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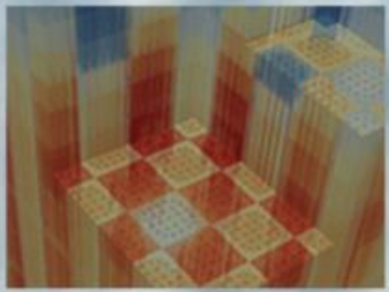

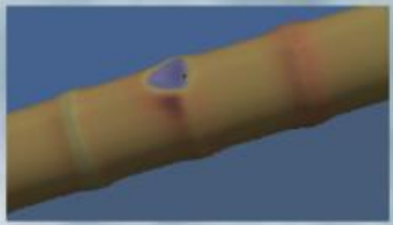

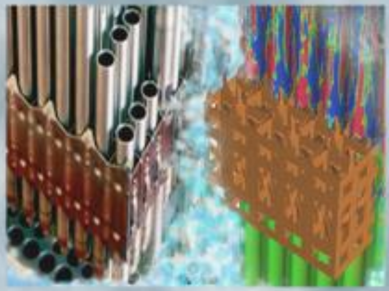

Initial Accident-Tolerant Fuel/Cladding Extensions to the VERA-to-Bison Offline Coupling

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CONTENTS

FIGURES

ACRONYMS

APMT	advanced powder metallurgical (FeCrAl alloy)
ATF	accident-tolerant fuel
BOC	beginning of cycle
CASL	Consortium for Advanced Simulation of Light Water Reactors
EOC	end of cycle
INL	Idaho National Laboratory
MOC	middle of cycle
ORNL	Oak Ridge National Laboratory
PWR	pressurized water reactor
VERA	Virtual Environment for Reactor Analysis

1. INTRODUCTION AND BACKGROUND

The Virtual Environment for Reactor Applications (VERA) [1] being developed by the Consortium for Advanced Simulation of Light-Water Reactors (CASL) allows a user to run numerous modeling codes with a single input file. This includes modeling codes such as MPACT/CTF [2,3], a neutronics/thermal hydraulics code, and Bison [4,5], a fuel performance code. This is achieved through the use of preprocessors which act upon the common VERA input and subsequent inputs. These preprocessors output files to be used as inputs to the pieces of software contained in VERA. For example, consider the flow chart in Figure 1, which illustrates the preprocessors (`react2xml` and `xml2moose`) used to obtain an input for Bison using an "offline," one-way coupling between MPACT/CTF and Bison [6].

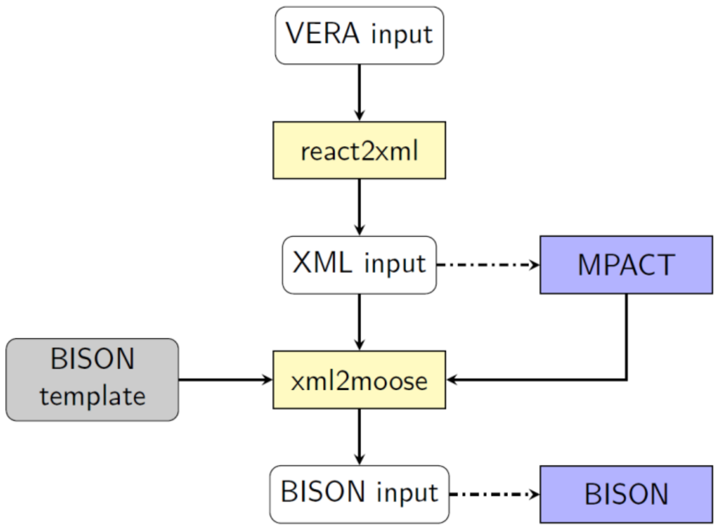

Figure 1. Input Parsing Process.

First, the VERA input is preprocessed with `react2xml`, producing an XML file suitable to run MPACT. This XML input, along with a Bison template file and rod histories from the MPACT simulation, are then preprocessed with `xml2moose`. This results in a standalone file which can then be run in BISON.

While developing advanced capabilities in a VERA component, one must ensure the associated preprocessor(s) are developed to accommodate these capabilities. CASL partners have expressed interest in modeling accident-tolerant fuel (ATF) materials in VERA. This report details the preprocessor development performed to accommodate Bison modeling of ATF materials in VERA.

1.1 ATF Materials

The work described here contributed to support for two ATF materials which are frequently considered: (1) FeCrAl cladding and (2) U_3Si_2 fuel. There are mature BISON material models for both of these materials. SiC cladding was also considered, but many critical material models have yet to be implemented in Bison. Adding VERA support for SiC cladding can be revisited once this occurs.

1.2 Default Model Selection

The default ATF material models in the 2D tensor mechanics template were adapted from ATF Bison modeling examples provided by the Bison development team. At the time of this writing, these examples can be found at the following locations in the VERA source:

- FeCrAl: `VERA/MOOSEExt/MOOSE/examples/tensor_mechanics/accident_tolerant_fuel/uo2_fecral.i`
- U_3Si_2: `VERA/MOOSEExt/MOOSE/examples/tensor_mechanics/accident_tolerant_fuel/u3si2_zircaloy.i`

2. IMPLEMENTATION

Adding support for these materials involved changes to (1) the Bison tensor mechanics template (`Bison_2D_tm.template`), (2) the `xml2moose` preprocessor, and (3) the `react2xml` preprocessor. The changes made to `react2xml` were minor.

2.1 `bison_2D_tm.template` Modificiations

Changes to the `[Materials]` block of the template were made to include default material models for each possible material type. This is best illustrated with an example. Before the changes were made, there was a single block to describe the thermal expansion of the cladding:

```
[./thermal_expansion]
  type = ZryThermalExpansionMatproEigenstrain
  block = 1
  temperature = temp
  stress_free_temperature = 293.0
  eigenstrain_name = clad_thermal_eigenstrain
[../]
```

The above block, as evidenced by `type = ZryThermalExpansionMatproEigenstrain`, is a ZIRLO model [7]. With the modifications to support ATF materials, there are now multiple blocks that describe the thermal expansion of the cladding, and xml2moose will delete the appropriate blocks based on the cladding material specified in the VERA input.

```
[./thermal_expansion_Zry]
  type = ZryThermalExpansionMatproEigenstrain
  block = 1
  temperature = temp
  stress_free_temperature = 293.0
  eigenstrain_name = clad_thermal_eigenstrain
[../]

[./thermal_expansion_FeCrAl]
  type = FeCrAlThermalExpansionEigenstrain
  block = 1
  temperature = temp
  stress_free_temperature = 293.0
  eigenstrain_name = clad_thermal_eigenstrain
  fecral_material_type = C35M
[../]
```

Note that, in addition to the second block the model for ZIRLO cladding is still present, although it has a different block name. The model is a thermal expansion model for FeCrAl cladding. Depending on the VERA input, `xml2moose` will discard whichever block is unnecessary. All material-specific blocks are named with a suffix identifying the material. The suffixes are as follows:

- `_Zry` for ZIRLO
- `_FeCrAl` for FeCrAl,
- `_UO2` for UO_2, and
- `_U3Si2` for U_3Si_2.

2.2 `xml2moose` Modifications

For `xml2moose` to retain only the necessary material blocks, modifications were made to allow for the identification of materials present in the input file. This is accomplished through the new members (`fuel_type` and `clad_type`) in the `PinData` structure of `CASL_MOOSE_Data.hpp`. The following snippet of a VERA input describes a single fuel rod composed of U_3Si_2 fuel and ZIRLO cladding.

```
[ASSEMBLY]
  title "Westinghouse 17x17"
  npin 1        ! *** scaled to 1x1 rod
  ppitch 1.270  ! *** increased for 1x1 to get rid of gap

  fuel U3Si2 11.59 95.0 / 3.1

  cell 1     0.4096 0.418 0.475 / U3Si2 he zirc
```

In this snippet, `xml2moose` determines the materials present by examining the materials given on the final line: `U3Si2 he zirc`. The first material determines `fuel_type`, and the final material determines the `clad_type`. (An annular fuel rod case is also functional; if `he` is the first material listed, then the second entry is interrogated to determine `fuel_type`). The member `fuel_type` and the `clad_type` are both integer data types. See **Table 1** designations indicating which material corresponds to which `_type` value.

Table 1. Material Type Designations

Fuel Material	
fuel_type = 0	UO_2
fuel_type = 1	U_3Si_2

Cladding Material	
clad_type = 0	ZIRCALOY
clad_type = 1	FeCrAl

Both members default to 0 if unexpected behavior (i.e., improper input) occurs. The code for these assignments can be found in `CASL_MOOSE_InputFileGenerator.cpp`.

After the materials present are properly identified and other determinations made, a call is made for each pin to `MOOSEInputFileParser::parseFile` or *the parser* of `CASL_MOOSE_InputFileParser.cpp`. Among other things, the parser takes in `fuel_type` and `clad_type` as arguments and then purges the unnecessary blocks.

The unnecessary blocks are identified by the suffix in their block titles. In the single fuel rod example from above, all blocks with a `_UO2` or `_FeCrAl` suffix would be removed.

2.3 `react2xml` Modifications

An addition was made to CORE.ini to allow for FeCrAl cladding to be specified in a cell without defining it as a material elsewhere. The addition is shown below.

```
mat fecral       7.25    al-27   -9.68720E-02 ! SCALE 6.2
                          cr-50   -8.73663E-03
                          cr-52   -1.88477E-01
                          cr-53   -1.91040E-02
                          cr-54   -4.75538E-03
                          fe-54   -4.10351E-02
                          fe-56   -6.44163E-01
                          fe-57   -1.48769E-02
                          fe-58   -1.97979E-03
                          / thexp=15.0
```

This entry should be verified before using these atomic fractions with MPACT. Additional entries may be needed for the different FeCrAl alloys. The atomic fractions do not factor into the Bison input.

2.4 Improvements to Consider

2.4.1 UO_2 Cracking

Ideally, the default UO_2 elasticity model would incorporate cracking. Below is an implementation of a smeared cracking model identified to be the most appropriate default setting.

```
[./fuel_elastic_stress_UO2]
  type = ComputeSmearedCrackingStress
  block = fuel
  cracking_stress = 1.68e8
  inelastic_models = 'fuel_creep'
  shear_retention_factor = 0.1
  max_stress_correction = 0
  output_properties = crack_damage
  outputs = exodus
[../]
```

Unfortunately, this block results in convergence issues. At the time of writing, the following fully elastic model is used in its place. It should be replaced with a cracking model when possible and is a topic on on-going work with the Bison team.

```
[./fuel_elastic_stress_UO2]
  type = ComputeFiniteStrainElasticStress
  block = 3
[../]
```

2.4.2 U_3Si_2 Relocation and Cracking

As of October 2018, there are no relocation or cracking models for U_3Si_2 implemented in Bison. If they are implemented in the future, they should be added as default models to the template.

2.4.3 FeCrAl Material Parameters

There are several alloys of FeCrAl being considered for ATF applications. Currently, the most mature material models in Bison are mixed between the advanced powder metallurgical FeCrAl alloy (APMT) and the C35M alloy. As such, in the template, some FeCrAl material blocks use APMT models, and others use C35M models. As additional alloy models are added, this discrepancy can be addressed.

Once this is accomplished, a mechanism for entering the FeCrAl alloy type must be developed, and `xml2moose` modifications must be made to appropriately propagate this input throughout the output file.

3. RESULTS

Two sets of results are presented herein to demonstrate VERA's ability to model FeCrAl cladding and U_3Si_2 fuel in Bison. These results have not been validated as they are preliminary. Longer term, validation, sensitivity, and uncertainty analyses would be necessary before industry partners could use the results in a very meaningful way to drive any safety determinations. The set first compares single fuel rods composed of various materials, and the second examines a quarter core containing a U_3Si_2 lead test assembly.

3.1 Single Rod Comparison

Three single fuel rods, detailed in **Table 2**, were considered.

Table 2. Single Fuel Rod Characteristics

Configuration	Fuel	Clad	Clad Width [cm]	Gap Width [µm]	Pellet Radius [cm]
Standard	UO_2	ZIRLO	0.057	84	0.4096
FeCrAl	UO_2	FeCrAl	0.035	84	0.4316
U_3Si_2	U_3Si_2	ZIRLO	0.057	84	0.4096

The far left column lists the names used when referring to the configurations. The standard configuration is typical of the fuel currently used in commercial nuclear reactors. The remaining configurations use the ATF materials incorporated as part of this work.

Apart from the FeCrAl configuration, these are Westinghouse 17 × 17 [8] assembly rod geometries. Relative to ZIRLO, FeCrAl cladding has a neutronic penalty, and the geometry given in **Table 2** was one identified by Idaho National Laboratory (INL) to address this issue [9]. The fuel pellet radius has been elongated, and the clad width has been reduced in equal amounts. This allows for a gap width and an overall fuel rod radius equal to the other configurations.

Each fuel rod was modeled using three representative power cycles adapted from a Watts Bar rod history. The Bison results for minimum gap width, maximum clad hoop stress, fuel centerline temperature, and fuel average temperature will be examined.

3.1.1 Minimum Gap Width

Figure 2 depicts the minimum gap width over time for each configuration, as well as the rod power used in the simulations.

Gap closure occurs first in the standard configuration, followed by the U_3Si_2 and FeCrAl configurations. As will be discussed later, the U_3Si_2 rod operates at lower temperatures, which results in less thermal expansion when compared to the standard rod. This leads to an extended time to gap closure. FeCrAl has a much slower creep rate than ZIRLO, driving the FeCrAl configuration to experience gap closure at around 1,000 days.

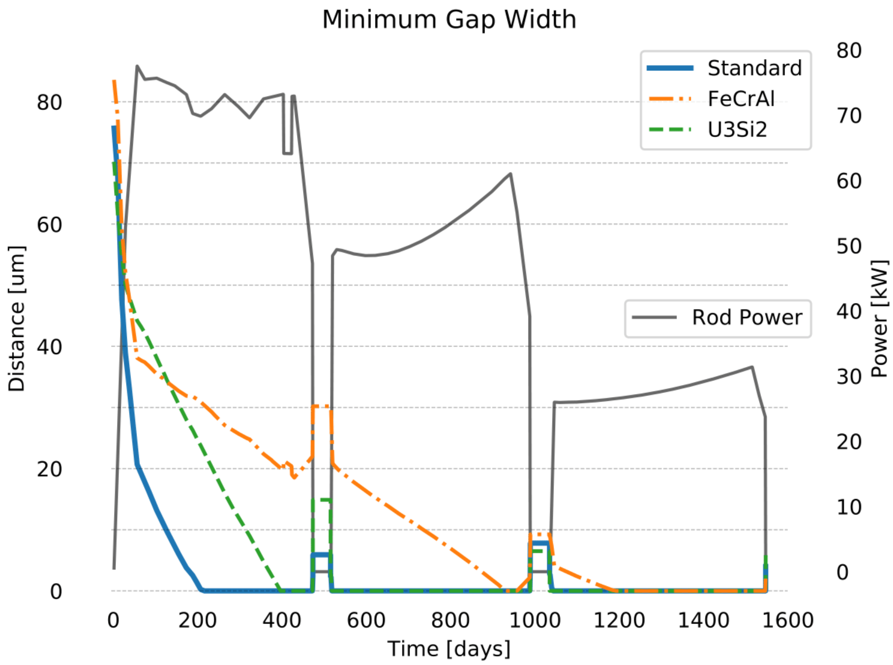

Figure 2. Minimum Gap Width, Single Rod.

3.1.2 Maximum Clad Hoop Stress

Figure 3 depicts the maximum clad hoop stress over time for each configuration.

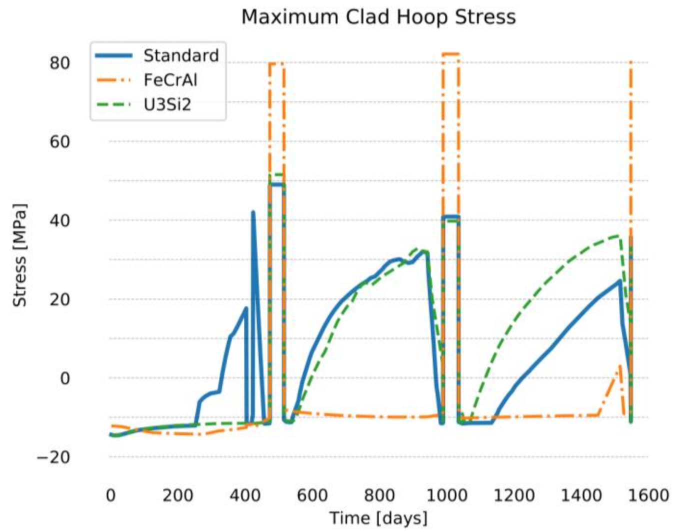

Figure 3. Maximum Clad Hoop Stress, Single Rod.

Negative maximum clad hoop stresses such as those at the beginning of the first cycle are observed when the system pressure exceeds the internal pressure of the rod. After gap closure, maximum clad hoop stress begins to increase in all of the configurations. The spiking behavior seen around 300 days for the standard configuration is attributable to the power changes shown in **Figure 2**. During outages, the maximum clad hoop stress climbs to an elevated plateau due to the system's depressurization to atmospheric pressure.

3.1.3 Average Fuel Temperature

Figures 4a and 4b depict the average fuel temperature over time for each configuration.

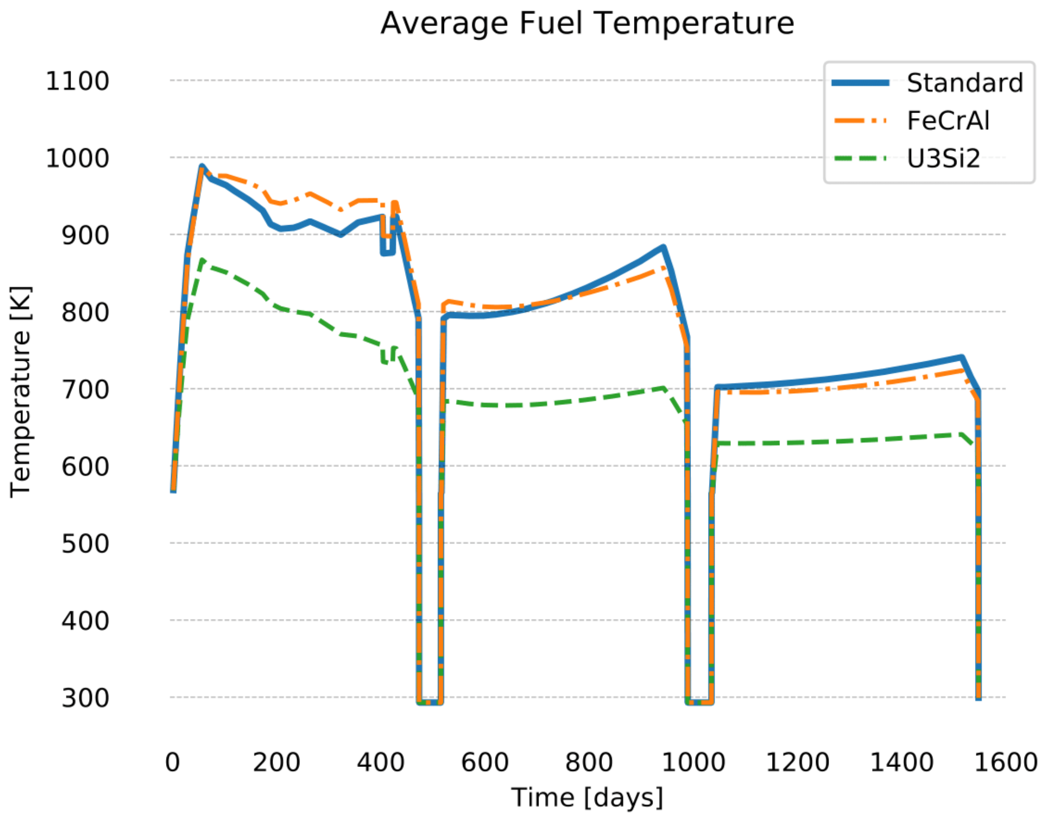

Figure 4a. Average Fuel Temperature, Single Rod.

The results are largely influenced by the fuel type present in each configuration. The standard and FeCrAl cases, which both feature UO_2 fuel, exhibit very similar behaviors. The U_3Si_2 configuration has a much lower maximum fuel centerline temperature due to the fuel's high thermal conductivity. The average temperature of the FeCrAl configuration might be expected to exceed that of the standard configuration until gap closure occurs in the former case. However, this is not observed due to the differing geometries. With equal geometries, however, this expectation is met, as can be seen in **Figure 4b**.

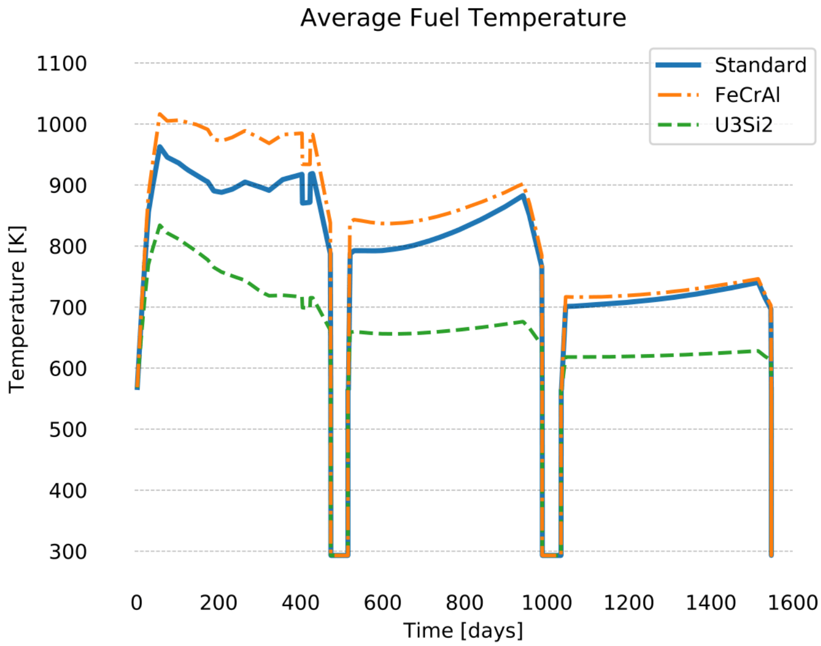

Figure 4b. Equal Geometries, Average Fuel Temperature, Single Rod.

3.1.4 Maximum Fuel Centerline Temperature

Figure 5 depicts the maximum fuel centerline temperature over time for each configuration.

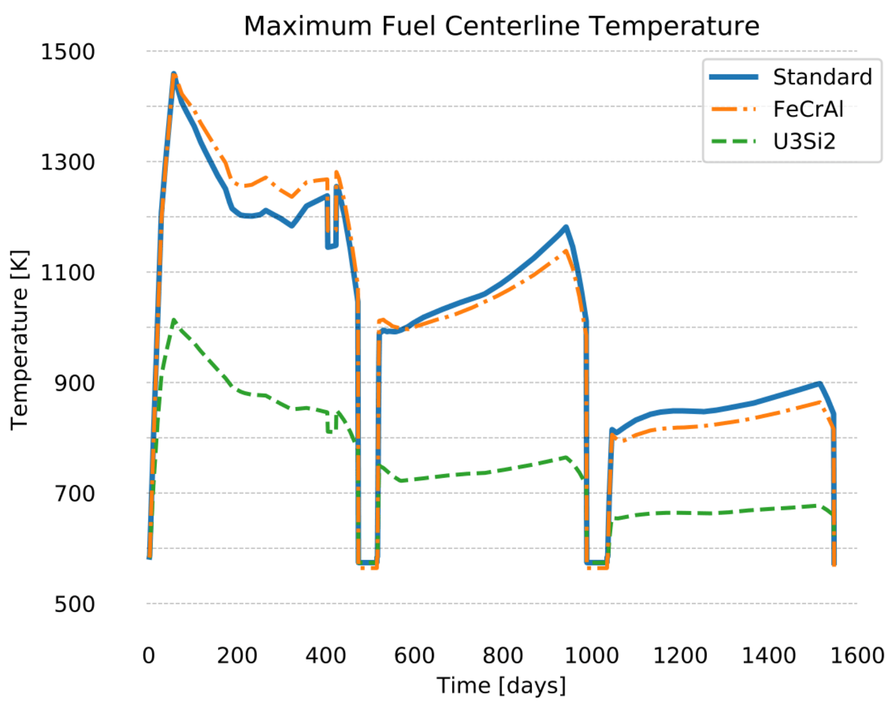

Figure 5. Maximum Fuel Centerline Temperature, Single Rod.

The trends observed in the previous section continue here; the standard and FeCrAl configurations demonstrate similar behavior, while the U_3Si_2 configuration experiences relatively lower temperatures.

3.2 U_3Si_2 Lead Test Assembly in Watts Bar Unit 1, Cycle 1

A quarter core with a U_3Si_2 lead test assembly was modeled to demonstrate VERA's ATF performance modeling in a multi-assembly application. The simulation was completed for a first cycle in Watts Bars Unit 1, a Westinghouse Electric Company four-loop pressurized water reactor (PWR) operated by the Tennessee Valley Authority. It is currently licensed for 3,459 MWth and has completed over 6,000 effective full power days of operation [8].

The test assembly was located at position D-12 and was enriched to 4.2%. The other assemblies, which were comprised of UO_2 and ZIRLO fuel rods, were enriched to 2.11%, 2.619%, or 3.1%. The axial cross section was taken at level 19 unless noted otherwise. In the figures below, results for each parameter are shown at three different points in time (from left to right): beginning of cycle (BOC), middle of cycle (MOC), and end of cycle (EOC).

3.2.1 Pin Powers

The lead test assembly, which had the highest enrichment, consistently experienced the highest powers.

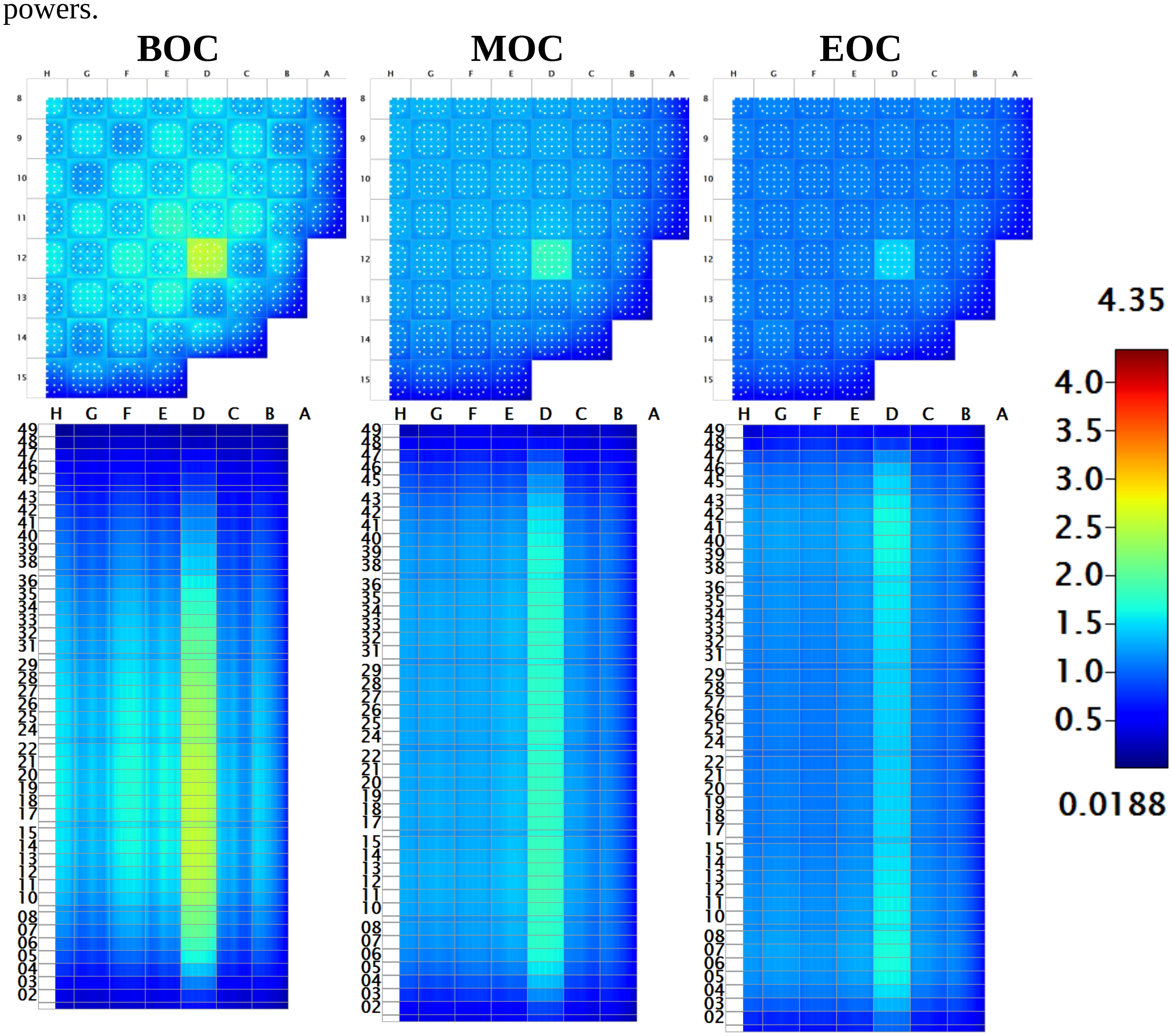

Figure 6. Pin Powers (Normalized to Unity), Quarter Core.

3.2.2 Moderator Temperature

The moderator temperature serves as the boundary condition for the simulation. An increase in the moderator temperature was observed around the lead test assembly due to higher assembly power and the high thermal conductivity of U_3Si_2.

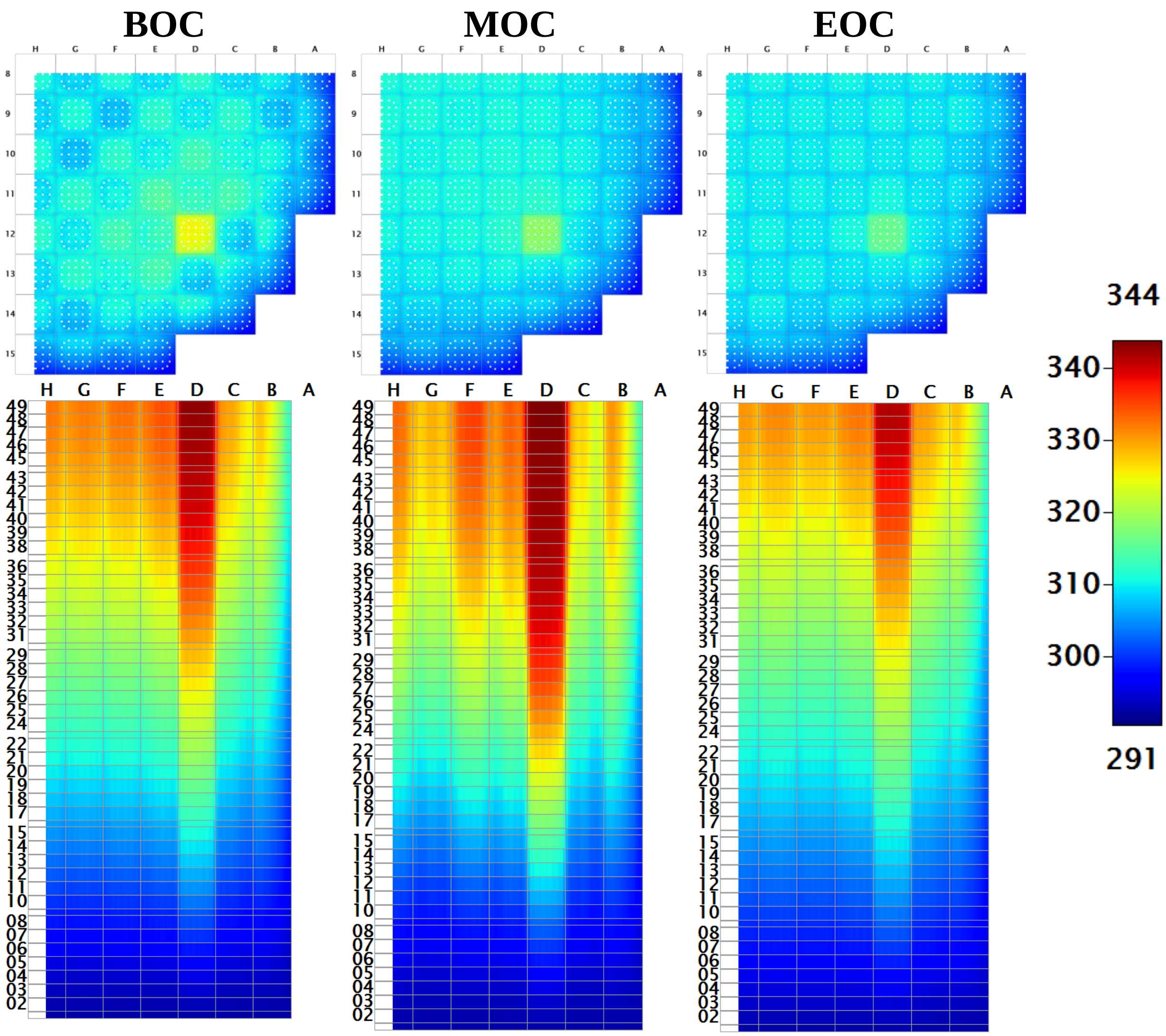

Figure 7. Moderator Temperature (K), Quarter Core.

3.2.3 Average Gap Width

Gap closure occurred in numerous rods by midcycle and in a significant majority of rods by the end of the cycle. In contrast to the results described in **Section 3.1.1,** gap closure occurs first in and around the lead test assembly due to the elevated lead test assembly power.

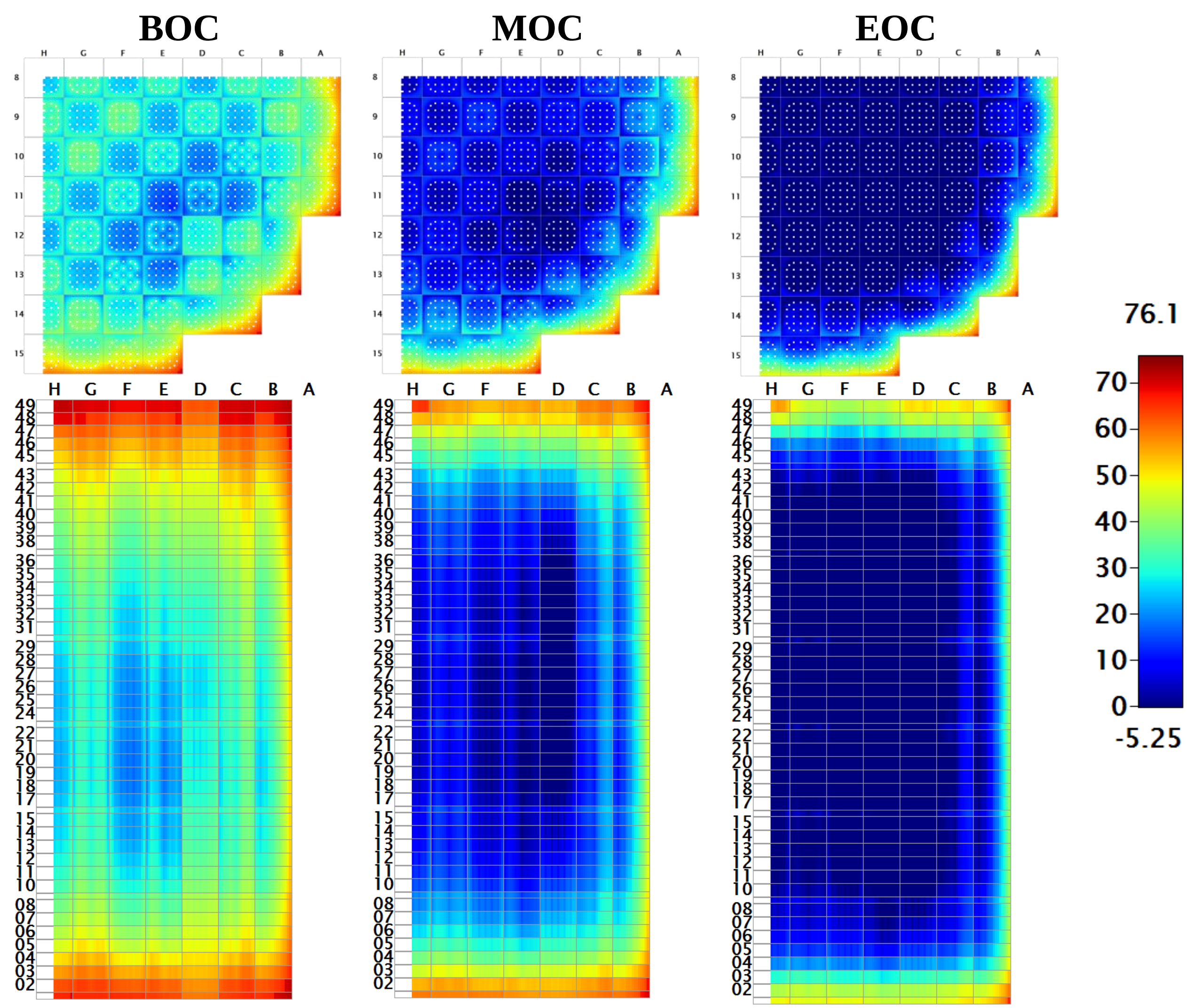

Figure 8. Average Gap Width [μm], Quarter Core.

3.2.3 Maximum Clad Hoop Stress

As in the single rod simulations, maximum hoop stress begins to increase after gap closure occurs. The images presented in the figure below are not from a single axial level; the maximum clad hoop stress can occur in different axial levels between pins.

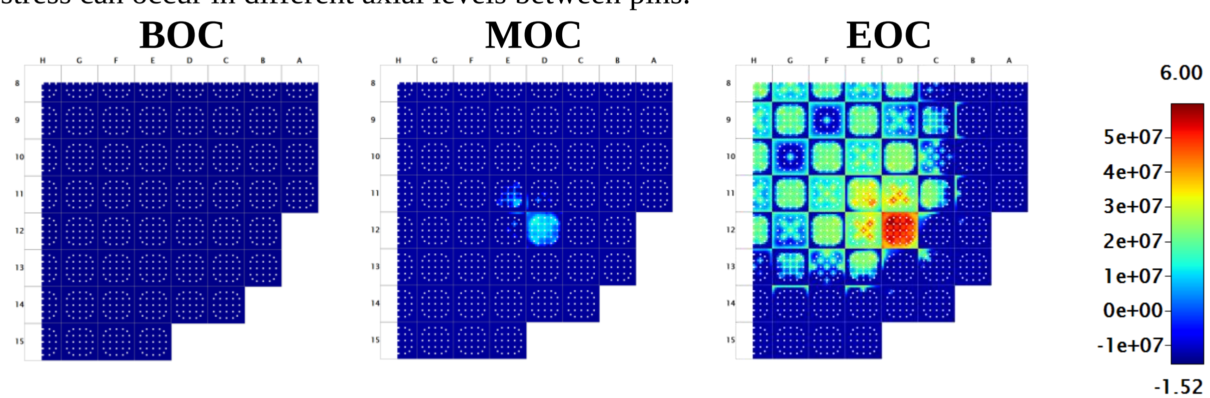

Figure 9. Maximum Clad Goop Stress (Pa), Quarter Core.

3.2.4 Fuel Centerline Temperature

Despite having the highest power, the lead test assembly experienced much lower temperatures due to the high thermal conductivity of U_3Si_2. The melting point of U_3Si_2 is 1938.15 K. The smallest margin to melting observed in the test assembly was 754.87 K. The smallest margin observed in the UO_2-fueled assemblies was 1531.02 K in assembly E-11.

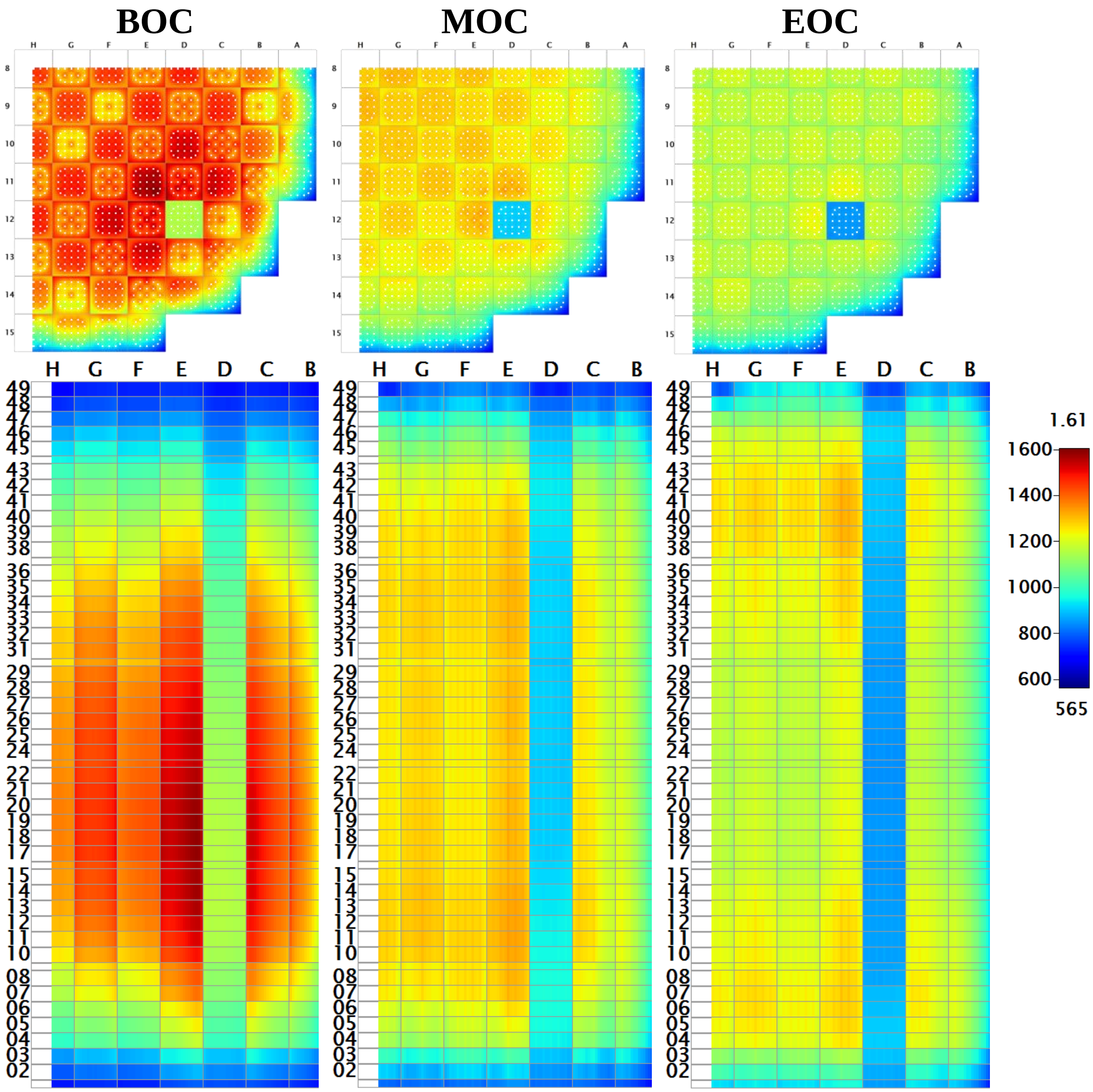

Figure 10. Fuel Centerline Temperature (K), Quarter Core.

3.2.5 Fuel Average Temperature

The lead test assembly experienced lower average fuel temperatures, as well.

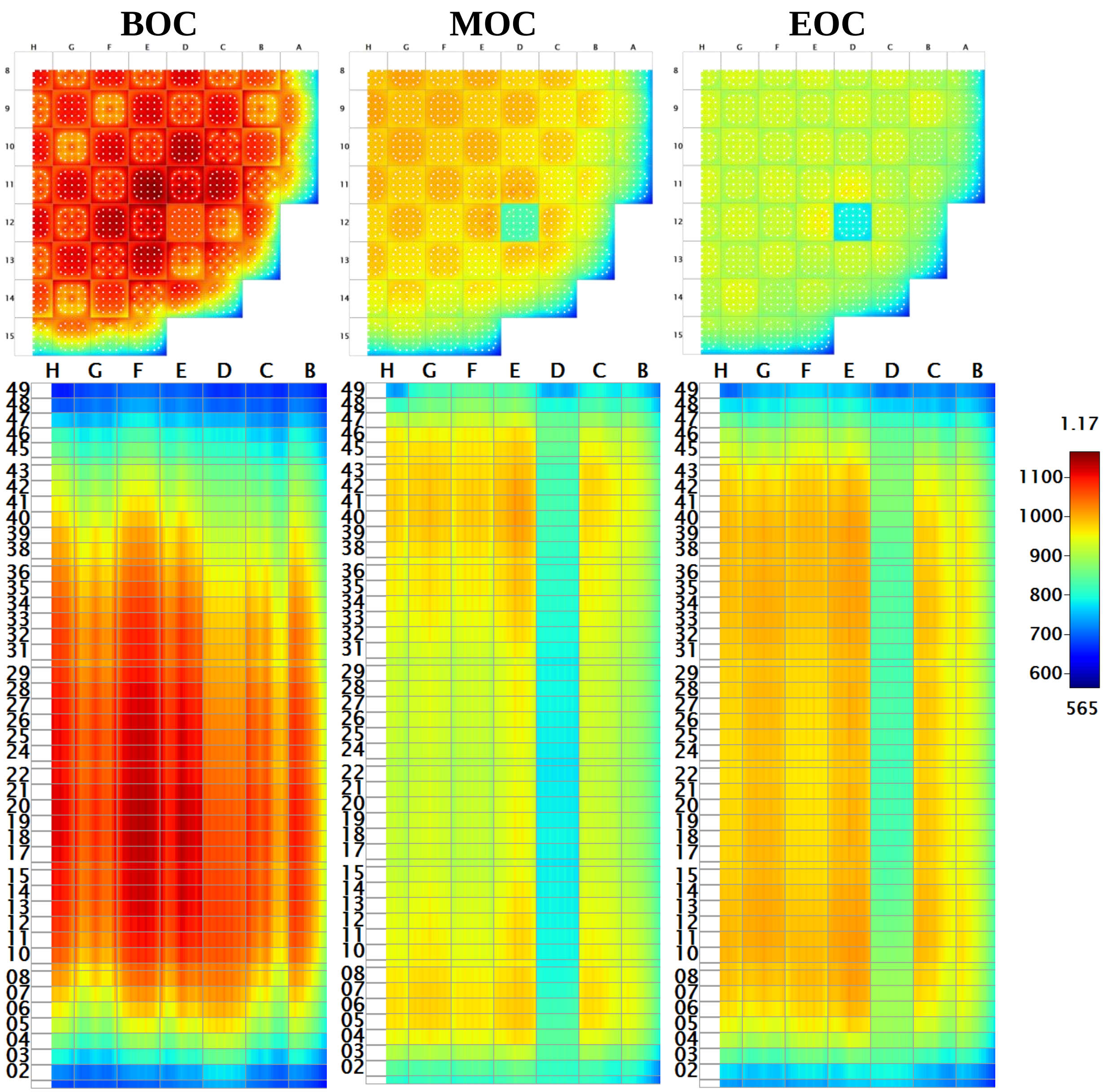

Figure 11. Fuel Average Temperature (K), Quarter Core.

4. CONCLUSION

`VERA` preprocessors were modified to allow for the fuel performance modeling of ATF materials with Bison. The default models within the `Bison_2D_tm.template` should be updated as material models are added to Bison.

Using the modified preprocessors, `VERA` demonstrated the ability to successfully generate Bison inputs for cases with FeCrAl cladding and U_3Si_2. This ability functions in single rod applications, as well as U_3Si_2 multiple assembly applications. The single rod simulations reflected the slow creep rate of FeCrAl clad and the low temperature operation of U_3Si_2, which both resulted in an extended time to gap closure. The quarter core U_3Si_2 lead test assembly simulation continued to demonstrate the low temperature operation of U_3Si_2 relative to a UO_2 assembly.

5. FUTURE WORK

5.1 GUIDANCE FOR FUTURE MODIFICATIONS

The following sections offer examples on common modifications.

5.1.1 Modifying Default Parameters on Existing Blocks

Consider the default block in the 2D tensor mechanics template, which implements a thermal expansion model for U_3Si_2:

```
[./fuel_thermal_strain_U3Si2]
  type = ComputeThermalExpansionEigenstrain
  block = 3
  thermal_expansion_coeff = 15.0e-6
  temperature = temp
  stress_free_temperature = 293.0
  eigenstrain_name = fuel_thermal_strain
[../]
```

If the user wants to change the default `thermal_expansion_coeff` value to 12.0e-6, then the user must simply change this entry in the template. The updated block is shown below.

```
[./fuel_thermal_strain_U3Si2]
  type = ComputeThermalExpansionEigenstrain
  block = 3
  thermal_expansion_coeff = 12.0e-6
  temperature = temp
  stress_free_temperature = 293.0
  eigenstrain_name = fuel_thermal_strain
[../]
```

In a similar manner, other parameters can be modified, removed, or added for existing blocks.

5.1.2 Adding New Blocks for Existing Materials

Assume a model for U_3Si_2 is introduced in Bison and needs to be added as a default model to the template. To do so, the user simply adds the block implementing the new model to the template file while paying careful attention to the block title; the block title must have the `_U3Si2` suffix to ensure that it is correctly purged for non-silicide cases. Below is a hypothetical example of what the block may look like.

```
[./fuel_relocation_U3Si2]
  type = U3Si2RelocationEigenstrain # This model doesn't actually exist
  block = 3
  burnup_function = burnup
  linear_heat_rate_function = q
[../]
```

Whenever a block with a material-specific model is added, the block title must contain the appropriate suffix.

5.1.3 Adding New Blocks for New Materials

After a number of critical material models for SiC cladding are added to BISON, the 2D tensor mechanics template may need to be updated to support SiC modeling. The following must be done:

1. Modify `CASL_MOOSE_InputFileGenerator.cpp` to identify SiC cladding from a VERA input and set `clad_type = 2` (another value could be chosen, but this is consistent with the current convention)
2. Add the default SiC blocks to the `Bison_2D_tm.template` with appropriate suffixes (`_SiC` seems reasonable)
3. Add conditional statements to `MOOSEInputFileParser::parseFile` for the case when `clad_type = 2`, and also update the purge lists.
4. Add a loop in `MOOSEInputFileParser::parseFile`, similar to the others present, which loops through `purgeSiC` and determines whether to purge or retain a block.

Some of the finer details of this process have been omitted, but this is the general procedure. A similar process acting on `fuel_type` can be implemented to add support for additional fuel materials.

5.2 POTENTIAL ISSUES

5.2.1 Coated Cladding

As mentioned in **Section 2.2**, the cladding material is determined from the last material in the cell definition. If a coated cladding was modeled explicitly, then this determination would need to be made in another manner, as the coating would occupy the last material in the cell definition.

5.2.2 FeCrAl Number Densities

As mentioned in **Section 2.3**, the atomic fractions included in CORE.ini for FeCrAl have not been verified. This should be addressed before this material definition is used with MPACT.

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[9] K. A. Gamble et al., "Behavior of U_3Si_2 Fuel and FeCrAl Cladding under Normal Operating and Accident Reactor Conditions," Table 4.7, INL tech. rep. INL/EXT-16-40059 Rev. 0, 2016.

7. ACKNOWLEDGMENTS

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