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Revision 0

BISON Investigation of the Effect of the Fuel-Cladding Contact Irregularities on the Peak Cladding Temperature and FCCI Observed in AFC-3A Rodlet 4

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SUMMARY

The primary objective of this report is to document results of BISON analyses supporting Fuel Cycle Research and Development (FCRD) activities. Specifically, the present report seeks to provide explanation for the microstructural features observed during post irradiation examination of the helium-bonded annular U-10Zr fuel irradiated during the AFC-3A experiment.

Post irradiation examination of the AFC-3A rodlet revealed microstructural features indicative of the fuel-cladding chemical interaction (FCCI) at the fuel-cladding interface. Presence of large voids was also observed in the same locations. BISON analyses were performed to examine stress and temperature profiles and to investigate possible correlation between the voids and FCCI. It was found that presence of the large voids lead to a formation of circumferential temperature gradients in the fuel that may have redirected migrating lanthanides to the locations where fuel and cladding are in contact. Resulting localized increase of lanthanide concentration is expected to accelerate FCCI.

The results of this work provide important guidance to the post irradiation examination studies. Specifically, the hypothesis of lanthanides being redirected from the voids to the locations where the fuel and the cladding are in contact should be verified by conducting quantitative electron microscopy or Electron Probe Micro-Analyzer (EPMA). The results also highlight the need for computer models capable of simulating lanthanide diffusion in metallic fuel and establish a basis for validation of such models.

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BISON Investigation of the Effect of the Fuel-Cladding Contact Irregularities on the Peak Cladding Temperature and FCCI Observed in AFC-3A Rodlet 4

1. OBJECTIVE

The primary objective of this report is to document results of BISON analyses supporting Fuel Cycle Research and Development (FCRD) activities. Specifically, the present report seeks to provide explanation for the microstructural features observed during post irradiation examination (PIE) of the helium-bonded annular U-10Zr fuel irradiated during the AFC-3A experiment.

Post irradiation examination of the AFC-3A rodlet revealed microstructural features indicative of the fuel-cladding chemical interaction (FCCI) at the fuel-cladding interface. Presence of large voids was also observed in the same locations. BISON analyses were performed to examine stress and temperature profiles and to investigate possible correlation between the voids and FCCI.

This work constitutes a research and development activity that is exploratory, preliminary, or investigative in nature.

2. BACKGROUND

2.1 Description of the BISON Fuel Performance Code

The fuel performance modeling effort described in the present report was executed at Idaho National Laboratory (INL) using the BISON fuel performance code. BISON[1] is a finite element-based engineering scale fuel performance code based on the Multiphysics Object-Oriented Simulation Environment (MOOSE) framework.[2] BISON solves the fully-coupled thermomechanics and species diffusion equations in two- or three-dimensional space. The code is currently under development and is being actively advanced by including multiphysics constitutive behavior models, and coupling to lower-length scale material models. Applicable to both steady and transient operation, BISON is designed for efficient use on parallel computers. Current applications include oxide, metal, and tristructural-isotropic (TRISO) nuclear fuels.

BISON is being developed by the Nuclear Energy Advanced Modeling & Simulation (NEAMS) Fuels Product Line to support advanced fuels development. NEAMS Fuels Product Line will develop and deliver a mechanistic (i.e., truly predictive) computational toolset for nuclear fuel design and/or analysis and integrate this toolset into the NEAMS ToolKit. NEAMS vision is to enhance the value of the Office of Nuclear Energy's research and development portfolio through the use of advanced computational methods.

2.2 AFC-3A Experiment Design and Operating Conditions

The motivation for the AFC-3 series experiments is the development of the advanced ultra-high burnup sodium-cooled fast reactor (SFR) metallic fuel concepts.[3] The irradiation experiment seeks to investigate advanced fuel designs with the following features: decreased fuel smeared density (SD), venting of the fission gas to the sodium coolant, a uranium-molybdenum (UMo) based alloy fuel system, coating or liner on the cladding inner surface, and/or targeted fuel alloy additions to reduce FCCI, and an advanced fabrication method that includes consideration of annular fuel and co-extruded fuel and cladding. The AFC-3A annular U-10Zr rodlet addresses the latter concept of the annular fuel coextruded with the cladding. Extrusion of metallic fuel alloy within cladding during fabrication could dramatically reduce process waste, eliminate volatile constituent losses during fabrication, and eliminate need for sodium bond.

The behavior of the low SD annular fuel early in life as initial fuel swelling occurs is identified as a principal area of uncertainty in the overview of the project.[3]

AFC-3A experiment design and operating conditions are described in detail in the experiment thermal evaluation,[4] and the as-run and projected physics evaluations.[5] Design and operating conditions information critical for the execution of the present study are summarized in Table 1 and Table 2. Detailed dimensions of the AFC-3 annular fuel rodlet assembly are given in the corresponding engineering drawings.[6] [7]A schematic of the AFC-3A annular rodlet assembly is given in Figure 1. A schematic of the AFC-3 annular fuel slug is given in Figure 2.

Table 1. Design of the AFC-3A annular U-10Zr irradiation experiment.

Rodlet	Composition	Density (g/cm^3)	As-built fuel height (cm)	As-built fuel outer diameter (cm)	Fuel inner diameter (cm)	Smeared density
3A-R4	U-10Zr	15.73	3.80492	0.48641	0.330	55%

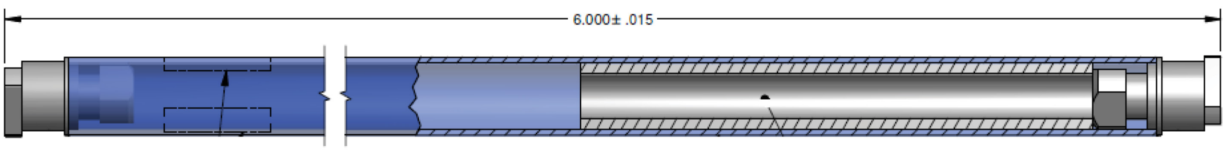

Figure 1. A schematic of the AFC-3A annular rodlet assembly.

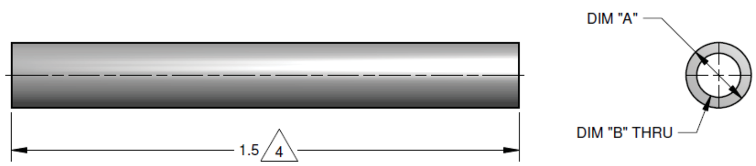

Figure 2. A schematic of the AFC-3 annular fuel slug.

Table 2. Irradiation history of the AFC-3A rodlet 4.

ATR cycle	Cumulative irradiation time, days	LHGR, W/cm
150B	0	313.43
	18	305.14
	31	320.20
151A	53	313.27
	68	332.92
	87	332.86
151B	109.1	315.29
	132.1	

2.3 AFC-3A Rodlet 4 PIE observations

Post irradiation examination of the AFC-3A rodlet revealed microstructural features indicative of the FCCI at the fuel-cladding interface[8]. Presence of large voids was also observed in the same locations. Optical micrographs of the AFC-3A rodlet 4 cross-section including high magnification images emphasizing FCCI are shown in Figure 3 through Figure 5.

Elevated temperature and lanthanide presence are two prerequisites for the FCCI. Fission-gas filled voids at the fuel-cladding interface are expected to impact the peak cladding temperature because low thermal conductivity of the fission gas greatly reduces heat conduction through the voids. These observations and analyses of the PIE images warranted computational investigations described herein.

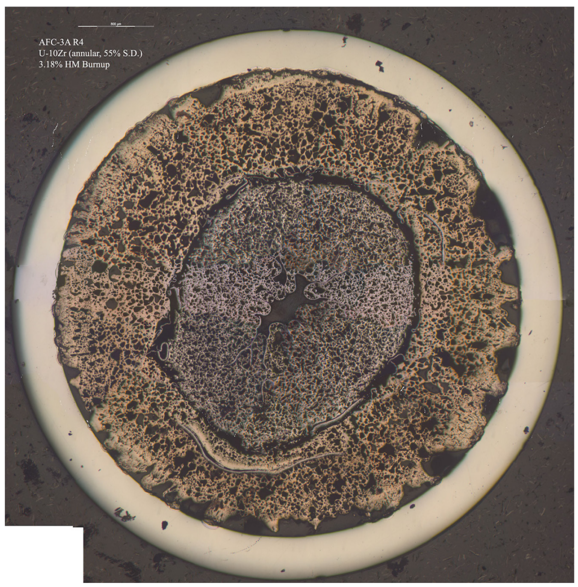

Figure 3. Optical micrograph of the AFC-3A Rodlet 4.

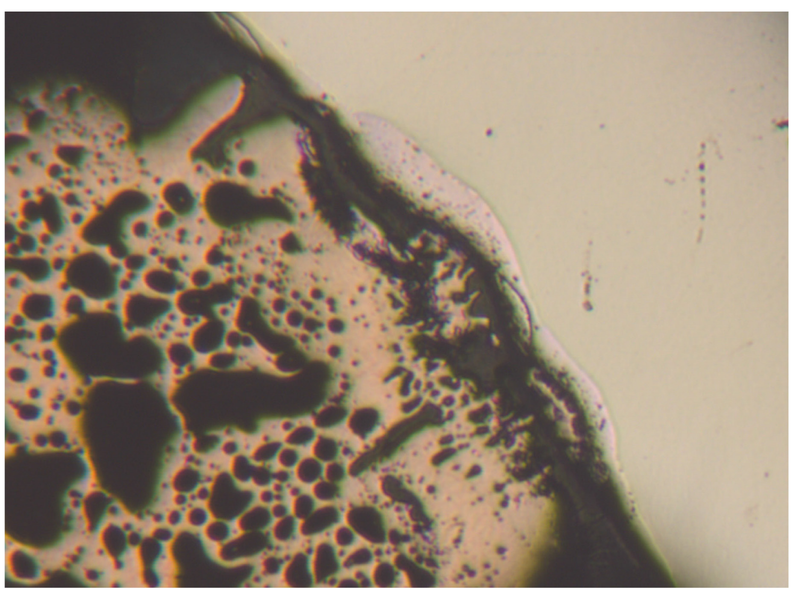

Figure 4. Optical micrograph of the fuel cladding interface showing FCCI.

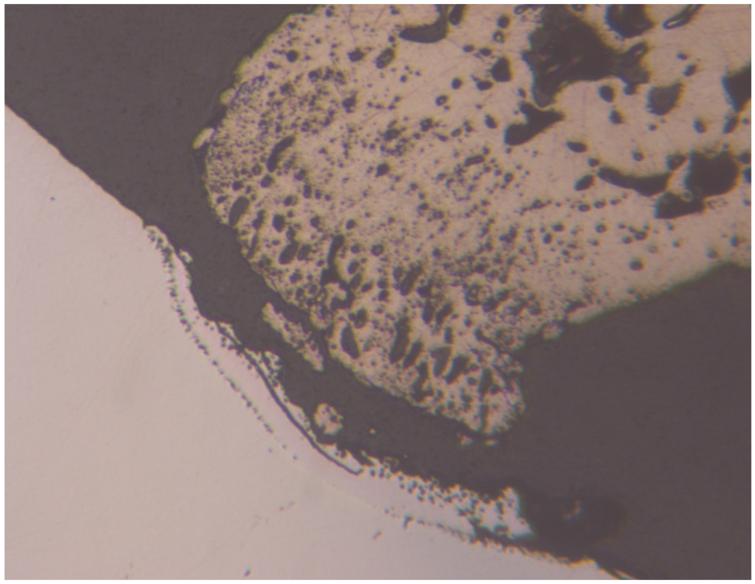

Figure 5. High magnification optical micrograph showing FCCI.

3. PROBLEM STATEMENT

Given the power history, material properties, and rodlet assembly design, investigate possible correlation between the voids and FCCI observed at the fuel cladding interface during PIE examination of AFC-3A rodlet 4.

4. CALCULATION PROCEDURE

Execution of the fuel performance calculation using BISON requires two problem-specific files: (1) a mesh file that contains two-dimensional description of the problem geometry, and (2) an input file that includes information on material properties, power history, boundary conditions, and parameters that control numerical algorithms in BISON.

4.1 Mesh Files

4.1.1 Mesh File for AFC-3A experiment modeling

For modeling the AFC-3A experiment, a 2D mesh of a thin horizontal fuel rod slice was chosen. The choice is based upon the necessity to capture the voids in the process of the thermo mechanical analysis of the rodlet. Using the chosen mesh allowed to focus the analysis on the fuel cross-sections that were subjected to PIE. To evaluate the impact of the voids, a central void having a diameter equal to that reported by the PIE was incorporated into the mesh. The mesh utilized QUAD8 elements shown in Figure 6. The image of the mesh featuring a central void is shown in Figure 7.

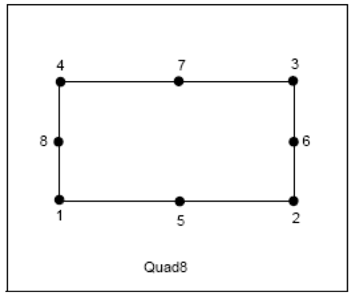

Figure 6. A diagram of the QUAD8 element.

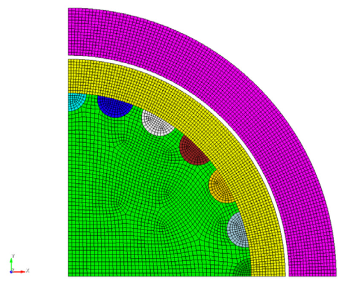

Figure 7. Image of the AFC-3A mesh featuring voids at the fuel cladding interface.

4.2 Input Files

The input files developed to meet the objectives of the present study included the main input files that list behavior models and material properties, and the input files containing power history, coolant conditions, and axial power distribution.

4.3 Computer Platforms and Software Version

BISON is designed to run on a variety of UNIX and Mac-based computer platforms. All the simulations described in this study were run on a MacPro workstation (model name: Mac Pro; model identifier: MacPro 5.1; operating system: Mac OS X 10.6.7; processor name: 6-Core Intel Xeon; processor speed: 2.93 GHz; number of processors: 2; total number of cores: 12), typically using all twelve cores. In all cases, the parallel nature of the calculation is handled completely by the software, with the user simply specifying the number of processors at execution time.

All simulations described in this report were run using BISON with a documented revision number. BISON version control is performed by the Fuel Modeling and Simulation Department of the INL.

4.4 Code Verification

Verification tests for the kernels/operators used in this work were successfully executed after the code was compiled. This implies that the agreement was confirmed between the numerical solution produced by the BISON and an analytical solution for each verification test. BISON verification tests are developed, maintained, and archived by the Fuel Modeling and Simulation Department of the INL. Full verification and validation of BISON has not occurred because the code is in a development stage.

5. RESULTS

5.1 Modeling of the AFC-3A rodlet 4

A temperature contour in the cladding for a case with small voids on the fuel-cladding interface is shown in Figure 8. The most prominent feature of this temperature contour is the hot spots in the location of the fuel-cladding contact. The peak cladding temperature in the hot spots is 30 degrees higher than in the locations that lack contact with the fuel. The appearance of the hot spots is consistent with the FCCI-affected areas of the cladding shown in Figure 4 and Figure 5.

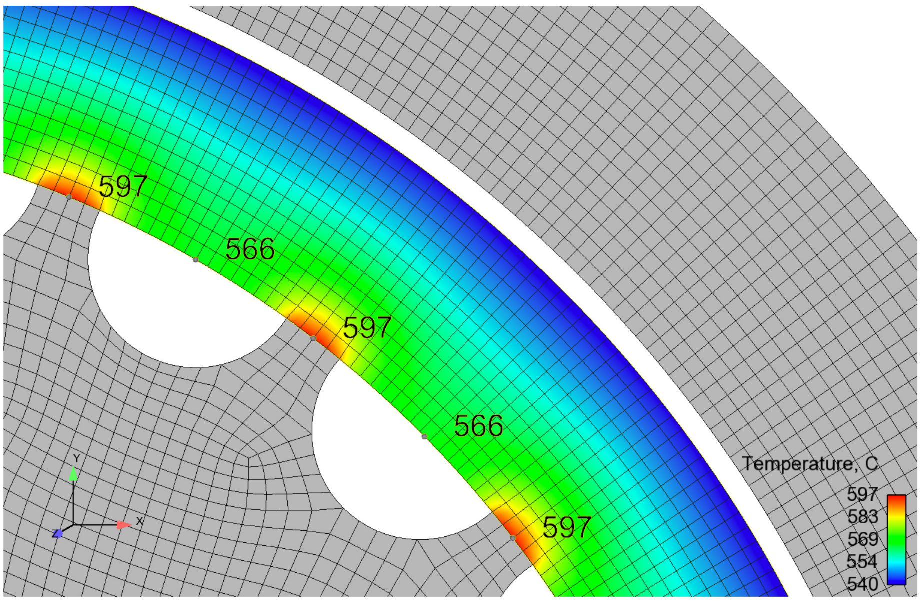

Figure 8. Effect of small voids at the fuel cladding interface on peak cladding temperature.

A temperature contour in the cladding for a case with large voids on the fuel-cladding interface is shown in Figure 9. The plot shows that the peak cladding temperature in the areas of the fuel-cladding contact is 87 degrees greater than in the areas that lack contact with the fuel. These observations prove that any disruptions of the fuel-cladding contact in helium-bonded metallic fuel result in localized hot spots in the cladding.

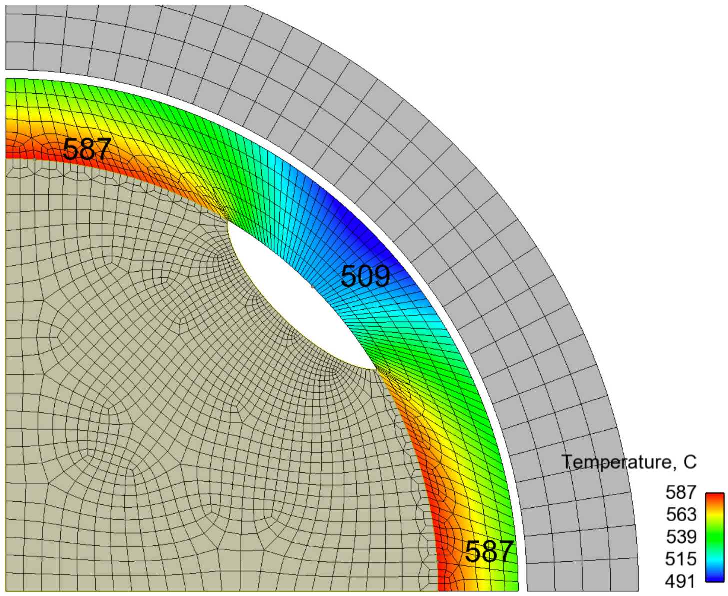

Figure 9. Effect of large voids at the fuel cladding interface on peak cladding temperature.

Disruption of the fuel-cladding contact results in some variation of cladding stress as illustrated in Figure 10. Theoretical investigations provide no link between cladding stress and FCCI. Recognizing that the variation of stress seen in Figure 10 is about 13%, it could be assumed that cladding stress is an unlikely parameter impacting FCCI in the given case.

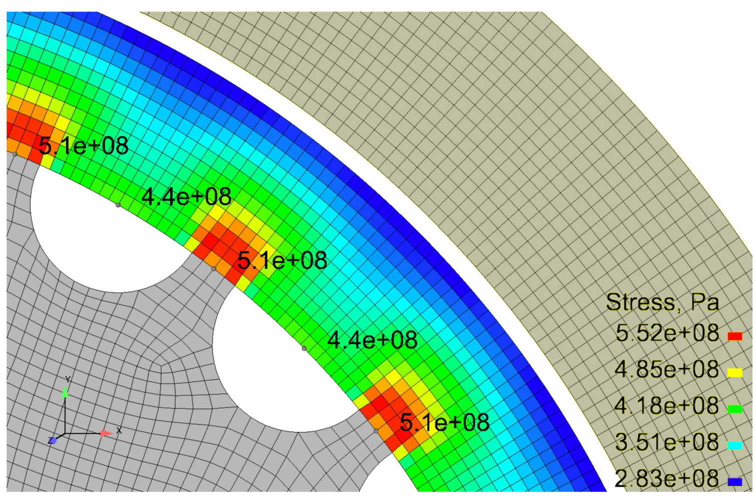

Figure 10. Effect of small voids at the fuel cladding interface on peak cladding stress.

Examination of the creep strain contour in the cladding shown in Figure 11 reveals a significant increase of creep strain. As mentioned above, theoretical investigations provide no link between cladding deformation and FCCI. The calculations presented here show that cladding creep strain in the locations of the fuel-cladding contact is 19 times greater. Because areas of high creep strain coincide with the presumed FCCI-affected areas in the cladding, there may be a correlation between the creep strain in the cladding and FCCI. Since FCCI relies on diffusion, there may be some enhancement of diffusion of species in cladding due to creep.

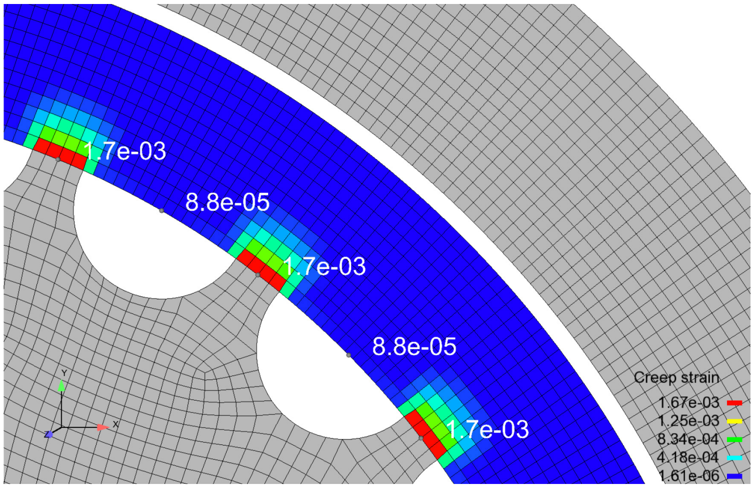

Figure 11. Effect of small voids at the fuel cladding interface on peak cladding strain.

Temperature distribution in the fuel is shown in Figure 12. The key observation is that areas of the fuel that are in contact with the cladding are 142 degrees colder than the areas that are not in contact. Since lanthanides are known to migrate towards the colder areas of the fuel, it is expected that lanthanides would concentrate in the areas where the fuel is in contact with the cladding. Examination of Figure 12 suggests that additional amounts of lanthanides may migrate the along the surfaces of the voids towards the cold spots in the fuel, thus promoting FCCI in those locations.

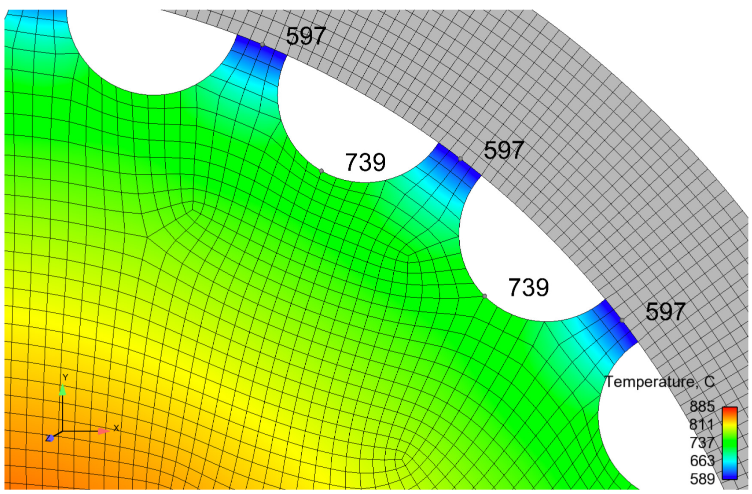

Figure 12. Effect of small voids on the fuel temperature distribution at the fuel cladding interface.

Finally, the case deemed most conservative in terms of impairment of the ability to transport heat from the fuel with the contact between the fuel and the cladding still present was examined. The results are shown in Figure 13 and Figure 14. In this case, the fuel is assumed to be slightly ovalized, so that just two points of contact exist between the fuel and the cladding. As evident from Figure 13, such configuration results in a significantly higher fuel temperature. Yet the cladding temperature is comparable to the cases discussed above. This result caps the peak temperature that can be possible due to irregularities of the fuel cladding contact and establishes a specific temperature envelope for this experiment design.

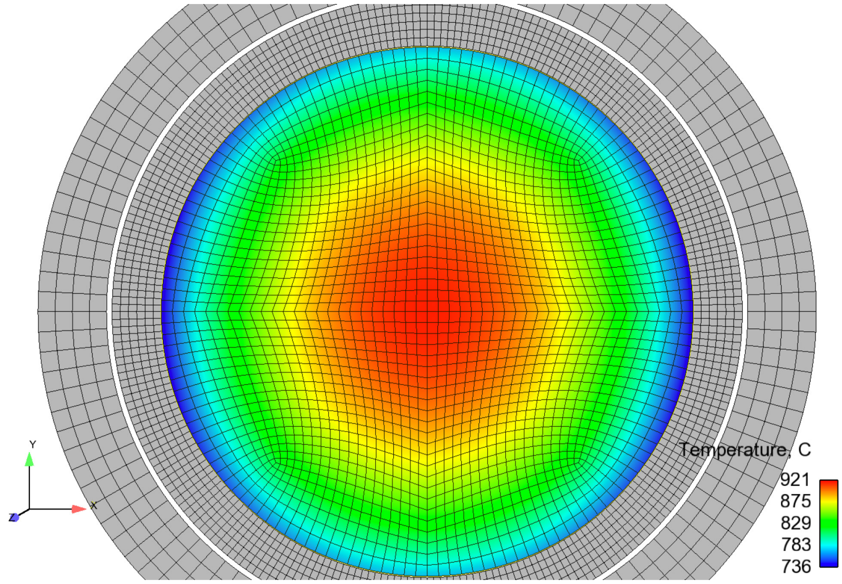

Figure 13. Temperature distribution in the fuel due to a single point of contact between fuel and cladding due to elliptical fuel shape.

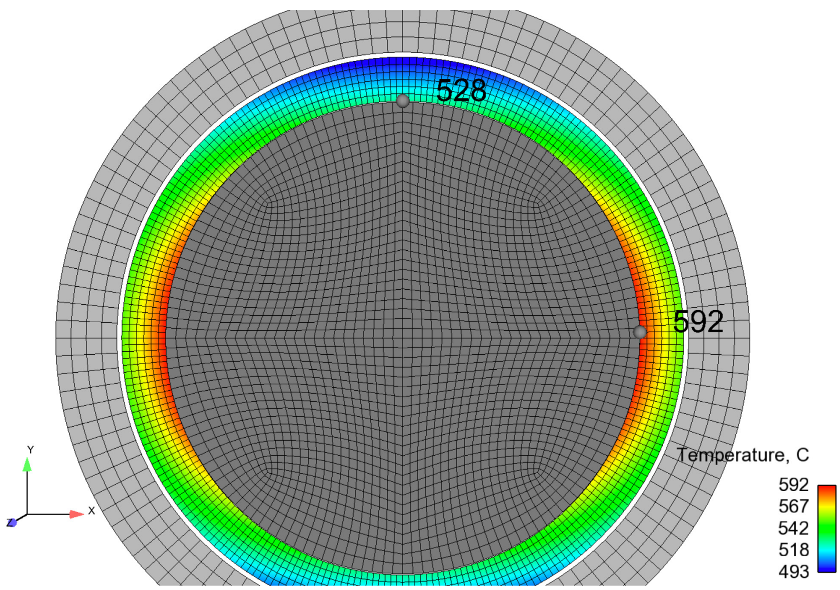

Figure 14. Temperature distribution in the cladding due to a single point of contact between fuel and cladding due to elliptical fuel shape.

Results of the calculations discussed above are summarized in Table 3. As evident from Table 3, irregularities of the fuel-cladding contact do not cause significant increase of the peak cladding temperature as compared to the nominal case where the fuel is in full contact with the cladding. Therefore, it is hypothesized that the nuances of temperature distribution on the fuel such as shown in Figure 12 may have caused lanthanides to diffuse towards the cold spots, which enhanced FCCI. This hypothesis should be verified using qualitative microscopy by comparing lanthanide concentrations between the cold spots in the fuel and the surface of the void.

Table 3. Summary results table

	Nominal	Large void	Single point	Small voids
Peak cladding temperature, C	585	587	591	597
Peak fuel temperature, C	776	806	921	885
Peak cladding stress, Pa	5.62E+08	5.87E+08	2.97E+08	5.52E+08
Peak cladding creep strain	1.14E-03	1.38E-03	4.06E-04	1.67E-03

6. CONCLUSIONS

Observed voids on the fuel cladding surface do not cause significant elevation in cladding temperature. Voids do cause noticeable circumferential temperature gradients in the cladding and in the fuel. Migrating lanthanides could concentrate in the resulting cold spots in the fuel, resulting in the enhancement of FCCI. The Electron Probe Micro-Analyzer (EPMA) or quantitative scanning electron microscope (SEM) can be used to explore the latter claim

This report provides important guidance to the NEAMS Program Fuel Product Line by identifying BISON development needs necessary for adequate simulation of fast reactor fuel. Specifically, it highlights the need for modeling of lanthanide diffusion and FCCI. It also helps to guide PIE activity carried out by the Advanced Fuels Campaign of the FCRD Program.

7. REFERENCES

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