and bottom of the pellet to a higher average exterior fuel pellet average temperature. The current 1.5D



(a) Average Pellet Exterior Temperature **(b)** Fuel Pellet Volume Change **(c)** Simulation Run Time

Figure 5: FUMEXII Simplified Pellet Only Simulation with Modified Average Temperature Postprocessor: The comparison disparity among the 1.5D BISON capability and the 2D axisymmetric simulations results for the average fuel pellet exterior temperature was successfully removed by calculating the average exterior pellet temperature on only the exterior radial side of the pellet in the 2D axisymmetric simulation.

post processor capability is not able to capture the increase in the average exterior fuel pellet temperature due to the significant contributions from the pellet top and bottom in this case.

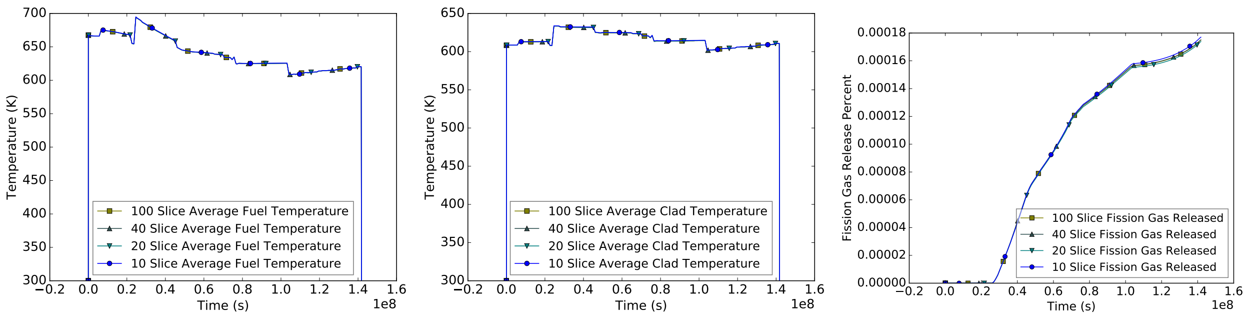
To demonstrate that the discrepancy among the 1.5D capability and the 2D axisymmetric simulations was due only to this difference in the post processor calculation of the average pellet exterior temperature, we ran the 2D axisymmetric simulation with a modified average pellet exterior temperature post processor that only used the exterior radial pellet surface. The simulation comparison results of this modified average exterior temperature post processor in the 2D axisymmetric simulation with the 1.5D simulation are shown in Figure 5. The modification of the post processor calculation produces results that agree across the 2D axisymmetric and 1.5D capability simulation results.

5 Validation Study on Number Axial Slices

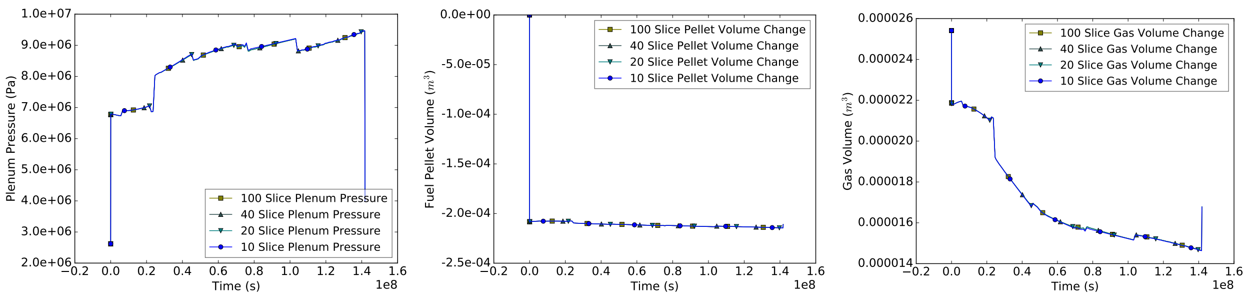
The validation effort also included a study on the number of axial fuel slices required to generate an accurate representation of a full length fuel rod with a minimum number of fuel slices. Additional fuel slices reduce the computational efficiency of the 1.5D capability, yet it is critical to ensure that a sufficient number of axial fuel slices are used in the simulation to capture the relevant solution information. We performed a convergence type study on the number of fuel slices required to model a full length fuel rod using the 1.5D simulation of the TSQ002 solid fuel pellets rod, presented in Figure 2. The comparison results for a series varying numbers of axial fuel slices, 10 slices, 20 slices, 40 slices, and 100 slices, are presented in Figures 6, 7, 8, and 9.

In this convergence study we found temperature, fission gas release, plenum pressure, and volume change are relatively insensitive to the number of axial fuel slices used in the model of the full length fuel rod, shown in Figure 6. In simulations concerned primarily with temperature profiles and radial heat transfer, 10 axial fuel slices are an acceptable number for a 1.5D BISON simulation.

On the other hand, the gap size and the EOL radial displacement along the fuel rod axial direction demonstrate a slight dependence on the number of axial fuel slices used to model the full length fuel rod. While the general shape of the fuel pellet radial displacement matches across the four convergence study cases compared here, the 10 slice and 20 slice cases are not able to capture as much of the full pellet stack radial displacement simply because these convergence study cases have few axial points at which to collect radial displacement information. This dependence on the number of axial slices for the gap and radial displacement is expected: these quantities are strongly connected to axial position, and a smaller number of axial slices results in a greater loss of axial position dependent information in the 1.5D simulations.

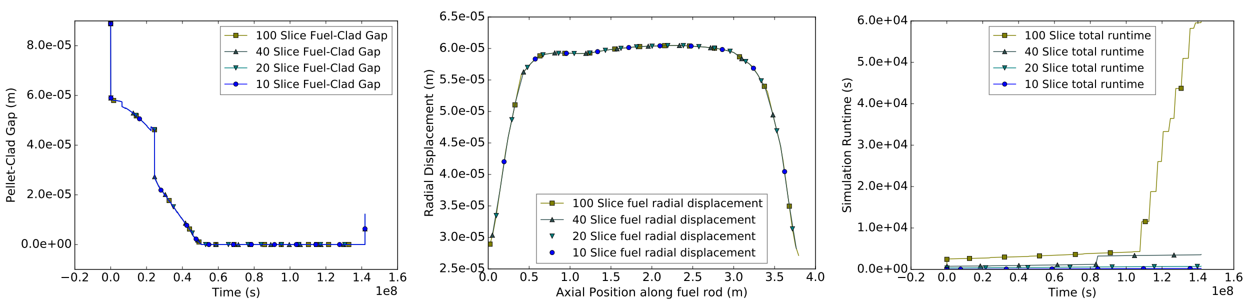


(a) Fuel Centerline Temperature **(b)** Average Clad Temperature **(c)** Fission Gas Release



(d) Plenum Pressure **(e)** Pellet Volume Change **(f)** Internal Gas Volume Change

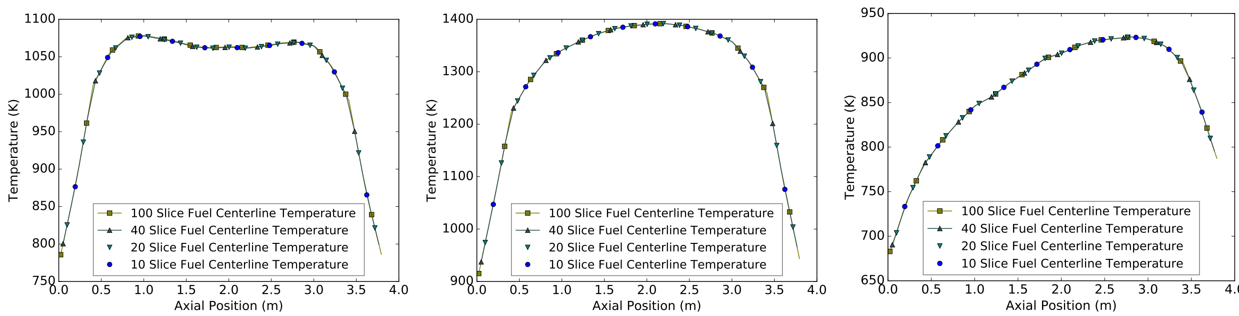
Figure 6: The axial slice convergence study using the US PWR 16x16 solid pellets rod indicates that fuel and clad temperatures, fission gas release, plenum pressure, and volume change of the pellet and the internal gas space is insensitive to the number of axial fuel slices used to model a full length rod.



(a) Pellet-Clad Gap at Mid-Stack **(b)** Fuel Axial Radial Displacement at EOL **(c)** Simulation Run Time

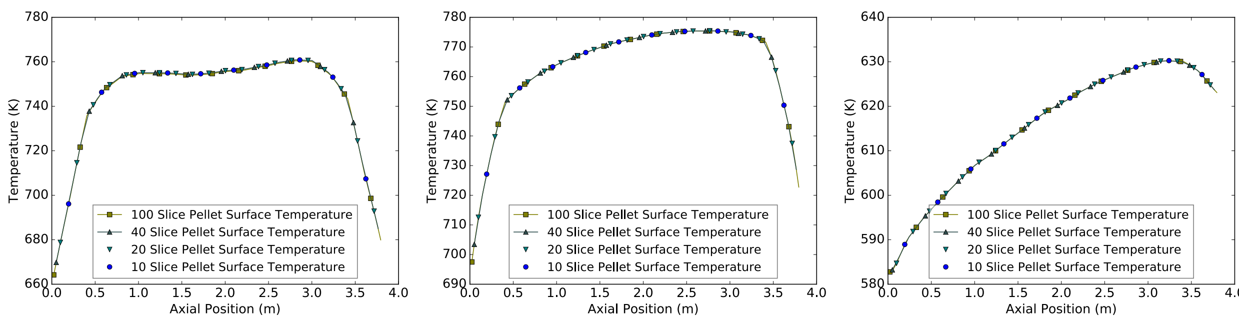
Figure 7: The axial slice convergence study using the US PWR 16x16 solid pellets rod demonstrates a dependence of the pellet-clad gap, axial EOL fuel radial displacement, and simulation time on the number of axial fuel slices used to model a full length rod with the 1.5D BISON capability.

In addition to the time history of the fuel centerline temperature at a specific node, we have also compared the variation of the fuel centerline and fuel pellet exterior surface temperature as a function of axial position at three specific points within the simulation: start up power, peak power which occurs fairly early in mid-life, and a significant power drop in the later stages of the power history curve. In all three time points selected for the comparison of fuel temperature as function of axial position, the results from the four 1.5D slice convergence study demonstrate nearly perfect alignment. This agreement in temperature among the 10 slice, 20 slice, 40 slice, and 100 slice 1.5D simulations justifies the use of the computationally efficient 10 slice 1.5D BISON capability to model a full length fuel rod.



(a) Startup Power (54 kW/m) **(b)** Peak Power, Mid Life (87 kW/m) **(c)** Power Drop, Near EOL (30 kW/m)

Figure 8: The axial slice convergence study using the US PWR 16x16 solid pellets rod demonstrates fuel centerline temperature is calculated consistently with different numbers of 1.5D axial fuel slices, even at significant power changes. The three power changes selected for the axial position of fuel centerline temperature correspond to significant and abrupt changes in the power history (see Figure 2 for the complete power history of the TSQ002 rod).



(a) Startup Power (54 kW/m) **(b)** Peak Power, Mid Life (87 kW/m) **(c)** Power Drop, Near EOL (30 kW/m)

Figure 9: The fuel pellet exterior surface temperature also demonstrates consistent results in the axial slice convergence study using the US PWR 16x16 solid pellets rod. The three power changes selected for the axial position of fuel centerline temperature correspond to significant and abrupt changes in the power history (see Figure 2 for the complete power history of the TSQ002 rod).

The significant increase in the simulation runtime with the increasing number of axial fuel slices, shown in Figure 7, highlights the impact of the 1.5D BISON capability to capture the important physics of a fuel rod, demonstrated in Figures 6, 8, and 9, with a minimal number of axial fuel slices (10) to achieve a substantial improvement in computational efficiency.

6 Summary and Future Work

This report documents the continued development and initial validation efforts for the 1.5D BISON modeling capability as applied to full length LWR fuel rods. The presented validation results show good agreement among the 1.5D simulations and the 2D axisymmetric validation cases, [3], for both solid and annular fuel pellets. The 1.5D assessment case simulations also demonstrate the significantly faster runtime of the 1.5D BISON capability: the 1.5D TSQ022 annular pellet simulation runs 50x faster than the original 2D axisymmetric case and the 1.5D TSQ002 solid pellet simulation runs to completion 140x faster than the analog 2D axisymmetric assessment case.

The usabilty improvements to the 1.5D capability have been added to the current BISON development code repository and are available for testing and use. Initial verification simulations, with results that align with analytical solutions, have been developed to ensure the correct formulation of the 1.5D BISON capability. These input files have been added to the BISON repository. The assessment case simulation input files and the comparison plot generation scripts have also been added to the BISON assessment case repository.

Additional work remains to be completed to ensure the 1.5D capability is ready for widespread use, including further usability improvements to mitigate input file errors, continued verification efforts, and expanded validation against existing 2D axisymmetric BISON assessment cases.

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