

# **Early User Experience with BISON Fuel Performance Code**

D. M. Perez

August 2012



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**August 2012**

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**Prepared for the  
U.S. Department of Energy  
Office of Nuclear Energy  
Under DOE Idaho Operations Office  
Contract DE-AC07-05ID14517**



**Fuel Modeling and Simulation Department**

# **Early User Experience with BISON Fuel Performance Code**

**INL/EXT-12-26947  
Revision 0**

**August 2012**

## **SUMMARY**

Three Fuel Modeling Exercise II (FUMEX II) LWR fuel irradiation experiments were simulated and analyzed using the fuel performance code BISON to demonstrate code utility for modeling of the LWR fuel performance. Comparisons were made against the BISON results and the experimental data for the three assessment cases. The assessment cases reported within this report include IFA-597.3 Rod 8, Riso AN3 and Riso AN4.



# CONTENTS

SUMMARY .....	iv
1. Introduction .....	1
2. IFA-597.3 Rod 8.....	1
2.1 Problem Overview .....	1
2.2 Problem Reference Documents.....	3
2.3 Problem Description.....	3
2.3.1 Problem Geometry .....	3
2.3.2 Problem Operating Parameters .....	3
2.3.3 Modeling Assumptions and Simplifications .....	5
2.4 Results .....	5
2.4.1 BISON Inputs.....	5
2.4.2 Comparison to Data .....	7
2.4.3 Execution Summary.....	7
3. Riso AN3 .....	8
3.1 Problem Overview .....	8
3.2 Problem Reference Documents.....	9
3.3 Problem Description.....	10
3.3.1 Problem Geometry .....	10
3.3.2 Problem Operating Parameters .....	10
3.3.3 Modeling Assumptions and Simplifications .....	13
3.4 Results .....	13
3.4.1 BISON Inputs.....	13
3.4.2 Comparison to Data .....	15
3.4.3 Execution Summary.....	17
4. Riso AN4 .....	18
4.1 Problem Overview .....	18
4.2 Problem Reference Documents.....	19
4.3 Problem Description.....	20
4.3.1 Problem Geometry .....	20
4.3.2 Problem Operating Parameters .....	20
4.3.3 Modeling Assumptions and Simplifications .....	23
4.4 Results .....	23
4.4.1 BISON Inputs.....	23
4.4.2 Comparison to Data .....	25
4.4.3 Execution Summary.....	26
5. Conclusions .....	27
6. References .....	27
APPENDIX A: IFA-597.3 ROD 8 BISON INPUT FILE .....	28

APPENDIX B: RISO AN3 BISON INPUT FILE .....	40
APPENDIX C: RISO AN4 BISON INPUT FILE .....	54

## FIGURES

Figure 2.1: Base irradiation history for IFA-597.3, carried out at Ringhals BWR.....	2
Figure 2.2: Halden irradiation periods for IFA-597.3 rod 8. ....	2
Figure 2.3: BISON input power history for IFA-597.3 rod 8. ....	4
Figure 2.4: BISON input clad surface temperature as a function of time.....	5
Figure 2.5: 2-D axi-symmetric linear mesh for IFA-597.3 Rod 8 simulation. ....	6
Figure 2.6: BISON fuel centerline temperature comparison to Halden experimental data. ....	7
Figure 3.1: Base irradiation history for fuel segment CB8, carried out at Biblis A PWR.....	8
Figure 3.2: Riso DR3 irradiation period for test AN3 (CB8-2R). ....	9
Figure 3.3: BISON input axial power profile for Riso AN3.....	11
Figure 3.4: BISON input power history for Riso AN3. ....	11
Figure 3.5: BISON input clad surface temperature as a function of time.....	12
Figure 3.6: 2-D axi-symmetric linear mesh for Riso AN3 simulation. Note: the axial aspect ratio has been scaled by 0.05. ....	14
Figure 3.7: BISON fuel centerline temperature comparison to Riso experimental data. ....	15
Figure 3.8: BISON plenum pressure comparison to Riso AN3 experimental data. ....	16
Figure 3.9: BISON total fission gas release comparison to Riso AN3 experimental data. ....	16
Figure 4.1: Base irradiation history for fuel segment CB7, carried out at Biblis A PWR.....	18
Figure 4.2: Riso DR3 irradiation period for test AN4 (CB7-2R). ....	19
Figure 4.3: BISON input axial power profile for Riso AN4.....	21
Figure 4.4: BISON input power history for Riso AN4. ....	21
Figure 4.5: 2-D axi-symmetric linear mesh for Riso AN4 simulation.....	24
Figure 4.6: BISON fuel centerline temperature comparison to Riso AN4 experimental data.....	25
Figure 4.7: BISON plenum pressure comparison to Riso An4 experimental data. ....	26

## TABLES

Table 2.1: IFA-597.3 rod 8 gometeric input parameters.....	3
Table 2.2: IFA-597.3 rod 8 operational input parameters.....	4
Table 2.3: Execution summary for IFA-597.3 rod 8.....	7
Table 3.1: Riso AN3 gometeric input parameters.....	10
Table 3.2: Riso AN3 operational input parameters.....	12
Table 3.3: Execution summary for Riso AN3.....	17
Table 4.1: Riso AN4 gometeric input parameters.....	20
Table 4.2: Riso AN4 operational input parameters.....	22
Table 4.3: Execution summary for Riso AN4.....	26

# Early User Experience with BISON Fuel Performance Code

## 1. Introduction

A series of published LWR fuel irradiation experiments were chosen to demonstrate BISON's utility for fuel performance analysis. The original intent was to examine the capability to predict the fuel centerline temperature, plenum pressure and total fission gas released. It was found that the fission gas release model is only partially functional, therefore, for two of the three cases summarized within this report; the fission gas release was not modeled.

The three assessment cases summarized within this report are IFA-597.3 Rod 8, Riso AN3 and Riso AN4. BISON predicts the fuel centerline temperature well in all three cases; however, the plenum pressure and total fission gas release were not predicted well (see detailed sections below). All of the files and documentation associated with each assessment problem can be found in the MOOSE repository under the `/bison/assessment/` directory.

## 2. IFA-597.3 Rod 8

### 2.1 Problem Overview

The IFA-597.3 Rod 8 experiment utilized a re-fabricated rod from the Ringhals BWR reactor. The mother rod was irradiated at a low average power of  $\sim 16\text{kW/m}$  for approximately 12 years (to a discharge burnup of  $\sim 67\text{ MWd/kgU}$ ). The re-fabricated rod, rod 8, was irradiated in the Halden reactor for approximately 4 months. Figure 2.1 shows the Ringhals base irradiation power history for rod 8 and Figure 2.2 shows the Halden power history for rod 8.

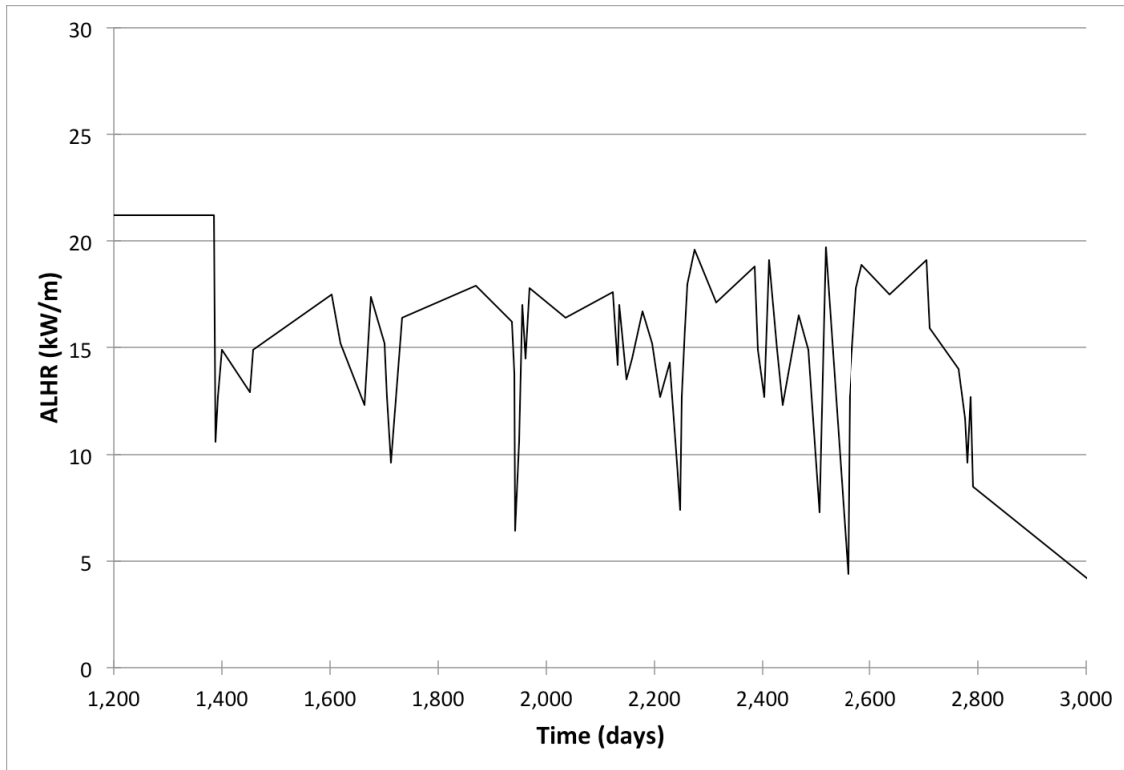


Figure 2.1: Base irradiation history for IFA-597.3, carried out at Ringhals BWR.

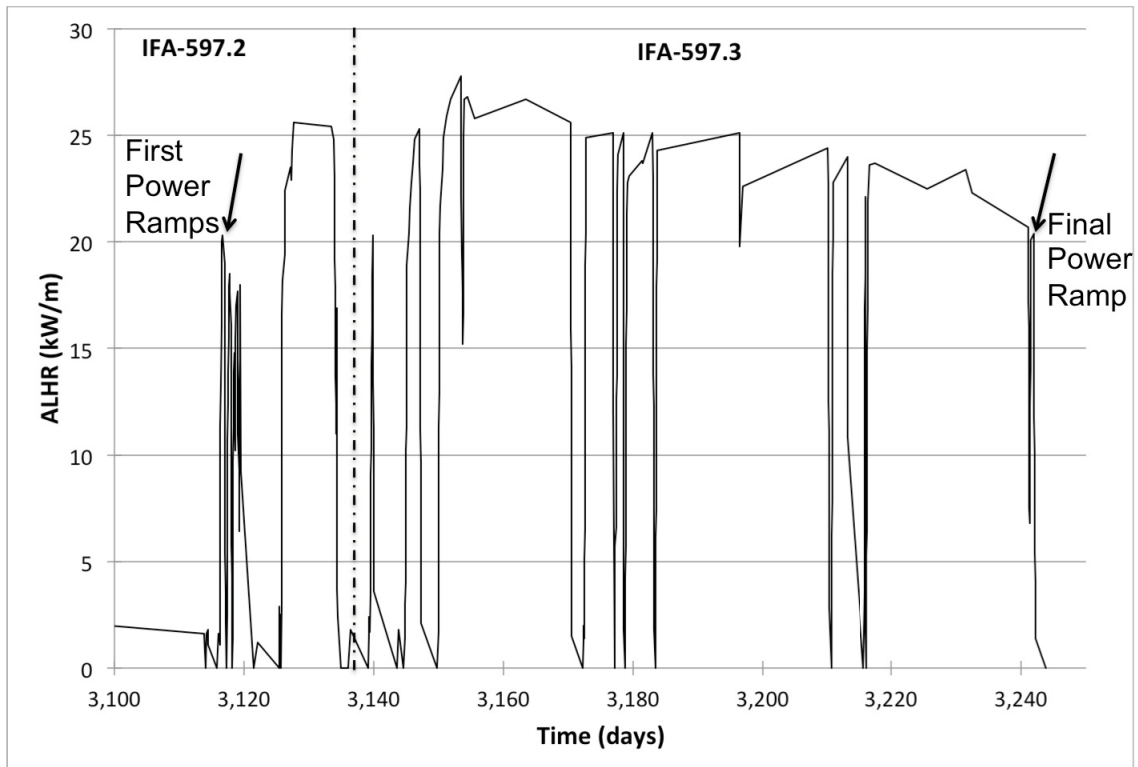


Figure 2.2: Halden irradiation periods for IFA-597.3 rod 8.

## 2.2 Problem Reference Documents

1. PIE of High Burnup BWR Fuel Rod IFA-597.3 Rod 8 [1]
2. The Integral Fuel Rod Behavior Test IFA-597.2: Pre-Characterization and Analysis of the Measurements [2]
3. The Integral Fuel Rod Behavior Test IFA-597.3: Analysis of the Measurements [3]
4. FUMEX II Final Report 2002-2007 [4]

## 2.3 Problem Description

### 2.3.1 Problem Geometry

The geometric input parameters for rod 8 are summarized in Table 2.1.

Table 2.1: IFA-597.3 rod 8 gometric input parameters.

<b>Fuel Rod</b>		
Fuel stack height	cm	35.39
Effective plenum volume	cm <sup>3</sup>	4.58
Mean diametral gap	cm	0.0211
<b>Fuel Pellet</b>		
Outer diameter	cm	1.0439
Inner diameter	cm	0.25
Grain diameter	um	7.83
Surface roughness	um	1.38
Length of hollow section	cm	3.4
<b>Dishing – One end</b>		
Dish diameter	cm	0.5
Dish depth	cm	0.01
Chamfer width	cm	0.07
Chamfer depth	cm	0.02
<b>Cladding – Zr2</b>		
Outer diameter	cm	1.1225
Inner diameter	cm	1.065
Surface roughness	um	1.3

### 2.3.2 Problem Operating Parameters

The power history described in Section 2.1 was modified to smooth out the base irradiation. The power history used as an input parameter for this simulation is shown in Figure 2.3. The other operating parameters are summarized in Table 2.2. The provided measured clad surface temperature as a function of time is shown in Figure 2.4.

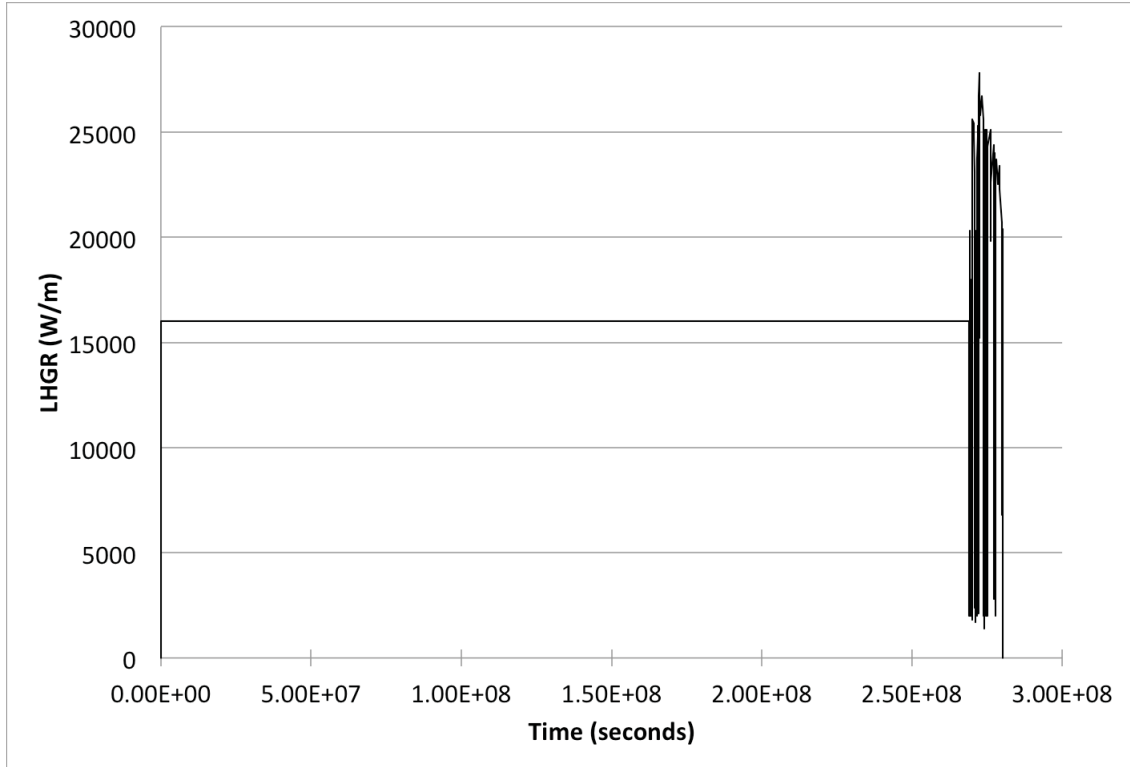


Figure 2.3: BISON input power history for IFA-597.3 rod 8.

Table 2.2: IFA-597.3 rod 8 operational input parameters.

<b>Base Irrdiation</b>		
Plenum pressure	MPa	0.1
Fill gas		He
Coolant inlet temperature	C	286
Coolant pressure	MPa	7.0
Fast neutron flux	n/(cm <sup>2</sup> *s) per (kW/m)	2.3*10 <sup>12</sup>
<b>Power Ramps</b>		
Plenum pressure	Mpa	0.5
Fill gas		He
Coolant inlet temperature	C	232
Coolant pressure	MPa	3.2
Fast neutron flux	n/(cm <sup>2</sup> *s) per (kW/m)	1.6*10 <sup>11</sup>

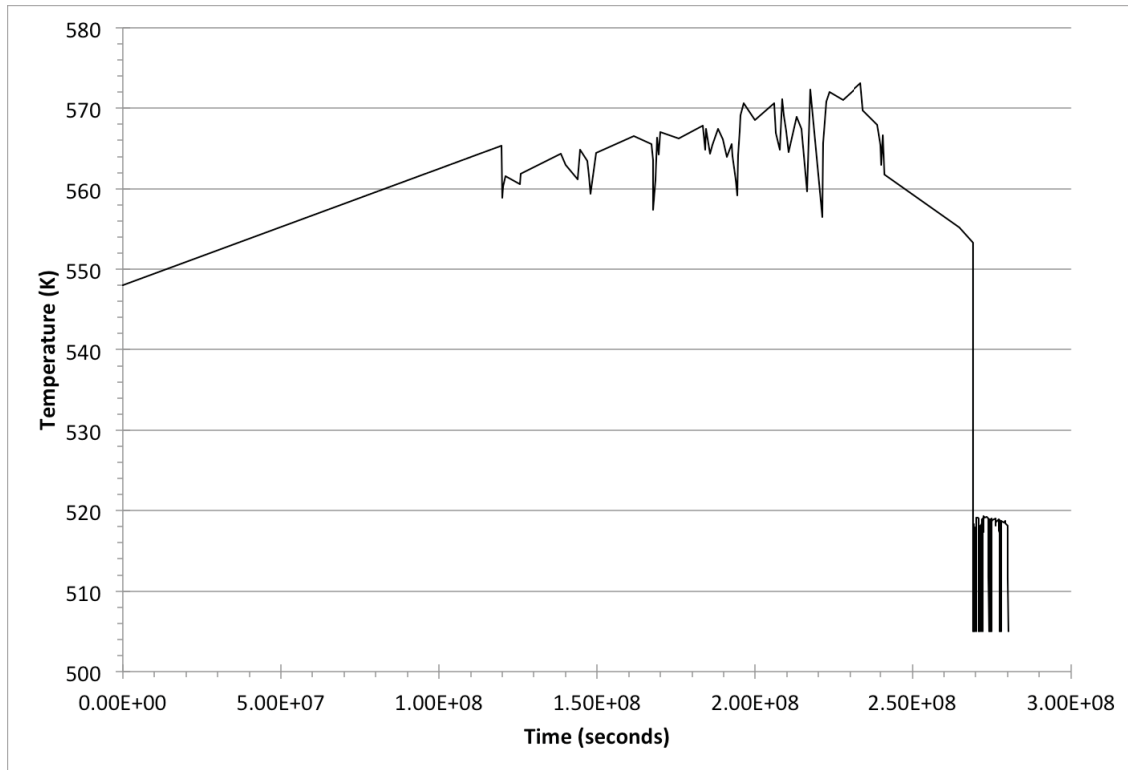


Figure 2.4: BISON input clad surface temperature as a function of time.

### 2.3.3 Modeling Assumptions and Simplifications

1. Fuel rod was modeled as one smeared pellet.
2. Density of fuel is  $10450 \text{ kg/m}^3$ .
3. The thermocouple hole was modeled as a hole through the entire length of the fuel rod.
4. Dish and Chamfer were not modeled.
5. Substituted Zr-2 cladding material with Zr-4 material properties.
6. Fission gas release is zero throughout the simulation.

## 2.4 Results

### 2.4.1 BISON Inputs

A 2-dimensional axi-symmetric linear mesh was used to model the geometry of rod 8. The fuel mesh consisted of 17 axial nodes and 12 radial nodes and the clad mesh consisted of 9 axial nodes and 5 radial nodes, the meshed fuel pellet is shown in Figure 2.5. The input file for this experiment can be found in Appendix A.

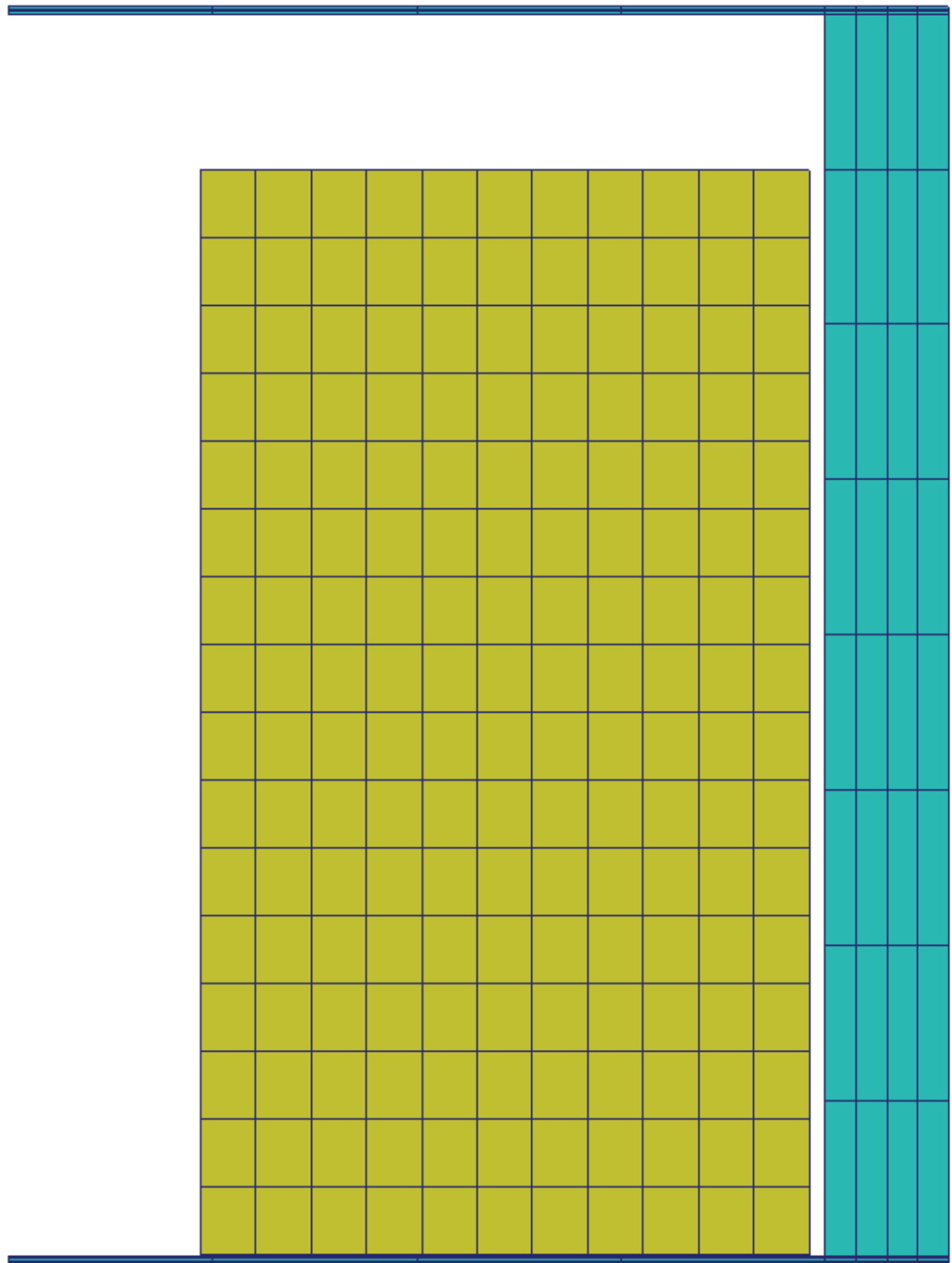


Figure 2.5: 2-D axi-symmetric linear mesh for IFA-597.3 Rod 8 simulation.

## 2.4.2 Comparison to Data

The IFA-597.3 Rod 8 experiment irradiated at Halden is used to demonstrate the codes' capability to capture the fuel centerline temperature and the total fission gas released. At this time BISON is not capable of capturing the total fission gas release during transient analysis, therefore, the only comparison made for this case was the fuel centerline temperature during the first four power ramps and the final power ramps (see Figure 2.1).

BISON predicts the fuel centerline temperature well; however, the temperature falls slightly under the measured experiment values (see Figure 2.6). This is likely due to zero fission gas release modeled for this problem.

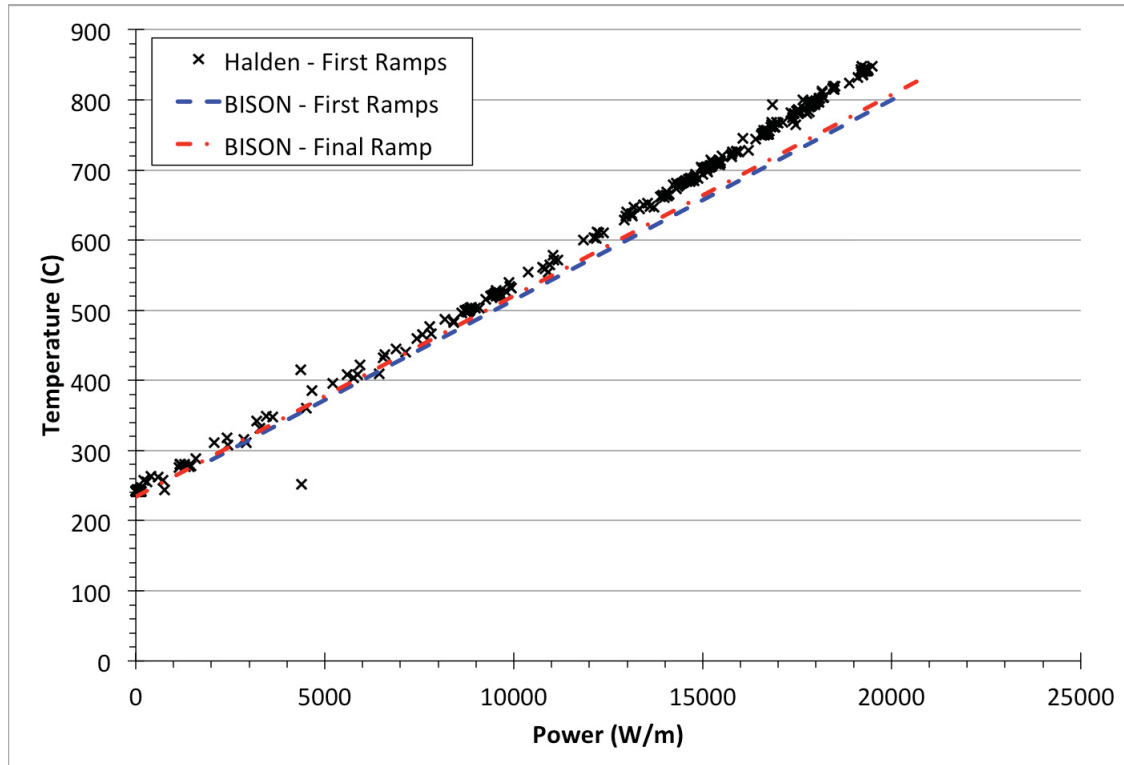


Figure 2.6: BISON fuel centerline temperature comparison to Halden experimental data.

## 2.4.3 Execution Summary

Table 2.3: Execution summary for IFA-597.3 rod 8.

Date	Machine	Number of Processors	Time to Completion	MOOSE Version
20120814	Mac Workstation, OS X	1	0 h, 45 min	12622

### 3. Riso AN3

#### 3.1 Problem Overview

The Riso AN3 experiment utilized a re-fabricated rod from the Biblis A PWR reactor. The mother rod, CB8, was irradiated over four reactor cycles from July 1982 to October 1986 (to an average discharge burnup of  $\sim 41.4$  MWd/kgU). The re-fabricated rod, CB8-2R (test AN4), was irradiated in the Riso R3 water-cooled HP1 rig under PWR conditions for three days from January 8, 1988 to January 11, 1988. Figure 3.1 shows the Biblis base irradiation power history for test AN3 and Figure 3.2 shows the Riso DR3 power history for test AN3.

Test AN3 was fitted with a fuel centerline thermocouple and a pressure transducer. The fuel centerline temperature, fission gas release and rod internal pressure can be used for comparison.

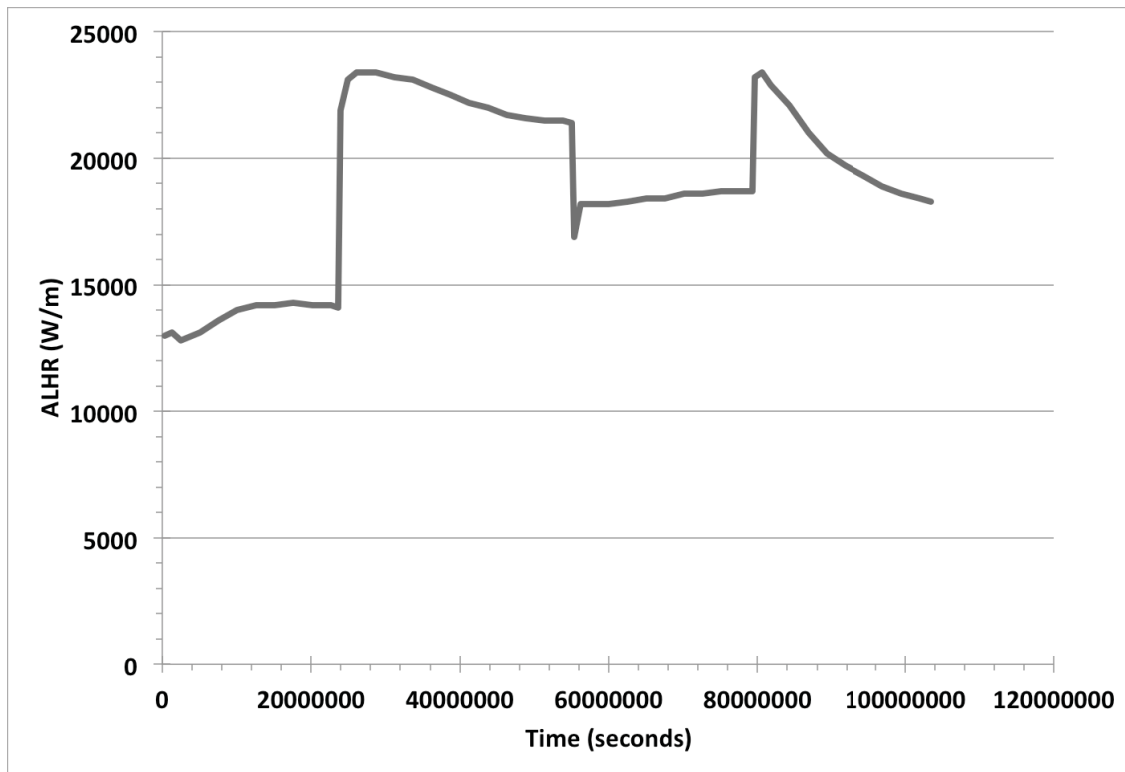


Figure 3.1: Base irradiation history for fuel segment CB8, carried out at Biblis A PWR.

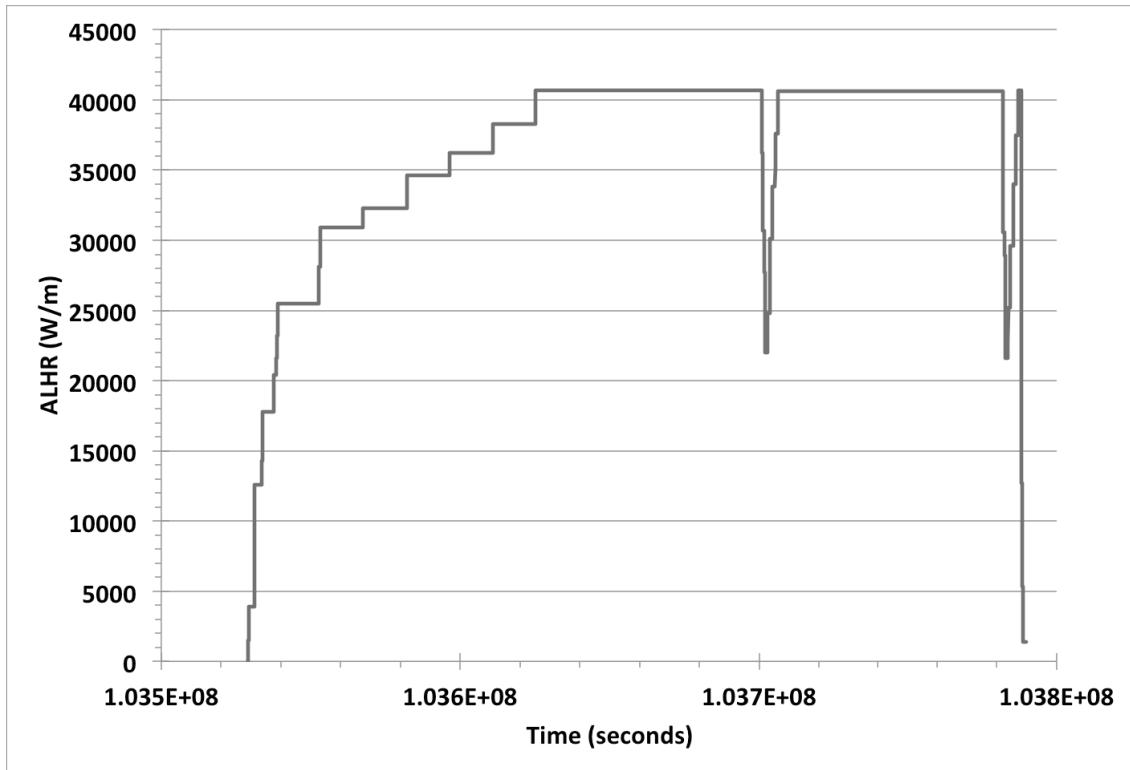


Figure 3.2: Riso DR3 irradiation period for test AN3 (CB8-2R).

### 3.2 Problem Reference Documents

1. The Third Riso Fission Gas Project: Burnup Test AN3 (CB8-2R) [5]
2. FUMEX II Final Report 2002-2007 [4]

### 3.3 Problem Description

#### 3.3.1 Problem Geometry

The geometric input parameters for the Riso AN3 test are summarized in Table 3.1.

Table 3.1: Riso AN3 gometric input parameters.

<b>Fuel Rod</b>		
Fuel stack height	cm	28.6
Plenum height	cm	6.1
Mean diametral gap	cm	0.0205
<b>Fuel Pellet</b>		
Outer diameter	cm	0.9053
Inner diameter	cm	0.25
Grain diameter	um	6.0
Surface roughness	um	1.0
Length of hollow section	cm	4.1
<b>Cladding – Zr2</b>		
Outer diameter	cm	1.081
Inner diameter	cm	0.9258
Surface roughness	um	1.0

#### 3.3.2 Problem Operating Parameters

The power histories described in Section 3.1 were combined together with an axial power profile shown in Figure 3.3. The power history used as an input parameter for this simulation is shown in Figure 3.4. The other operating parameters are summarized in Table 3.2. The provided measured clad surface temperature as a function of time is shown in Figure 3.5.

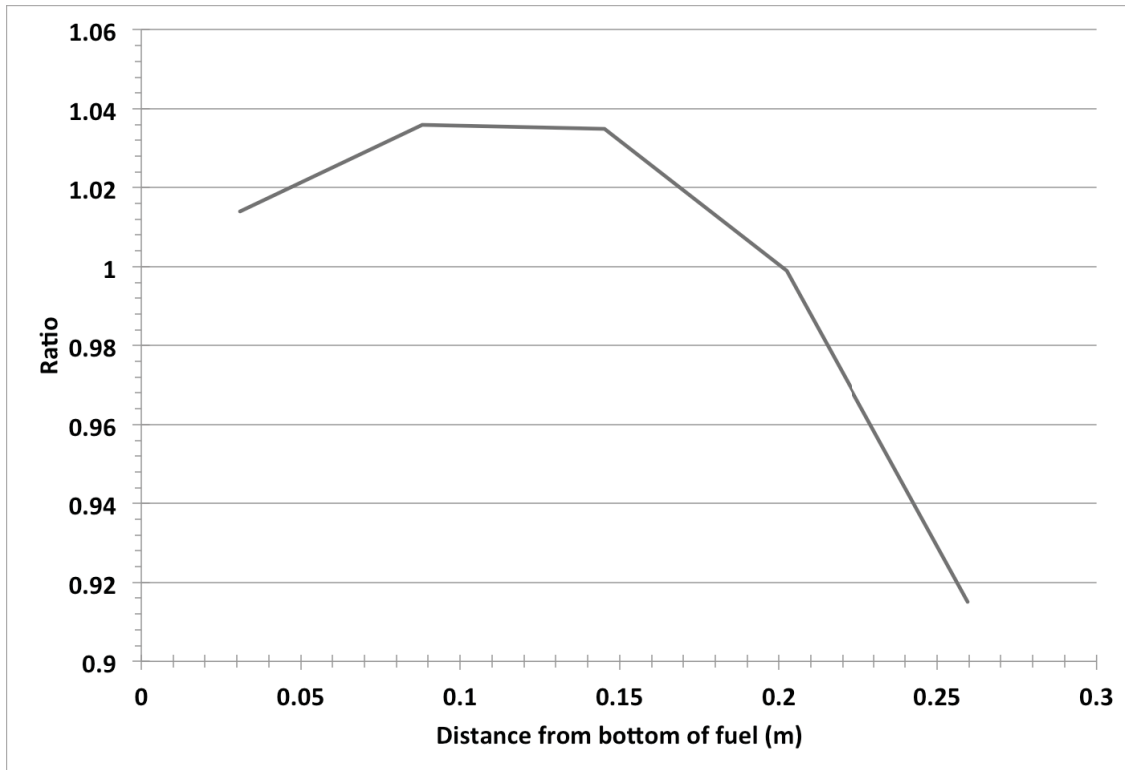


Figure 3.3: BISON input axial power profile for Riso AN3.

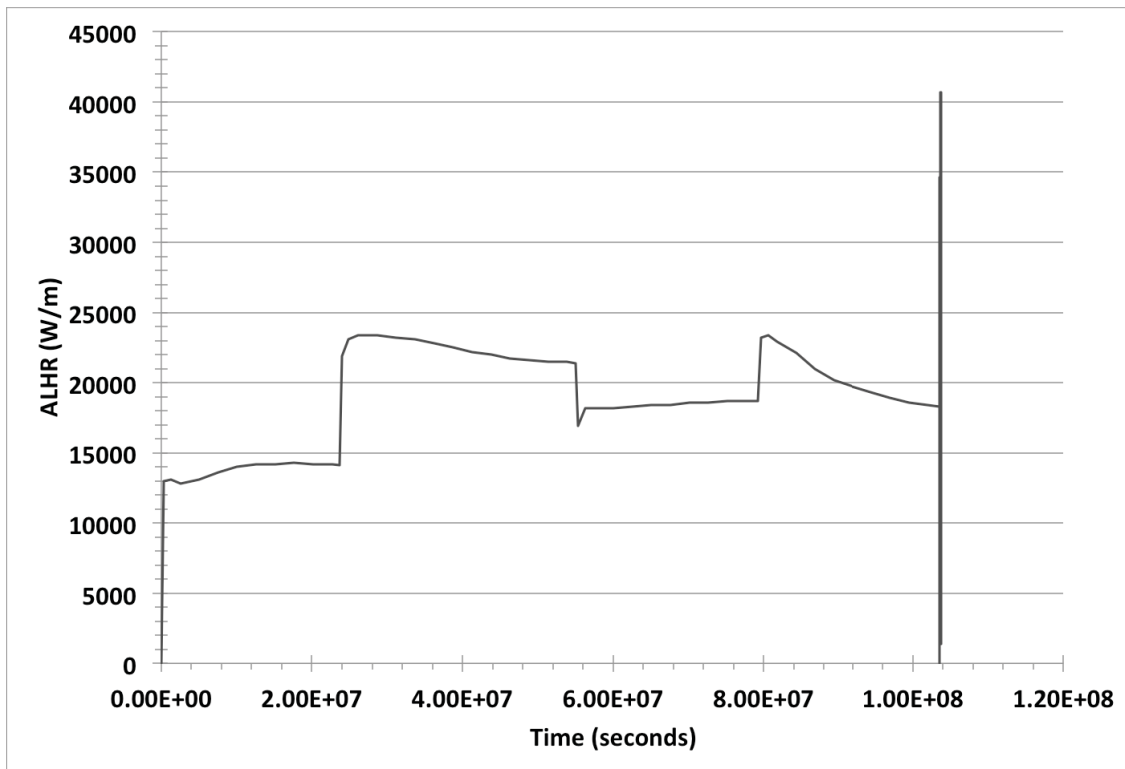


Figure 3.4: BISON input power history for Riso AN3.

Table 3.2: Riso AN3 operational input parameters.

<b>Base Irrdiation</b>		
Plenum pressure	MPa	2.31
Fill gas		He
Coolant inlet temperature	C	287.7
Coolant pressure	MPa	15.52
Fast neutron flux	n/(cm <sup>2</sup> *s) per (kW/m)	3.4*10 <sup>12</sup>
<b>Power Ramps</b>		
Plenum pressure	Mpa	1.57
Fill gas		He
Coolant inlet temperature	C	NA
Coolant pressure	MPa	15.3
Fast neutron flux	n/(cm <sup>2</sup> *s) per (kW/m)	4.0*10 <sup>11</sup>

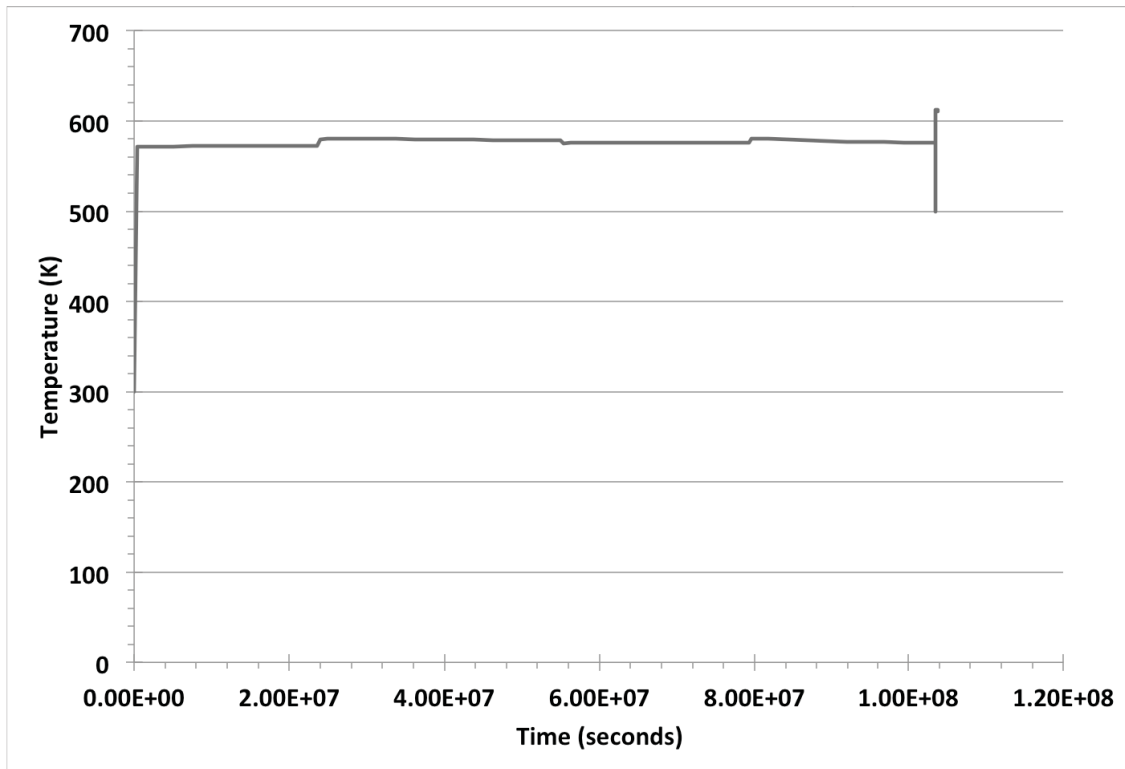


Figure 3.5: BISON input clad surface temperature as a function of time.

### 3.3.3 Modeling Assumptions and Simplifications

1. Fuel rod was modeled as one smeared pellet.
2. Density of fuel is  $10303 \text{ kg/m}^3$ .
3. The plenum height was adjusted such that the plenum volume at the beginning of the bump test was approximately  $7.0 \text{ cm}^3$ .
4. Based off the observations made in the Riso AN4 assessment problem, the maximum grain radius measured during post-irradiation examination (PIE) of  $11.7 \text{ um}$  was used for the simulation.
5. The contact pressure specified for the gap heat transfer calculation was  $35 \text{ MPA}$  (which is approximately the pressure required to plastically deform the clad based on a yield stress of  $230 \text{ MPa}$ ).
6. The clad temperature was assumed to be  $500\text{K}$  during the re-fabrication down time.
7. The total jump distance for the gap heat transfer term was set to  $10 \text{ um}$  [6].
8. The entire fuel stack was shifted up from the bottom of the cad by  $5.1 \text{ mm}$ , which is the height of the insulator pellet at the bottom of the fuel rod.

## 3.4 Results

### 3.4.1 BISON Inputs

A 2-dimensional axi-symmetric linear element mesh was used to model the geometry of the rod used in the AN3 experiment. The fuel was meshed using two fuel pellets. The first pellet was  $4.1 \text{ cm}$  in length with a hole down the center, the second pellet was  $24.5 \text{ cm}$  in length with no hole down the center the first pellet's mesh consisted of 29 axial nodes and 10 radial nodes (for an aspect ratio of 4.07). The second pellet's mesh consisted of 166 axial nodes and 13 radial nodes (for an aspect ratio of 3.93). The clad mesh consisted of 131 axial nodes and 3 radial nodes (see Figure 3.6). The input file for this experiment can be found in Appendix B.

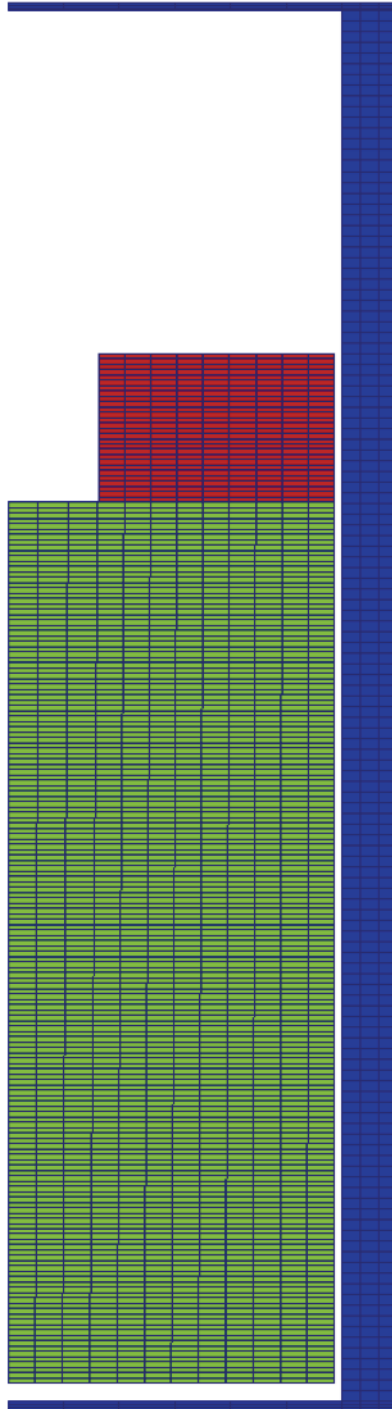


Figure 3.6: 2-D axi-symmetric linear mesh for Riso AN3 simulation. Note: the axial aspect ratio has been scaled by 0.05.

### 3.4.2 Comparison to Data

The Riso AN3 experiment is used to assess the codes' capability to capture the fuel centerline temperature, plenum pressure and the total fission gas released. At this time BISON is not capable of capturing the total fission gas release during transient analysis accurately; however, the total fission gas released model was used for this simulation and therefore is used for comparison.

BISON predicts the fuel centerline temperature well (see Figure 3.7); however, the plenum pressure stays relatively low and fairly constant throughout the bump test (see Figure 3.8). The total fission gas released is shown in Figure 3.9.

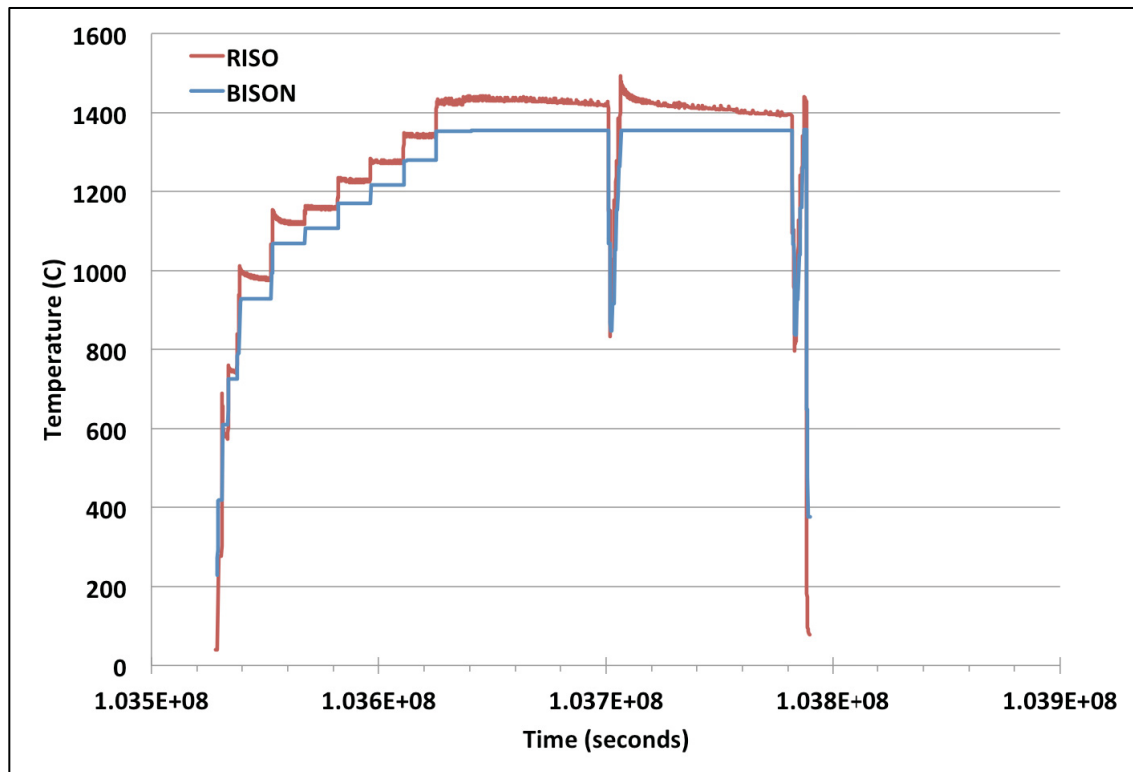


Figure 3.7: BISON fuel centerline temperature comparison to Riso experimental data.

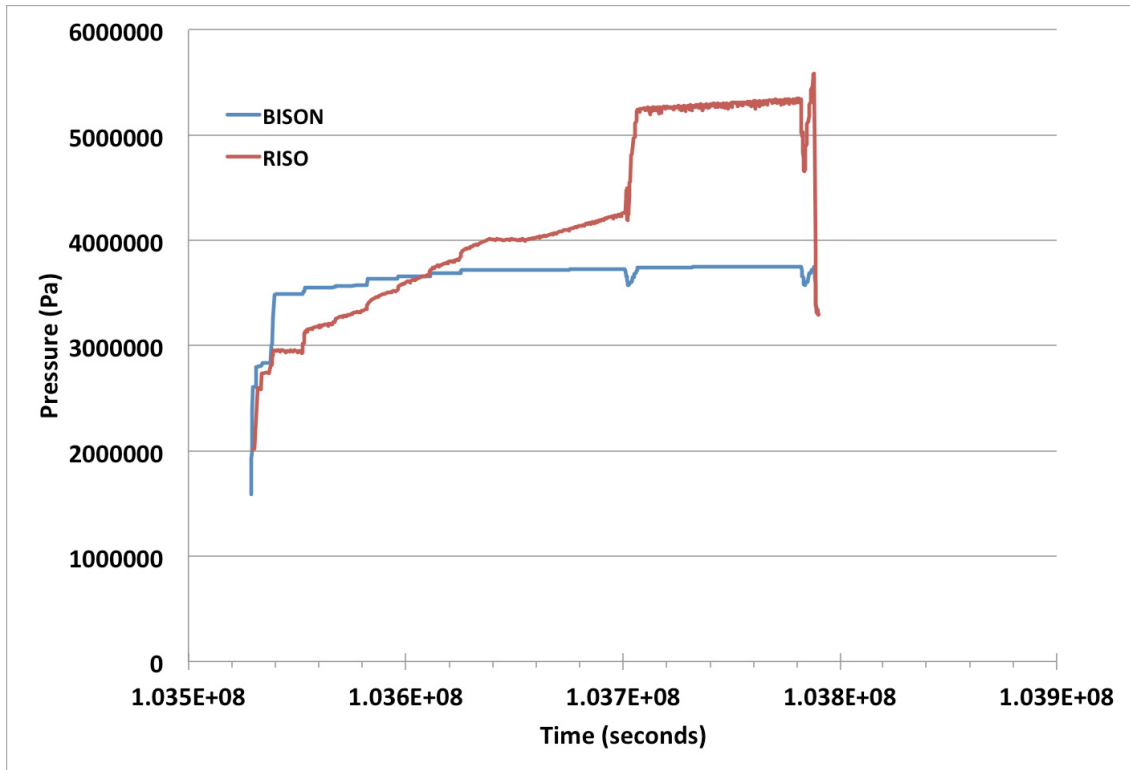


Figure 3.8: BISON plenum pressure comparison to Riso AN3 experimental data.

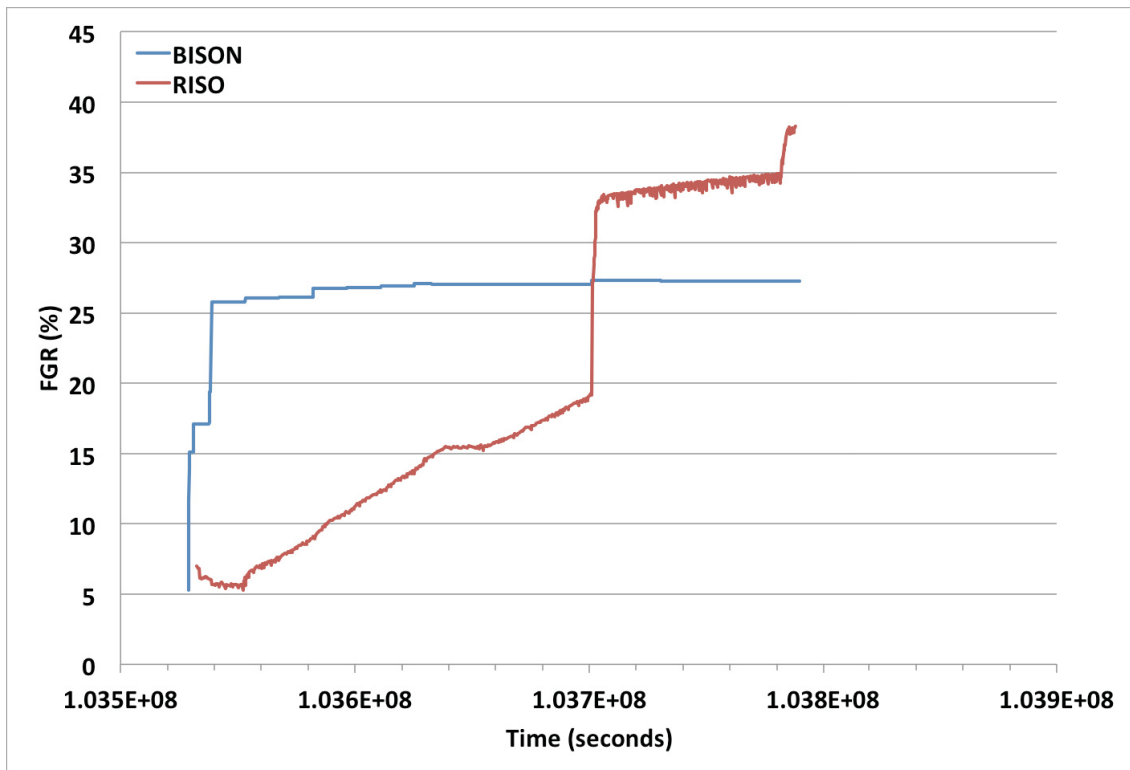


Figure 3.9: BISON total fission gas release comparison to Riso AN3 experimental data.

### 3.4.3 Execution Summary

Table 3.3: Execution summary for Riso AN3.

Date	Machine	Number of Processors	Time to Completion	MOOSE Version
20120622	Mac Workstation, OS X	8	6h, 15min	11266

## 4. Riso AN4

### 4.1 Problem Overview

The Riso AN4 experiment utilized a re-fabricated rod from the Biblis A PWR reactor. The mother rod, CB7, was irradiated over four reactor cycles from July 1982 to October 1986 (to an average discharge burnup of  $\sim 41.4$  MWd/kgU). The re-fabricated rod, CB7-2R (test AN4), was irradiated in the Riso DR3 water-cooled HP1 rig under PWR conditions for three days from December 4, 1987 to December 7, 1987. Figure 4.1 shows the Riso DR3 power history for test AN4.

Test AN4 was fitted with a fuel centerline thermocouple and a pressure transducer. The fuel centerline temperature, fission gas release and rod internal pressure can be used for comparison.

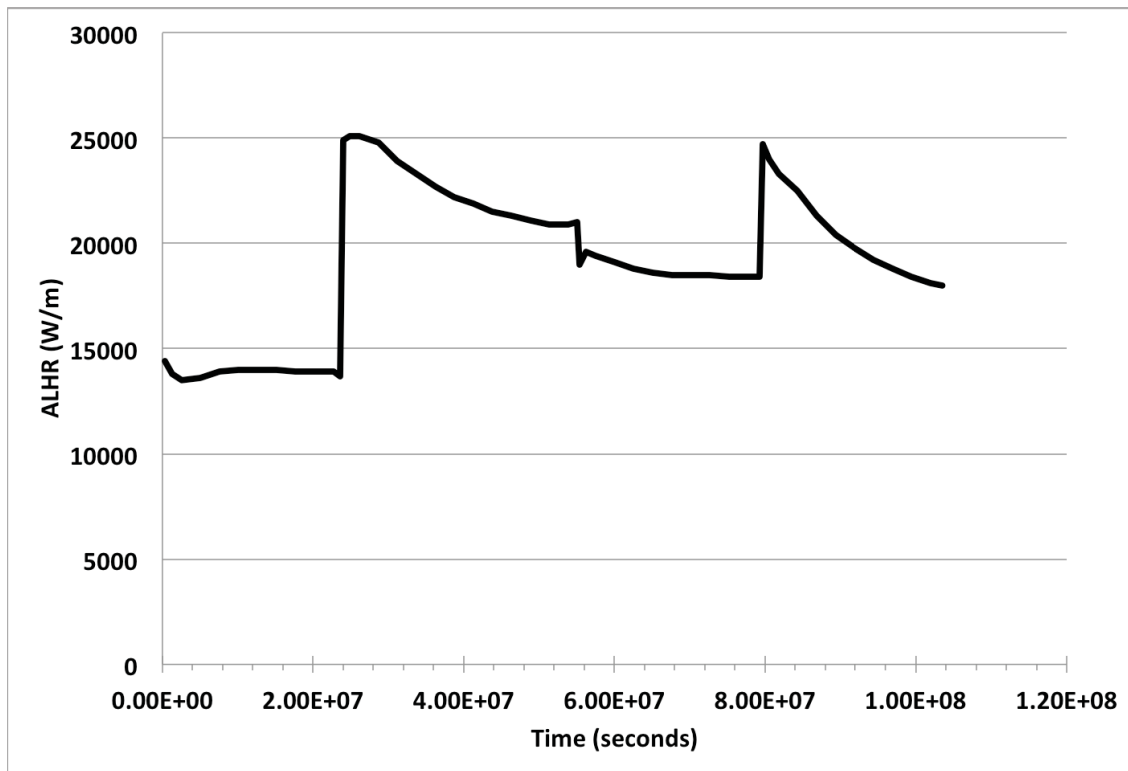


Figure 4.1: Base irradiation history for fuel segment CB7, carried out at Biblis A PWR.

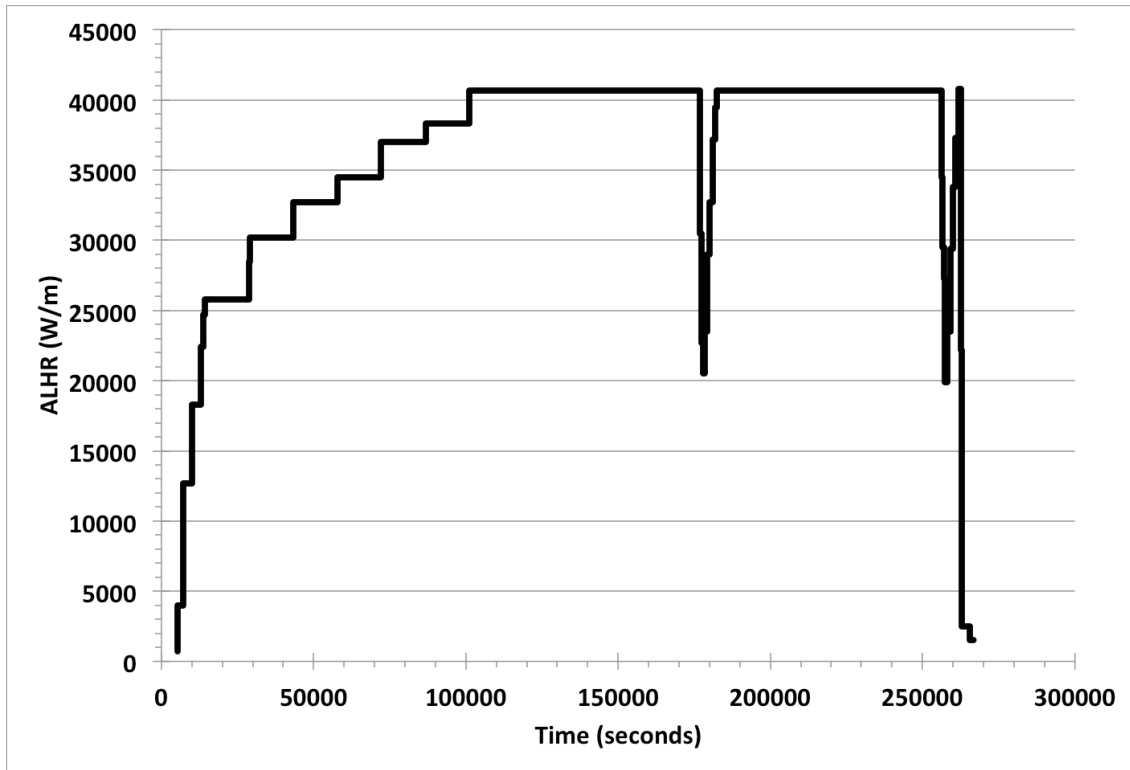


Figure 4.2: Riso DR3 irradiation period for test AN4 (CB7-2R).

## 4.2 Problem Reference Documents

1. The Third Riso Fission Gas Project: Bump Test AN4 (CB7-2R) [7]
2. FUMEX II Final Report 2002-2007 [4]

## 4.3 Problem Description

### 4.3.1 Problem Geometry

The geometric input parameters for the Riso AN4 test are summarized in Table 4.1.

Table 4.1: Riso AN4 gometric input parameters.

<b>Fuel Rod</b>		
Fuel stack height	cm	29.2
Plenum height	cm	3.4
Mean diametral gap	cm	0.0205
<b>Fuel Pellet</b>		
Outer diameter		
Inner diameter		
Grain diameter		
Surface roughness		
Length of hollow section		
<b>Dishing – Both ends</b>		
Dish diameter	cm	0.665
Dish depth	cm	0.013
Chamfer width	cm	0.046
Chamfer depth	cm	0.016
<b>Cladding – Zr2</b>		
Outer diameter	cm	1.081
Inner diameter	cm	0.9258
Surface roughness	um	1.0

### 4.3.2 Problem Operating Parameters

The power histories described in Section 4.1 were combined together with an axial power profile shown in Figure 4.3. The power history used as an input parameter for this simulation is shown in Figure 4.4. The other operating parameters are summarized in Table 4.2.

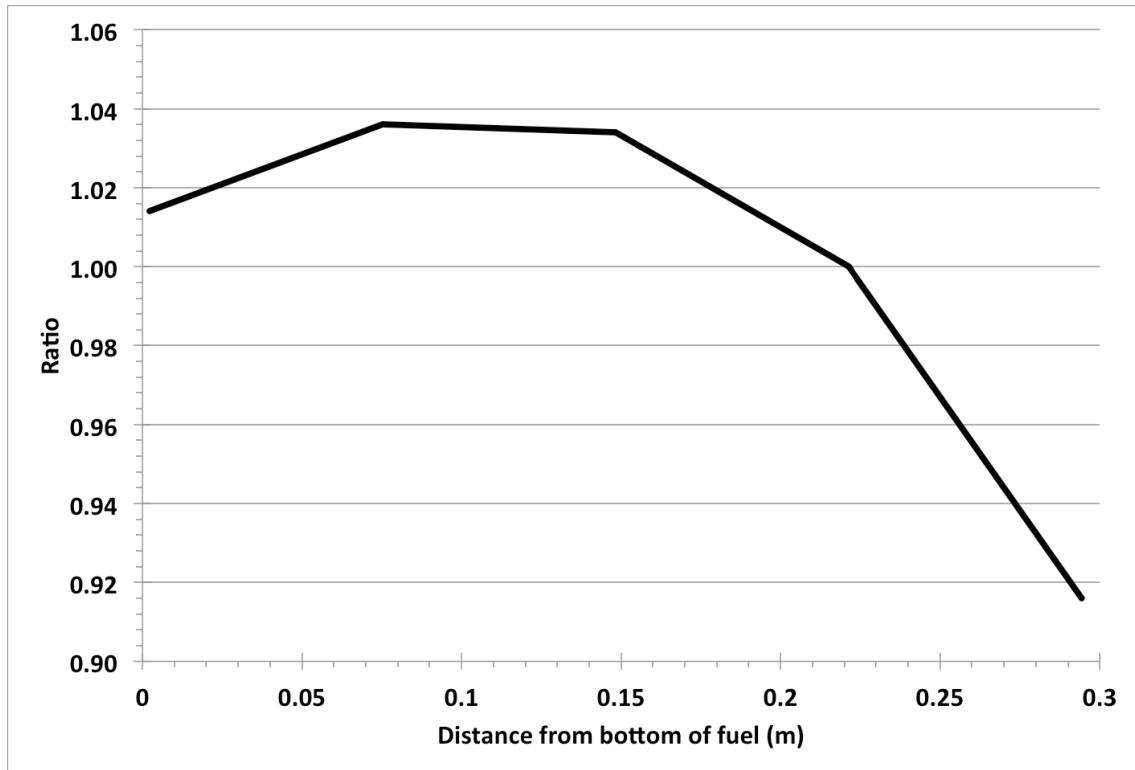


Figure 4.3: BISON input axial power profile for Riso AN4.

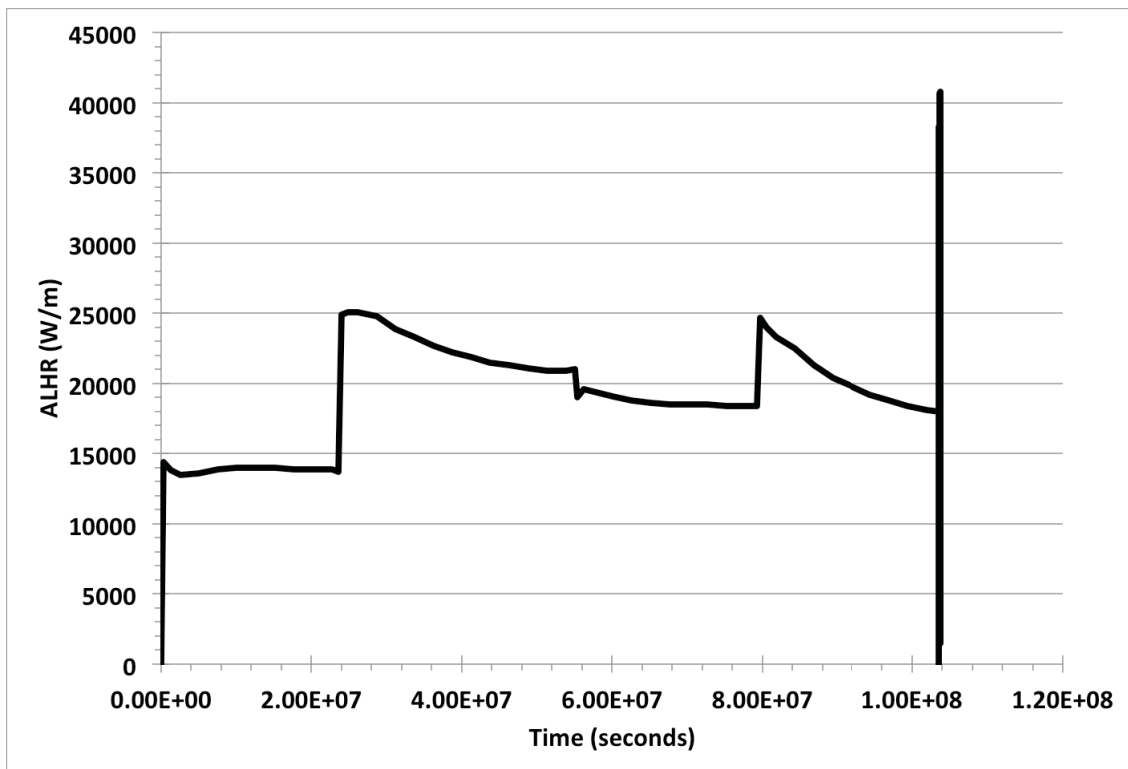


Figure 4.4: BISON input power history for Riso AN4.

Table 4.2: Riso AN4 operational input parameters.

<b>Base Irrdiation</b>		
Plenum pressure	MPa	2.31
Fill gas		He
Coolant inlet temperature	C	287.7
Coolant pressure	MPa	15.52
Fast neutron flux	n/(cm <sup>2</sup> *s) per (kW/m)	3.4*10 <sup>12</sup>
<b>Power Ramps</b>		
Plenum pressure	Mpa	0.1
Fill gas		Xe
Coolant inlet temperature	C	NA
Coolant pressure	MPa	15.3
Fast neutron flux	n/(cm <sup>2</sup> *s) per (kW/m)	4.0*10 <sup>11</sup>

### **4.3.3 Modeling Assumptions and Simplifications**

1. Fuel rod was modeled as one smeared pellet.
2. Density of fuel is 10303 kg/m<sup>3</sup>.
3. The thermocouple hole was modeled as a hole through the entire length of the fuel rod.
4. The maximum grain radius measured during post-irradiation examination (PIE) of 9.8  $\mu\text{m}$  was used for the simulation.
5. The contact pressure specified for the gap heat transfer calculation was 35 MPa (which is approximately the pressure required to plastically deform the clad).

## **4.4 Results**

### **4.4.1 BISON Inputs**

A 2-dimensional axi-symmetric linear element mesh was used to model the geometry of the rod used in the AN4 experiment. The fuel mesh consisted of 141 axial nodes and 9 radial nodes (for an aspect ratio of 5.1); the clad mesh consisted of 113 axial nodes and 5 radial nodes (see Figure 4.5). The input file for this experiment can be found in Appendix C.

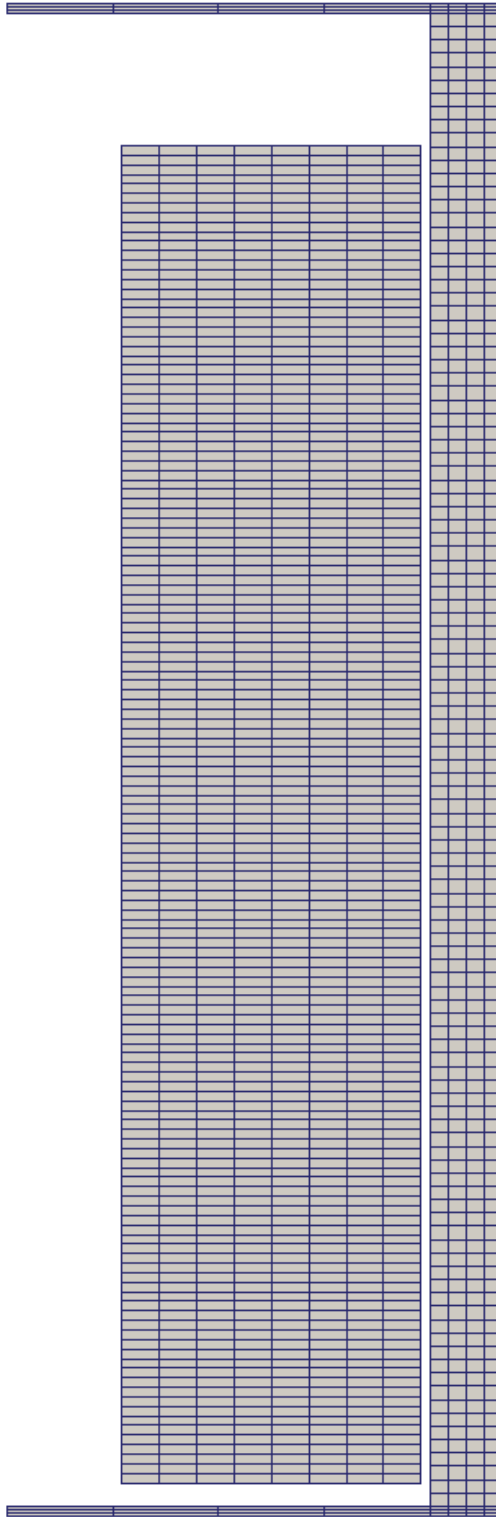


Figure 4.5: 2-D axi-symmetric linear mesh for Riso AN4 simulation.

#### 4.4.2 Comparison to Data

The Riso AN4 experiment is used to demonstrate the codes' capability to capture the fuel centerline temperature, plenum pressure and the total fission gas released. At this time BISON is not capable of capturing the total fission gas released during transient analysis, therefore, the only comparisons made were the fuel centerline temperature and plenum pressure.

BISON predicts the fuel centerline temperature well (see Figure 4.6); however, the plenum pressure stays relatively low and fairly constant throughout the bump test (see Figure 4.7). This is likely because the fission gas release model in the code was turned off for this simulation.

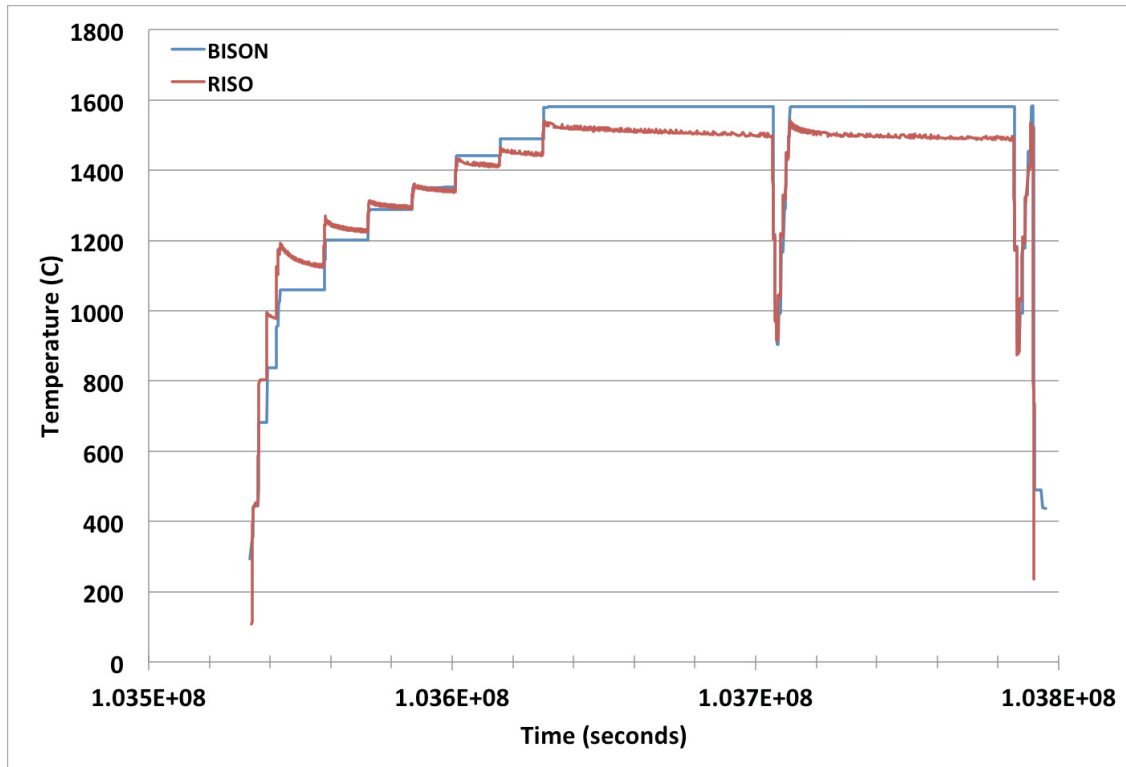


Figure 4.6: BISON fuel centerline temperature comparison to Riso AN4 experimental data.

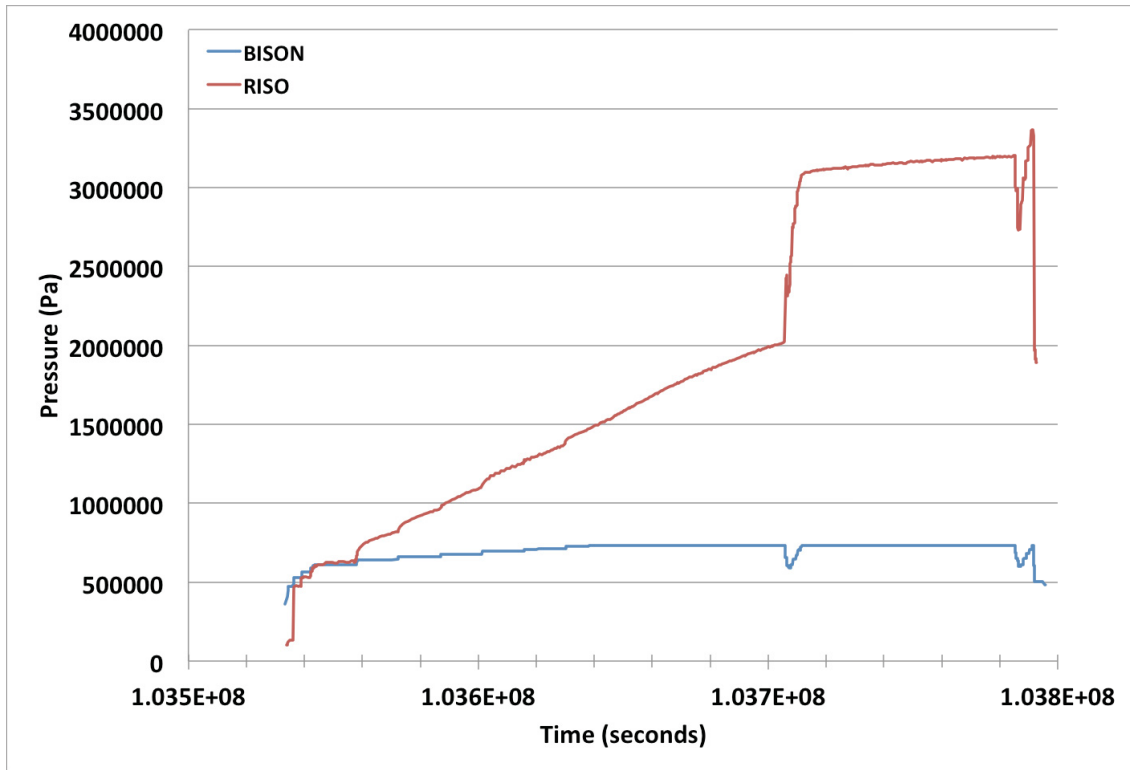


Figure 4.7: BISON plenum pressure comparison to Riso An4 experimental data.

#### 4.4.3 Execution Summary

Table 4.3: Execution summary for Riso AN4.

Date	Machine	Number of Processors	Time to Completion	MOOSE Version
20120614	Mac Workstation, OS X	8	1h, 20min	11181

## 5. Conclusions

Over the course of this work, the models of three LWR fuel irradiation experiments were developed and executed using the fuel performance code BISON. The starting information for model development was attained from publications detailing the experiments. The effort consisted of development of the input and mesh files describing fuel design and materials, development of the power history files, execution of the code, examination of the output files to plot the results summarized in this report, and comparison of the BISON results with the measurements obtained during the experiments.

The highlights of the early user experience are as follows:

- Code installation was performed by the development team. Periodic code updates were performed by the operator.
- BISON input capability encompassed necessary functions to accurately describe fuel design and operating conditions. The power history capability included axial and radial power profiles. Development of the input and mesh files was greatly assisted by the example problems and BISON workshop materials. In some cases, errors in the input file are flagged during code execution attempts.
- BISON execution on a Mac Workstation is a simple process requiring minimum effort from the operator. The execution time varies and can reach several hours.
- Use of the PARAVIEW software to examine the input required initial training. ENSIGHT is a second software option to examine the output file also requires training to use.

As the BISON code is still under development, less emphasis was placed in this study on the agreement of the code results with experimental data. Nevertheless, code predictions of the fuel centerline temperature were found adequate in all three analyzed cases. BISON fission gas release model is only partially functional and was not utilized in two of the three analyzed cases.

## 6. References

1. K. Malen et al., "PIE of high burn-up BWR fuel rod IFA-597.3 rod 8," HRP-356/18, Halden.
2. M. Vankeerbergen, "The Integral Fuel Rod Behaviour Test IFA-597.2: Pre-characterization and Analysis of Measurements," HWR-442, Halden, March 1996.
3. I. Matsson and J. A. Turnbull, "The Integral fuel rod behavior test IFA-597.3: Analysis of the Measurements," HWR-543, Halden, January 1998.
4. "Fuel Modeling at Extended Burnup (FUMEX II): Report of a coordinated research project," IAEA-TECDPC-xxxxx, IAEA, 2002-2007.
5. "The Third Riso Fission Gas Project: Burnup Test AN3 (CB8-2R)," Riso-FGP3-AN3, Riso, September 1990.
6. A. M. Ross and R. L. Stoute, "Heat transfer coefficient between  $\text{UO}_2$  and Zircaloy-2," AECL-1552, Atomic Energy of Canada Limited, 1962.
7. "The Third Riso Fission Gas Project: Burnup Test AN4 (CB7-2R)," Riso-FGP3-AN4, Riso, September 1990.

## APPENDIX A: IFA-597.3 ROD 8 BISON INPUT FILE

```
[GlobalParams]
density = 10450.0
disp_x = disp_x
disp_y = disp_y
order = FIRST
family = LAGRANGE
energy_per_fission = 3.2e-11 # J/fission
[]

# Specify coordinate system type
[Problem]
coord_type = RZ
[]

# Set problem dimension (2d-rz here) and import mesh file
[Mesh]
file = pelletcladsmearmedium1_rz.e
displacements = 'disp_x disp_y'
patch_size = 1000
[]

# Define dependent variables, element order and shape function family, and initial conditions
[Variables]
[/disp_x]
[../]

[/disp_y]
[../]

[/temp]
initial_condition = 300.0 # set initial temp to ambient
[../]
[]

# Define auxillary variables, element order and shape function family
[AuxVariables]
[/fission_rate]
block = 2 # defined for the fuel material (block 2) only
[../]

[/fast_neutron_flux]
block = 1
[../]

[/fast_neutron_fluence]
block = 1
[../]
```

```

[/burnup]
  block = 2
[/]

[/stress_xx]  # stress aux variables are defined for output; this is a way to get integration point
variables to the output file
  order = CONSTANT
  family = MONOMIAL
[/]
[/stress_yy]
  order = CONSTANT
  family = MONOMIAL
[/]
[/stress_zz]
  order = CONSTANT
  family = MONOMIAL
[/]
[/vonmises]
  order = CONSTANT
  family = MONOMIAL
[/]
[/creep_strain_mag]
  order = CONSTANT
  family = MONOMIAL
[/]

[/hydrostatic_stress]
  order = CONSTANT
  family = MONOMIAL
[/]
[]

# Define functions to control power and boundary conditions
[Functions]

[/power_profile]
  type = PiecewiseLinearFile  # reads and interpolates an input file containing rod average linear power
vs time
  yourFileName = IFA-597_3_ROD8_power_history.csv
  scale_factor = 1
[/]

[/axial_peaking_factors]  # reads and interpolates an input file containing the axial power profile vs
time
  type = PiecewiseBilinear
  yourFileName = IFA-597_3_ROD8_axial_peaking.csv
  scale_factor = 1
  axis = 1
[/]

```

```

[./pressure_ramp]      # reads and interpolates input data defining amplitude curve for coolant and
fill gas pressure
    type = PiecewiseLinear
    x = '0 1e4 2.69e8 269247456 280265184'
    y = '0 1 1 0.457 0.457'
[../]

[./flux]               # reads and interpolates input data defining fast neutron flux
    type = PiecewiseLinearFile
    yourFileName = IFA-597_3_ROD8_fast_neutron_flux.csv
[../]

[./clad_temp_bc]
    type = PiecewiseLinearFile
    yourFileName = IFA-597_3_ROD8_clad_bc.csv
    format = columns
[../]

[./q]
    type = PiecewiseLinearFile # reads and interpolates an input file containing rod average linear power
vs time
    yourFileName = IFA-597_3_ROD8_power_history.csv
[../]

[]

# Specify that we need solid mechanics (divergence of stress)
[SolidMechanics]
[./solid]
    disp_r = disp_x
    disp_z = disp_y
    temp = temp
[../]
[]

# Define kernels for the various terms in the PDE system (in all cases here, the axisymmetric (RZ)
version is specified)
[Kernels]

[./gravity]            # body force term in stress equilibrium equation
    type = Gravity
    variable = disp_y
    value = -9.81
[../]

[./heat]              # gradient term in heat conduction equation
    type = HeatConduction
    variable = temp
[../]

```

```

[./heat_ie]    # time term in heat conduction equation
  type = HeatConductionImplicitEuler
  variable = temp
[../]

[./heat_source] # source term in heat conduction equation
  type = NeutronHeatSource
  variable = temp
  block = 2          # fission rate applied to the fuel (block 2) only
  fission_rate = fission_rate # coupling to the fission_rate aux variable
[../]
[]

# Define auxilliary kernels for each of the aux variables
[AuxKernels]
[./fissionrate]    # computes the volumetric fission rate as a function of time and space
  type = FissionRateAuxLWR
  variable = fission_rate
  block = 2
  function1 = power_profile      # using the power function defined above
  function2 = axial_peaking_factors # using the axial power profile function defined above
  pellet_diameter = 0.010439
# pellet_inner_diameter = 0.0 # ignore T/C hole at top of fuel stack
  pellet_inner_diameter = 0.0025
  execute_on = timestep_begin
[../]

[./fast_neutron_flux]
  type = FastNeutronFluxAux
  variable = fast_neutron_flux
  block = 1
  axial_power_profile = axial_peaking_factors
  function = flux
  factor = 3.728e17
  execute_on = timestep_begin
[../]

[./fast_neutron_fluence]
  type = FastNeutronFluenceAux
  variable = fast_neutron_fluence
  fast_neutron_flux = fast_neutron_flux
  execute_on = timestep_begin
[../]

[./burnup]      # computes burnup as a function of time and space
  type = BurnupAux
  variable = burnup
  block = 2
  fission_rate = fission_rate      # coupling to the fission rate aux variable
  molecular_weight = 0.270

```

```

    execute_on = timestep_begin
[../]

[/hydrostatic_stress]
    block = 2
    type = MaterialTensorAux
    tensor = stress
    variable = hydrostatic_stress
    quantity = hydrostatic
    execute_on = timestep
[../]

[/stress_xx]          # computes stress components for output
    type = MaterialTensorAux
    tensor = stress
    variable = stress_xx
    index = 0
    execute_on = timestep # for efficiency, only compute at the end of a timestep
[../]
[/stress_yy]
    type = MaterialTensorAux
    tensor = stress
    variable = stress_yy
    index = 1
    execute_on = timestep
[../]
[/stress_zz]
    type = MaterialTensorAux
    tensor = stress
    variable = stress_zz
    index = 2
    execute_on = timestep
[../]
[/vonmises]
    type = MaterialTensorAux
    tensor = stress
    variable = vonmises
    quantity = vonmises
    execute_on = timestep
[../]
[/creep_strain_mag]
    type = MaterialTensorAux
    tensor = creep_strain
    variable = creep_strain_mag
    quantity = plasticstrainmag
    execute_on = timestep
[../]

[]

```

```

# Define mechanical contact between the fuel (sideset=10) and the clad (sideset=5)

```

```

[Contact]
[./pellet_clad_mechanical]
  master = 5
  slave = 10
  disp_x = disp_x
  disp_y = disp_y
  penalty = 1e7
  model = experimental
# model = glued      # surfaces are tied upon contact
[../]
[]

# Define thermal contact between the fuel (sideset=10) and the clad (sideset=5)
[ThermalContact]
[./thermal_contact]
  type = GapHeatTransferLWR
  variable = temp
  master = 5
  slave = 10
  initial_moles = initial_moles    # coupling to a postprocessor which supplies the initial plenum/gap
gas mass
  gas_released = fis_gas_released  # coupling to a postprocessor which supplies the fission gas addition
  jumpdistance_clad = 5e-6
  jumpdistance_fuel = 5e-6
  roughness_clad = 1.3e-6
  roughness_fuel = 1.38e-6
  initial_gas_fractions = '1 0 0 0 0 0'
  refab_time = 269247456
  refab_gas_fractions = '1 0 0 0 0 0'
[../]
[]

# Define boundary conditions
[BCs]

# pin pellets and clad along axis of symmetry (y)
[./no_x_all]
  type = DirichletBC
  variable = disp_x
  boundary = 12
  value = 0.0
[../]

# pin clad bottom in the axial direction (y)
[./no_y_clad_bottom]
  type = DirichletBC
  variable = disp_y
  boundary = '1'
  value = 0.0
[../]

```

```

# pin fuel bottom in the axial direction (y)
[./no_y_fuel_bottom]
  type = DirichletBC
  variable = disp_y
  boundary = '1020'
  value = 0.0
[../]

[./temp]
  type = FunctionDirichletBC
  boundary = '1 2 3'
  variable = temp
  function = clad_temp_bc
[../]

[./Pressure]
# apply coolant pressure on clad outer walls
[./coolantPressure]
  boundary = '1 2 3'
  factor = 7.0e6 #changes to 3.2e6 after 59 MWd/kgUO2
  function = pressure_ramp # use the pressure_ramp function defined above
[../]
[../]

[./PlenumPressure]
# apply plenum pressure on clad inner walls and pellet surfaces
[./plenumPressure]
  boundary = 9
  initial_pressure = 1.0e5 #changes to 5e5 after 59 MWd/kgUO2
  startup_time = 1.0e4
  R = 8.3143
  output_initial_moles = initial_moles # coupling to post processor to get initial fill gas mass
  temperature = ave_temp_interior # coupling to post processor to get gas temperature
approximation
  volume = gas_volume # coupling to post processor to get gas volume
  material_input = fis_gas_released # coupling to post processor to get fission gas added
  output = plenum_pressure # coupling to post processor to output plenum/gap pressure
  refab_time = 269247456
  refab_pressure = 5e5
  refab_temperature = 293
  refab_volume = 6e-6
[../]
[../]

[ ]

# Define material behavior models and input material property data
[Materials]
[./density_clad]
  type = Density
  block = 1

```

```

    density = 6551.0
[../]

[./density_fuel]
    type = Density
    block = 2
[../]

[./fuel_thermal]          # temperature and burnup dependent thermal properties of UO2 (bison
kernel)
    type = ThermalUO2
    block = 2
    temp = temp
    burnup = burnup
[../]

[./fuel_solid_mechanics_swelling] # free expansion strains (swelling and densification) for UO2
(bison kernel)
    type = VSwellingUO2
    block = 2
    temp = temp
    burnup = burnup
[../]

[./fuel_creep]            # thermal and irradiation creep for UO2 (bison kernel)
    type = CreepUO2
    block = 2
    disp_r = disp_x
    disp_z = disp_y
    temp = temp
    fission_rate = fission_rate
    youngs_modulus = 2.e11
    poissons_ratio = .345
    thermal_expansion = 10e-6
    grain_radius = 3.915e-6
    oxy_to_metal_ratio = 2.0
    max_its = 10
    output_iteration_info = false
[../]

[./fuel_relocation]
    type = RelocationUO2
    block = 2
    burnup = burnup
    diameter = 0.010439 #Fuel pellet diameter in m
    q = q
    gap = 2.11e-4 #diametral gap in m
    burnup_relocation_stop = 0.051
[../]

[./clad_thermal]          # general thermal property input (elk kernel)

```

```

type = HeatConductionMaterial
block = 1
thermal_conductivity = 16.0
specific_heat = 330.0
[../]

[/clad_solid_mechanics]          # thermoelasticity and thermal and irradiation creep for Zr4 (bison
kernel)
type = ThermalIrradiationCreepZr4
block = 1
disp_r = disp_x
disp_z = disp_y
temp = temp
fast_neutron_flux = fast_neutron_flux
youngs_modulus = 7.5e10
poissons_ratio = 0.3
thermal_expansion = 5.0e-6
max_its = 5000
output_iteration_info = false
# output = max_creep_its
[../]

[/clad_irrgrowth]
type = IrradiationGrowthZr4
block = 1
fast_neutron_fluence = fast_neutron_fluence
[../]

[/fission_gas_release]          # Forsberg-Massih fission gas release mode
type = ForMas
block = 2
temp = temp
fission_rate = fission_rate      # coupling to fission_rate aux variable
grain_radius = 3.915e-6
plenum_pressure = plenum_pressure
hydrostatic_stress = hydrostatic_stress
calibration_factor = 100
[../]
[]

[Dampers]
[/limitT]
type = MaxIncrement
max_increment = 100.0
variable = temp
[../]
[]

[Executioner]
type = Transient

```

```

# PETSC options
petsc_options = '-snes_mf_operator -ksp_monitor -ksp_gmres_modifiedgramschmidt'
petsc_options_iname = '-snes_type -snes_ls -ksp_gmres_restart -pc_type -pc_composite_pcs -
sub_0_pc_hypre_type -sub_0_pc_hypre_boomeramg_max_iter -
sub_0_pc_hypre_boomeramg_grid_sweeps_all -sub_1_sub_pc_type -pc_composite_type -ksp_type -
mat_mffd_type'
petsc_options_value = 'ls      basic 201      composite hypre,asm      boomeramg      2
2      lu      multiplicative  fgmres  ds'

# controls for linear iterations
l_max_its = 100
l_tol = 8e-3

# controls for nonlinear iterations
nl_max_its = 15
nl_rel_tol = 1e-4
nl_abs_tol = 1e-10

# time control
start_time = 0.0
dt = 2.0e2
end_time = 280265184
num_steps = 5000.0

# direct control of time steps vs time (optional)
time_t = '0      1.0e4 1.0e7 5.6e7 5.8e7 6.8e7 8.0e7 2.660e8 2.6901e8 2.802e8'
time_dt = '2.0e2 4.0e3 2.0e6 2.0e6 2.0e6 2.0e6 2.0e6 2.00e6 4.0e3 4.0e3'
# time_t = '0      1.0e4 1.0e7 5.6e7 5.8e7 6.8e7 8.0e7'
# time_dt = '2.0e2 4.0e3 2.0e6 2.0e6 2.0e5 2.0e5 3.0e5'

[]

# Define postprocessors (some are required as specified above; others are optional; many others are
available)
[Postprocessors]
[./ave_temp_interior]      # average temperature of the cladding interior and all pellet exteriors
    type = SideAverageValue
    boundary = 9
    variable = temp
[../]

[./clad_inner_vol]      # volume inside of cladding
    type = InternalVolume
    boundary = 7
    variable = disp_x
    output = file
[../]

[./pellet_volume]      # fuel pellet total volume

```

```

type = InternalVolume
boundary = 8
variable = disp_x
output = file
[../]

[/avg_clad_temp]          # average temperature of cladding interior
type = SideAverageValue
boundary = 7
variable = temp
[../]

[/fis_gas_produced]       # fission gas produced (moles)
type = ElementIntegralFisGasProduce
variable = temp
block = 2
[../]

[/fis_gas_released]       # fission gas released to plenum (moles)
type = ElementIntegralFisGasRelease
variable = temp
block = 2
[../]

[/gas_volume]             # gas volume
type = InternalVolume
boundary = 9
variable = disp_x
[../]

[/plenum_pressure]        # pressure within plenum and gap
type = Reporter
[../]

[/initial_moles]          # initial fill gas mass (moles)
type = Reporter
output = file
[../]

[/flux_from_clad]         # area integrated heat flux from the cladding
type = SideFluxIntegral
variable = temp
boundary = 5
diffusivity = thermal_conductivity
[../]

[/flux_from_fuel]         # area integrated heat flux from the fuel
type = SideFluxIntegral
variable = temp
boundary = 10
diffusivity = thermal_conductivity

```

```

[../]

[./_dt]          # time step
    type = PrintDT
[../]

[./nonlinear_its]      # number of nonlinear iterations at each timestep
    type = PrintNumNonlinearIters
[../]

[./rod_total_power]
    type = ElementIntegralPower
    variable = temp
    fission_rate = fission_rate
    block = 2
[../]

[./average_fission_rate]
    type = AverageFissionRate
    rod_ave_lin_pow = power_profile
    fuel_outer_radius = 0.0052195
    fuel_inner_radius = 0.00125
    output = file
[../]

[]

# Define output file(s)
[Output]
    file_base = out_IFA-597_3_ROD8 # prefix of output file name
    postprocessor_csv = 1
    interval = 1
    output_initial = true
    exodus = true
    perf_log = true
    max_pps_rows_screen = 40
[]

```

## APPENDIX B: RISO AN3 BISON INPUT FILE

```
[GlobalParams]
density = 10303.0
disp_x = disp_x
disp_y = disp_y
order = FIRST
family = LAGRANGE
energy_per_fission = 3.2e-11 # J/fission
[]

# Specify coordinate system type
[Problem]
coord_type = RZ
[]

# Set problem dimension (2d-rz here) and import mesh file
[Mesh]
file = 2_smeared_pellets_MEDIUM_rz.e
displacements = 'disp_x disp_y'
patch_size = 1000
[]

# Define dependent variables, element order and shape function family, and initial conditions
[Variables]
[./disp_x]
[../]

[./disp_y]
[../]

[./temp]
initial_condition = 300.0 # set initial temp to ambient
[../]
[]

# Define auxillary variables, element order and shape function family
[AuxVariables]
[./fission_rate]
block = 'fuel_pellet_1 fuel_pellet_2' # defined for the fuel material with no hole only
[../]

[./fast_neutron_flux]
block = 'clad'
[../]

[./fast_neutron_fluence]
block = 'clad'
[../]
```

```

[/burnup]
  block = 'fuel_pellet_1 fuel_pellet_2'
[/]

[/hydrostatic_stress]
  order = CONSTANT
  family = MONOMIAL
[/]

[/stress_xx]    # stress aux variables are defined for output; this is a way to get integration point
variables to the output file
  order = CONSTANT
  family = MONOMIAL
[/]

[/stress_yy]
  order = CONSTANT
  family = MONOMIAL
[/]

[/stress_zz]
  order = CONSTANT
  family = MONOMIAL
[/]

[/creep_strain_xx]
  order = CONSTANT
  family = MONOMIAL
[/]

[/creep_strain_yy]
  order = CONSTANT
  family = MONOMIAL
[/]

[/creep_strain_xy]
  order = CONSTANT
  family = MONOMIAL
[/]

[/creep_strain_hoop]
  order = CONSTANT
  family = MONOMIAL
[/]

[/vonmises]
  order = CONSTANT
  family = MONOMIAL
[/]

```

```

[./creep_strain_mag]
  order = CONSTANT
  family = MONOMIAL
[../]
[]

# Define functions to control power and boundary conditions
[Functions]

[./power_profile]
  type = PiecewiseLinearFile # reads and interpolates an input file containing rod average linear power
vs time
  yourFileName = riso_an3_power_history.csv
  format = columns
  scale_factor = 1
[../]

[./axial_peaking_factors] # reads and interpolates an input file containing the axial power profile vs
time
  type = PiecewiseBilinear
  yourFileName = an3_axial_peaking.csv
  scale_factor = 1
  axis = 1
[../]

[./pressure_ramp] # reads and interpolates input data defining amplitude curve for coolant and
fill gas pressure
  type = PiecewiseLinear
  x = '0 1e4 103528800 103529000 103794477'
  y = '0 1 1 0.986 0.986'
[../]

[./flux] # reads and interpolates input data defining fast neutron flux
  type = PiecewiseLinearFile
  yourFileName = riso_an3_fast_flux.csv
  format = columns
[../]

[./clad_temp_bc]
  type = PiecewiseLinearFile
  yourFileName = riso_an3_clad_bc.csv
  format = columns
[../]

[./q]
  type = PiecewiseLinearFile # reads and interpolates an input file containing rod average linear power
vs time
  yourFileName = riso_an3_power_history.csv
  format = columns
[../]

```

```

[]

# Specify that we need solid mechanics (divergence of stress)
[SolidMechanics]
  [./solid]
    disp_r = disp_x
    disp_z = disp_y
    temp = temp
  [../]
[]

# Define kernels for the various terms in the PDE system (in all cases here, the axisymmetric (RZ)
version is specified)
[Kernels]

  [./gravity]    # body force term in stress equilibrium equation
    type = Gravity
    variable = disp_y
    value = -9.81
  [../]

  [./heat]       # gradient term in heat conduction equation
    type = HeatConduction
    variable = temp
  [../]

  [./heat_ie]    # time term in heat conduction equation
    type = HeatConductionImplicitEuler
    variable = temp
  [../]

  [./heat_source_] # source term in heat conduction equation
    type = NeutronHeatSource
    variable = temp
    block = 'fuel_pellet_1 fuel_pellet_2'          # fission rate applied to the fuel (block 2) only
    fission_rate = fission_rate # coupling to the fission_rate aux variable
  [../]
[]

# Define auxilliary kernels for each of the aux variables
[AuxKernels]
  [./fissionrate] # computes the volumetric fission rate as a function of time and space
    type = FissionRateAuxLWR
    variable = fission_rate
    block = 'fuel_pellet_1 fuel_pellet_2'
    function1 = power_profile # using the power function defined above
    function2 = axial_peaking_factors # using the axial power profile function defined above
    pellet_diameter = 0.009053
    pellet_inner_diameter = 0
    f_volume_reduction = 1.0112
    execute_on = timestep_begin

```

```
[../]
```

```
[./fast_neutron_flux]  
type = FastNeutronFluxAux  
variable = fast_neutron_flux  
block = 'clad'  
axial_power_profile = axial_peaking_factors  
function = flux  
factor = 4.9e17  
execute_on = timestep_begin  
[../]
```

```
[./fast_neutron_fluence]  
type = FastNeutronFluenceAux  
variable = fast_neutron_fluence  
fast_neutron_flux = fast_neutron_flux  
execute_on = timestep_begin  
[../]
```

```
[./burnup] # computes burnup as a function of time and space  
type = BurnupAux  
variable = burnup  
block = 'fuel_pellet_1 fuel_pellet_2'  
fission_rate = fission_rate # coupling to the fission rate aux variable  
molecular_weight = 0.270  
execute_on = timestep_begin  
[../]
```

```
[./hydrostatic_stress] # include hydrostatic stress for possible use in ForMas  
block = 'fuel_pellet_1 fuel_pellet_2'  
type = MaterialTensorAux  
tensor = stress  
variable = hydrostatic_stress  
quantity = hydrostatic  
execute_on = timestep  
[../]
```

```
[./stress_xx] # computes stress components for output  
type = MaterialTensorAux  
tensor = stress  
variable = stress_xx  
index = 0  
execute_on = timestep # for efficiency, only compute at the end of a timestep  
[../]
```

```
[./stress_yy]  
type = MaterialTensorAux  
tensor = stress  
variable = stress_yy  
index = 1
```

```

    execute_on = timestep
[../]

[./stress_zz]
    type = MaterialTensorAux
    tensor = stress
    variable = stress_zz
    index = 2
    execute_on = timestep
[../]

[./vonmises]
    type = MaterialTensorAux
    tensor = stress
    variable = vonmises
    quantity = vonmises
    execute_on = timestep
[../]

[./creep_strain_xx]          # computes stress components for output
    type = MaterialTensorAux
    tensor = creep_strain
    variable = creep_strain_xx
    index = 0
    execute_on = timestep    # for efficiency, only compute at the end of a timestep
[../]

[./creep_strain_yy]
    type = MaterialTensorAux
    tensor = creep_strain
    variable = creep_strain_yy
    index = 1
    execute_on = timestep
[../]

[./creep_strain_xy]
    type = MaterialTensorAux
    tensor = creep_strain
    variable = creep_strain_xy
    index = 3
    execute_on = timestep
[../]

[./creep_strain_hoop]
    type = MaterialTensorAux
    tensor = creep_strain
    variable = creep_strain_hoop
    index = 2
    execute_on = timestep
[../]

```

```

[/creep_strain_mag]
type = MaterialTensorAux
tensor = creep_strain
variable = creep_strain_mag
quantity = plasticstrainmag
execute_on = timestep
[/]

[]

# Define mechanical contact between the fuel (sideset=10) and the clad (sideset=5)
[Contact]
[/pellet_clad_mechanical]
master = 5
slave = 10
disp_x = disp_x
disp_y = disp_y
penalty = 1e7
model = experimental
[/]

[]

# Define thermal contact between the fuel (sideset=10) and the clad (sideset=5)
[ThermalContact]
[/thermal_contact]
type = GapHeatTransferLWR
variable = temp
master = 5
slave = 10
initial_moles = initial_moles    # coupling to a postprocessor which supplies the initial plenum/gap
gas mass
gas_released = fis_gas_released  # coupling to a postprocessor which supplies the fission gas addition
contact_pressure_input = 35e6    # set contact pressure equal to the pressure required to reach yeild
stress
roughness_clad = 1.0e-6
roughness_fuel = 1.0e-6
jumpdistance_fuel = 5e-6
jumpdistance_clad = 5e-6 # sum of jump distances = 10 um
initial_gas_fractions = '1 0 0 0 0 0'
refab_time = 103529000
refab_gas_fractions = '1 0 0 0 0 0'
[/]

[]

# Define boundary conditions
[BCs]

# pin pellets and clad along axis of symmetry (y)
[/no_x_all]
type = DirichletBC
variable = disp_x

```

```

boundary = 12
value = 0.0
[../]

# pin clad bottom in the axial direction (y)
[/no_y_clad_bottom]
type = DirichletBC
variable = disp_y
boundary = '1'
value = 0.0
[../]

# pin fuel bottom in the axial direction (y)
[/no_y_fuel_bottom]
type = DirichletBC
variable = disp_y
boundary = '1020'
value = 0.0
[../]

[/temp]
type = FunctionDirichletBC
boundary = '1 2 3'
variable = temp
function = clad_temp_bc
[../]

[/Pressure]
# apply coolant pressure on clad outer walls
[/coolantPressure]
boundary = '1 2 3'
factor = 1.552e7 #changes to 1.53e7 for bump tests
function = pressure_ramp # use the pressure_ramp function defined above
[../]
[../]

[/PlenumPressure]
# apply plenum pressure on clad inner walls and pellet surfaces
[/plenumPressure]
boundary = 9
initial_pressure = 2.31e6 #changes to 1e5 for bump tests
startup_time = 1.0e4
R = 8.3143
output_initial_moles = initial_moles # coupling to post processor to get initial fill gas mass
temperature = ave_temp_interior # coupling to post processor to get gas temperature
approximation
volume = gas_volume # coupling to post processor to get gas volume
material_input = fis_gas_released # coupling to post processor to get fission gas added
output = plenum_pressure # coupling to post processor to output plenum/gap pressure
refab_time = 103529000
refab_pressure = 1.57e6

```

```

    refab_temperature = 500
    refab_volume = 7.0e-6
[../]
[../]

[ ]

# Define material behavior models and input material property data
[Materials]
[./density1]
    type = Density
    block = 'clad'
    density = 6551.0
[../]
[./density2]
    type = Density
    block = 'fuel_pellet_1 fuel_pellet_2'
[../]

[./fuel_thermal]          # temperature and burnup dependent thermal properties of UO2 (bison
kernel)
    type = ThermalUO2
    block = 'fuel_pellet_1 fuel_pellet_2'
    temp = temp
    burnup = burnup
[../]

[./fuel_solid_mechanics_swelling]  # free expansion strains (swelling and densification) for UO2
(bison kernel)
    type = VSwellingUO2
    block = 'fuel_pellet_1 fuel_pellet_2'
    temp = temp
    burnup = burnup
[../]

[./fuel_creep]            # thermal and irradiation creep for UO2 (bison kernel)
    type = CreepUO2
    block = 'fuel_pellet_1 fuel_pellet_2'
    disp_r = disp_x
    disp_z = disp_y
    temp = temp
    fission_rate = fission_rate
    youngs_modulus = 2.e11
    poissons_ratio = .345
    thermal_expansion = 10e-6
    grain_radius = 5.85e-6 # maximum grain size measured during PIE
    oxy_to_metal_ratio = 2.0
    max_its = 10
    output_iteration_info = false
[../]

```

```

[/fuel_relocation]
type = RelocationUO2
block = 'fuel_pellet_1 fuel_pellet_2'
burnup = burnup
diameter = 0.009053 #Fuel pellet diameter in m
q = q
gap = 2.05e-4 #diametral gap in m
burnup_relocation_stop = 0.029
[../]

[/clad_thermal]          # general thermal property input (elk kernel)
type = HeatConductionMaterial
block = 'clad'
thermal_conductivity = 16.0
specific_heat = 330.0
[../]

[/clad_solid_mechanics]  # thermoelasticity and thermal and irradiation creep for Zr4 (bison
kernel)
type = ThermalIrradiationCreepZr4
block = 'clad'
disp_r = disp_x
disp_z = disp_y
temp = temp
fast_neutron_flux = fast_neutron_flux
youngs_modulus = 7.5e10
poissons_ratio = 0.3
thermal_expansion = 5.0e-6
max_its = 5000
output_iteration_info = false
[../]

[/clad_irrgrowth]
type = IrradiationGrowthZr4
block = 'clad'
fast_neutron_fluence = fast_neutron_fluence
[../]

[/fission_gas_release]   # Forsberg-Massih fission gas release mode
type = ForMas
block = 'fuel_pellet_1 fuel_pellet_2'
temp = temp
fission_rate = fission_rate    # coupling to fission_rate aux variable
grain_radius = 5.85e-6
plenum_pressure = plenum_pressure
hydrostatic_stress = hydrostatic_stress
calibration_factor = 6.5
[../]
[]

[Dampers]

```

```

[./limitT]
    type = MaxIncrement
    max_increment = 50.0
    variable = temp
[../]
[]

[Preconditioning]
[./SMP]
    type = SMP
    full = true
[../]
[]

[Executioner]
# type = Transient
type = AdaptiveTransient

# PETSC options
petsc_options = '-snes_mf_operator -ksp_monitor -ksp_gmres_modifiedgramschmidt'
petsc_options_iname = '-snes_type -snes_ls -ksp_gmres_restart -pc_type -pc_composite_pcs -
sub_0_pc_hypre_type -sub_0_pc_hypre_boomeramg_max_iter -
sub_0_pc_hypre_boomeramg_grid_sweeps_all -sub_1_sub_pc_type -pc_composite_type -ksp_type -
mat_mffd_type'
petsc_options_value = 'ls      basic 201      composite hypre,asm      boomeramg      2
2      lu      multiplicative fgmres ds'

# controls for linear iterations
l_max_its = 100
l_tol = 8e-3

# controls for nonlinear iterations
nl_max_its = 10
nl_rel_tol = 1e-4
nl_abs_tol = 1e-10

# time control
start_time = 0.0
dt = 2.0e2
end_time = 103789797
num_steps = 5000.0

# direct control of time steps vs time (optional)
time_t = '0      103528800 103529000 103529119 103531160 103533619 103537700 103552640
103567520 103582160 103596439 103611019 103625239 103701019 103701870 103781900
103782929'
time_dt = '2.0e2 1e2 1.0e1 1.0e2 1e2 1e2 1e2 1e2 1e2 1e2 1e2 1e2 1e2 1e2 1e2 1e2 1e2 '

dtmax = 1e6
dtmin = 1
optimal_iterations = 6

```

```

growth_factor = 1.3
iteration_window = 0.4
linear_iteration_ratio = 100

```

```

[]

```

# Define postprocessors (some are required as specified above; others are optional; many others are available)

```

[Postprocessors]

```

```

  [./ave_temp_interior]      # average temperature of the cladding interior and all pellet exteriors
    type = SideAverageValue
    boundary = 7
    variable = temp
  [../]

```

```

  [./clad_inner_vol]        # volume inside of cladding
    type = InternalVolume
    boundary = 7
    variable = disp_x
    output = file
  [../]

```

```

  [./pellet_volume]         # fuel pellet total volume
    type = InternalVolume
    boundary = 8
    variable = disp_x
    output = file
  [../]

```

```

  [./avg_clad_temp]         # average temperature of cladding interior
    type = SideAverageValue
    boundary = 7
    variable = temp
  [../]

```

```

  [./fis_gas_produced]      # fission gas produced (moles)
    type = ElementIntegralFisGasProduce
    variable = temp
    block = 'fuel_pellet_1 fuel_pellet_2'
  [../]

```

```

  [./fis_gas_released]      # fission gas released to plenum (moles)
    type = ElementIntegralFisGasRelease
    variable = temp
    block = 'fuel_pellet_1 fuel_pellet_2'
  [../]

```

```

  [./gas_volume]            # gas volume
    type = InternalVolume
    boundary = 9

```

```

    variable = disp_x
[../]

[./plenum_pressure]      # pressure within plenum and gap
    type = Reporter
[../]

[./initial_moles]        # initial fill gas mass (moles)
    type = Reporter
    output = file
[../]

[./flux_from_clad]       # area integrated heat flux from the cladding
    type = SideFluxIntegral
    variable = temp
    boundary = 5
    diffusivity = thermal_conductivity
[../]

[./flux_from_fuel]       # area integrated heat flux from the fuel
    type = SideFluxIntegral
    variable = temp
    boundary = 10
    diffusivity = thermal_conductivity
[../]

[./_dt]                  # time step
    type = PrintDT
[../]

[./nonlinear_its]        # number of nonlinear iterations at each timestep
    type = PrintNumNonlinearIters
[../]

[./rod_total_power]
    type = ElementIntegralPower
    variable = temp
    fission_rate = fission_rate
    block = 'fuel_pellet_1 fuel_pellet_2'
[../]

[./average_fission_rate]
    type = AverageFissionRate
    rod_ave_lin_pow = power_profile
    fuel_outer_radius = 0.0045265
    fuel_inner_radius = 0.00125
    output = file
[../]

[]

```

```
# Define output file(s)
[Output]
  file_base = output # prefix of output file name
  interval = 1
  output_initial = true
  exodus = true
  perf_log = true
  max_pps_rows_screen = 40
[]
```

## APPENDIX C: RISO AN4 BISON INPUT FILE

[GlobalParams]

density = 10303.0

disp\_x = disp\_x

disp\_y = disp\_y

order = FIRST

family = LAGRANGE

energy\_per\_fission = 3.2e-11

[]

[Problem]

coord\_type = RZ

[]

[Mesh]

file = pelletcladsmearmedium1\_rz.e

displacements = 'disp\_x disp\_y'

patch\_size = 1000

[]

[Variables]

[/disp\_x]

[../]

[/disp\_y]

[../]

[/temp]

initial\_condition = 300.0

[../]

[]

[AuxVariables]

[/fission\_rate]

block = 2

[../]

[/fast\_neutron\_flux]

block = 1

[../]

[./fast\_neutron\_fluence]

block = 1

[../]

[./burnup]

block = 2

[../]

[./hydrostatic\_stress]

order = CONSTANT

family = MONOMIAL

[../]

[./stress\_xx]

order = CONSTANT

family = MONOMIAL

[../]

[./stress\_yy]

order = CONSTANT

family = MONOMIAL

[../]

[./stress\_zz]

order = CONSTANT

family = MONOMIAL

[../]

[./creep\_strain\_xx]

order = CONSTANT

family = MONOMIAL

[../]

[./creep\_strain\_yy]

order = CONSTANT

family = MONOMIAL

[../]

[./creep\_strain\_xy]

order = CONSTANT

family = MONOMIAL

[../]

[./creep\_strain\_hoop]

order = CONSTANT

```
family = MONOMIAL
[../]
```

```
[./vonmises]
order = CONSTANT
family = MONOMIAL
[../]
[./creep_strain_mag]
order = CONSTANT
family = MONOMIAL
[../]
[]
```

#### [Functions]

```
[./power_profile]
type = PiecewiseLinearFile
yourFileName = an4_power_history.csv
scale_factor = 1
format = columns
[../]
```

```
[./axial_peaking_factors]
type = PiecewiseBilinear
yourFileName = an4_axial_peaking.csv
scale_factor = 1
axis = 1
[../]
```

```
[./pressure_ramp]
type = PiecewiseLinear
x = '0 1e4 103528800 103529000 103795758'
y = '0 1 1 0.986 0.986'
[../]
```

```
[./flux]
type = PiecewiseLinearFile
yourFileName = an4_fast_flux.csv
format = columns
[../]
```

```

[/clad_temp_bc]
    type = PiecewiseLinearFile
    yourFileName = an4_clad_bc.csv
    format = columns
[/]

[/q]
    type = PiecewiseLinearFile
    yourFileName = an4_power_history.csv
    format = columns
[/]

[]

[SolidMechanics]
[/solid]
    disp_r = disp_x
    disp_z = disp_y
    temp = temp
[/]

[]

[Kernels]

[/gravity]
    type = Gravity
    variable = disp_y
    value = -9.81
[/]

[/heat]
    type = HeatConduction
    variable = temp
[/]

[/heat_ie]
    type = HeatConductionImplicitEuler
    variable = temp
[/]

[/heat_source]

```

```

    type = NeutronHeatSource
    variable = temp
    block = 2
    fission_rate = fission_rate
[../]
[]

```

```

[AuxKernels]
[./fissionrate]
    type = FissionRateAuxLWR
    variable = fission_rate
    block = 2
    function1 = power_profile
    function2 = axial_peaking_factors
    pellet_diameter = 0.009053
    pellet_inner_diameter = 0.0025
    f_volume_reduction = 1
    execute_on = timestep_begin
[../]

```

```

[./fast_neutron_flux]
    type = FastNeutronFluxAux
    variable = fast_neutron_flux
    block = 1
    axial_power_profile = axial_peaking_factors
    function = flux
    factor = 4.9e17
    execute_on = timestep_begin
[../]

```

```

[./fast_neutron_fluence]
    type = FastNeutronFluenceAux
    variable = fast_neutron_fluence
    fast_neutron_flux = fast_neutron_flux
    execute_on = timestep_begin
[../]

```

```

[./burnup]
    type = BurnupAux
    variable = burnup

```

```
block = 2
fission_rate = fission_rate
molecular_weight = 0.270
execute_on = timestep_begin
[../]
```

```
[./hydrostatic_stress]
block = 2
type = MaterialTensorAux
tensor = stress
variable = hydrostatic_stress
quantity = hydrostatic
execute_on = timestep
[../]
```

```
[./stress_xx]
type = MaterialTensorAux
tensor = stress
variable = stress_xx
index = 0
execute_on = timestep
[../]
```

```
[./stress_yy]
type = MaterialTensorAux
tensor = stress
variable = stress_yy
index = 1
execute_on = timestep
[../]
```

```
[./stress_zz]
type = MaterialTensorAux
tensor = stress
variable = stress_zz
index = 2
execute_on = timestep
[../]
```

```
[./vonmises]
type = MaterialTensorAux
```

```
tensor = stress
variable = vonmises
quantity = vonmises
execute_on = timestep
[../]
```

```
[./creep_strain_xx]
type = MaterialTensorAux
tensor = creep_strain
variable = creep_strain_xx
index = 0
execute_on = timestep
[../]
```

```
[./creep_strain_yy]
type = MaterialTensorAux
tensor = creep_strain
variable = creep_strain_yy
index = 1
execute_on = timestep
[../]
```

```
[./creep_strain_xy]
type = MaterialTensorAux
tensor = creep_strain
variable = creep_strain_xy
index = 3
execute_on = timestep
[../]
```

```
[./creep_strain_hoop]
type = MaterialTensorAux
tensor = creep_strain
variable = creep_strain_hoop
index = 2
execute_on = timestep
[../]
```

```
[./creep_strain_mag]
type = MaterialTensorAux
tensor = creep_strain
```

```

    variable = creep_strain_mag
    quantity = plasticstrainmag
    execute_on = timestep
[../]

[]

[Contact]
[./pellet_clad_mechanical]
    master = 5
    slave = 10
    disp_x = disp_x
    disp_y = disp_y
    penalty = 1e8
    model = experimental
[../]

[]

[ThermalContact]
[./thermal_contact]
    type = GapHeatTransferLWR
    variable = temp
    master = 5
    slave = 10
    initial_moles = initial_moles
    gas_released = fis_gas_released
    contact_pressure_input = 35e6
    roughness_clad = 1.0e-6
    roughness_fuel = 1.0e-6
    initial_gas_fractions = '1 0 0 0 0 0 0'
    refab_time = 103529000
    refab_gas_fractions = '0 0 0 1 0 0 0'
[../]

[]

[BCs]
[./no_x_all]
    type = DirichletBC
    variable = disp_x
    boundary = 12
    value = 0.0

```

```
[../]
```

```
[./no_y_clad_bottom]
```

```
type = DirichletBC
```

```
variable = disp_y
```

```
boundary = '1'
```

```
value = 0.0
```

```
[../]
```

```
[./no_y_fuel_bottom]
```

```
type = DirichletBC
```

```
variable = disp_y
```

```
boundary = '1020'
```

```
value = 0.0
```

```
[../]
```

```
[./temp]
```

```
type = FunctionDirichletBC
```

```
boundary = '1 2 3'
```

```
variable = temp
```

```
function = clad_temp_bc
```

```
[../]
```

```
[./Pressure]
```

```
[./coolantPressure]
```

```
boundary = '1 2 3'
```

```
factor = 1.552e7
```

```
function = pressure_ramp
```

```
[../]
```

```
[../]
```

```
[./PlenumPressure]
```

```
[./plenumPressure]
```

```
boundary = 9
```

```
initial_pressure = 2.31e6
```

```
startup_time = 1.0e4
```

```
R = 8.3143
```

```
output_initial_moles = initial_moles
```

```
temperature = ave_temp_interior
```

```
volume = gas_volume
```

```
material_input = fis_gas_released
```

```

    output = plenum_pressure
    refab_time = 103529000
    refab_pressure = 1.0e5
    refab_temperature = 293
    refab_volume = 7.9e-6
    [../]
    [../]

[ ]

[Materials]
    [./density1]
        type = Density
        block = 1
        density = 6551.0
    [../]
    [./density2]
        type = Density
        block = 2
    [../]

    [./fuel_thermal]
        type = ThermalUO2
        block = 2
        temp = temp
        burnup = burnup
    [../]

    [./fuel_solid_mechanics_swelling]
        type = VSwellingUO2
        block = 2
        temp = temp
        burnup = burnup
    [../]

    [./fuel_creep]
        type = CreepUO2
        block = 2
        disp_r = disp_x
        disp_z = disp_y
        temp = temp

```

```

fission_rate = fission_rate
youngs_modulus = 2.e11
poissons_ratio = .345
thermal_expansion = 10e-6
grain_radius = 4.9e-6
oxy_to_metal_ratio = 2.0
max_its = 10
output_iteration_info = false
[../]

```

```

[/fuel_relocation]
type = RelocationUO2
block = 2
burnup = burnup
diameter = 0.009053
q = q
gap = 2.05e-4
burnup_relocation_stop = 0.029
[../]

```

```

[/clad_thermal]
type = HeatConductionMaterial
block = 1
thermal_conductivity = 16.0
specific_heat = 330.0
[../]

```

```

[/clad_solid_mechanics]
type = ThermalIrradiationCreepZr4
block = 1
disp_r = disp_x
disp_z = disp_y
temp = temp
fast_neutron_flux = fast_neutron_flux
youngs_modulus = 7.5e10
poissons_ratio = 0.3
thermal_expansion = 5.0e-6
max_its = 5000
output_iteration_info = false
[../]

```

```
[./clad_irrgrowth]
    type = IrradiationGrowthZr4
    block = 1
    fast_neutron_fluence = fast_neutron_fluence
[../]
```

```
[./fission_gas_release]
    type = ForMas
    block = 2
    temp = temp
    fission_rate = fission_rate
    grain_radius = 100 #Shut off fission gas production
    plenum_pressure = plenum_pressure
    hydrostatic_stress = hydrostatic_stress
    calibration_factor = 100
[../]
[]
```

```
[Dampers]
[./limitT]
    type = MaxIncrement
    max_increment = 25.0
    variable = temp
[../]
[]
```

```
[Preconditioning]
[./SMP]
    type = SMP
    full = true
[../]
```

```
[Executioner]
    type = AdaptiveTransient
```

```
# PETSC options
petsc_options = '-snes_mf_operator -ksp_monitor -ksp_gmres_modifiedgramschmidt'
petsc_options_iname = '-snes_type -snes_ls -ksp_gmres_restart -pc_type -pc_composite_pc -
sub_0_pc_hypre_type -sub_0_pc_hypre_boomeramg_max_iter -
sub_0_pc_hypre_boomeramg_grid_sweeps_all -sub_1_sub_pc_type -pc_composite_type -ksp_type -
mat_mffdt_type'
```

```

2  Petsc_options_value = 'ls      basic 201      composite hypre,asm      boomeramg      2
                                lu      multiplicative  fgmres  ds'

# controls for linear iterations
l_max_its = 100
l_tol = 8e-3

# controls for nonlinear iterations
nl_max_its = 10
nl_rel_tol = 1e-3
nl_abs_tol = 1e-8

# time control
start_time = 0.0
dt = 2.0e2
end_time = 103795758
num_steps = 50000.0

# direct control of time steps vs time (optional)
time_t = '0 103528800 103529000 103534230 103536080 103538960 103542079 103557860
103572319 103586899 103601180 103615760 103630099 103705820 103706970 103785380
103786350'
time_dt = '2.0e2 1e2 1.0e2 1.0e2 1e2 1e2 1e2 1e2 1e2 1e2 1e2 1e2 1e2 1e2 1e2 1e2 1e2'

dtmax = 1e6
dtmin = 1
optimal_iterations = 4
growth_factor = 1.3
iteration_window = 0.4
linear_iteration_ratio = 100

[]

[Postprocessors]
[./ave_temp_interior]
    type = SideAverageValue
    boundary = 9
    variable = temp
[./]

[./clad_inner_vol]
    type = InternalVolume

```

```
boundary = 7  
variable = disp_x  
output = file  
[../]
```

```
[./pellet_volume]  
type = InternalVolume  
boundary = 8  
variable = disp_x  
output = file  
[../]
```

```
[./avg_clad_temp]  
type = SideAverageValue  
boundary = 7  
variable = temp  
[../]
```

```
[./fis_gas_produced]  
type = ElementIntegralFisGasProduce  
variable = temp  
block = 2  
[../]
```

```
[./fis_gas_released]  
type = ElementIntegralFisGasRelease  
variable = temp  
block = 2  
[../]
```

```
[./gas_volume]  
type = InternalVolume  
boundary = 9  
variable = disp_x  
[../]
```

```
[./plenum_pressure]  
type = Reporter  
[../]
```

```
[./initial_moles]
```

```

type = Reporter
output = file
[../]

[/flux_from_clad]
type = SideFluxIntegral
variable = temp
boundary = 5
diffusivity = thermal_conductivity
[../]

[/flux_from_fuel]
type = SideFluxIntegral
variable = temp
boundary = 10
diffusivity = thermal_conductivity
[../]

[/_dt]
type = PrintDT
[../]

[/nonlinear_its]
type = PrintNumNonlinearIters
[../]

[/rod_total_power]
type = ElementIntegralPower
variable = temp
fission_rate = fission_rate
block = 2
[../]

[/average_fission_rate]
type = AverageFissionRate
rod_ave_lin_pow = power_profile
fuel_outer_radius = 0.0045265
fuel_inner_radius = 0.00125
output = file
[../]

```

```
[]
```

```
[Output]
```

```
file_base = output
```

```
interval = 1
```

```
output_initial = true
```

```
exodus = true
```

```
perf_log = true
```

```
max_pps_rows_screen = 40
```

```
[]
```