INL/EXT-12-25530

Application of the BISON Fuel Performance Code to the FUMEX-III Coordinated Research Project

R. L. Williamson
S. R. Novascone

April 2012

The INL is a U.S. Department of Energy National Laboratory
operated by Battelle Energy Alliance

INL/EXT-12-25530

Application of the BISON Fuel Performance Code to the FUMEX-III Coordinated Research Project

R. L. Williamson

S. R. Novascone

April 2012

Idaho National Laboratory
Idaho Falls, Idaho 83415

http://www.inl.gov

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

CONTENTS

FIGURES

TABLES

Error! Reference source not found.

1. INTRODUCTION

Since 1981, the International Atomic Energy Agency (IAEA) has sponsored a series of Coordinated Research Projects (CRP) in the area of nuclear fuel modeling. These projects have typically lasted 3-5 years and have had broad international participation. The objectives of the projects have been to assess the maturity and predictive capability of fuel performance codes, support interaction and information exchange between countries with code development and application needs, build a database of well-defined experiments suitable for code validation, transfer a mature fuel modeling code to developing countries, and provide guidelines for code quality assurance and code application to fuel licensing.

The fourth and latest of these projects, known as FUMEX-III[1] (FUel Modeling at EXtended Burnup-III), began in 2008 and ended in December of 2011. FUMEX-III was the first of this series of fuel modeling CRP's in which the INL participated.

Participants met at the beginning of the project to discuss and select a set of experiments ("priority cases") for consideration during the project. These priority cases were of broad interest to the participants and included reasonably well-documented and reliable data. A meeting was held midway through the project for participants to present and discuss progress on modeling the priority cases. A final meeting was held at close of the project to present and discuss final results and provide input for a final report.

Also in 2008, the INL initiated development of a new multidimensional (2D and 3D) multiphysics nuclear fuel performance code called BISON, with code development progressing steadily during the three-year FUMEX-III project. Interactions with international fuel modeling researchers via FUMEX-III played a significant role in the BISON evolution, particularly influencing the selection of material and behavioral models which are now included in the code.

The FUMEX-III cases are generally integral fuel rod experiments occurring late in fuel life (high burnup), and thus involve complex coupled multiphysics behavior. A mature fuel performance capability is needed to have any hope of reasonable comparison to experimental data. BISON's ability to model such integral fuel rod behavior did not mature until 2011, limiting the number of FUMEX-III cases considered during the CRP. In fact, only two FUMEX cases were considered in any detail. The first was actually from the earlier FUMEX-II project, and included a comparison of results from the BISON fission gas release model to what is known as the Vitanza[2] threshold. This comparison will be briefly described below for completeness. The only FUMEX-III case considered was the Riso3-GE7 experiment, which includes measurements of rod outer diameter following pellet clad mechanical interaction (PCMI) resulting from a power ramp late in fuel life.

2. BISON DESCRIPTION

2.1 Overview

BISON is a finite element-based nuclear fuel performance code based on the INL Multiphysics Object Oriented Simulation Environment (MOOSE).[3] The code is designed for steady and transient analysis and is applicable to a variety of fuel forms, including light water reactor fuel rods, TRISO particle fuel, and metallic rod and plate fuel. BISON solves the fully-coupled equations of thermomechanics and species diffusion, for either 2D axisymmetric or 3D geometries. Fuel models are included to describe temperature and burnup dependent thermal properties, fission product swelling, densification, thermal and irradiation creep, fracture, and fission gas production and release. Plasticity, irradiation growth, and thermal and irradiation creep models are implemented for clad materials. Models are also available to simulate gap heat transfer, mechanical contact, and the evolution of the gap/plenum pressure with plenum volume, gas temperature, and fission gas addition. Because BISON is a MOOSE-based application, it can efficiently solve problems using standard desktop workstations or massively parallel high-performance computers, which is essential for complex 3D simulations.

Computational meshes for BISON can be developed using a variety of existing mesh generation software, such as the CUBIT code (http://cubit.sandia.gov) developed at Sandia National Laboratory. The mesh provided as input to BISON determines the dimensionality of the analysis, thus either 2D or 3D simulations can be performed simply by supplying either a 2D or 3D finite element mesh. Scripts are available to automate meshing of complete fuel rods, containing either individual fuel pellets or a smeared fuel column. Output can be generated in a variety of popular graphics formats and viewed with existing software such as ENSIGHT (http ://www.ensight.com), TECPLOT (http://www.tecplot.com), or PARAVIEW (http://www.paraview.org/).

It is noteworthy that a companion code to BISON, called MARMOT[4], has also been developed that solves mesoscale phase-field equations, and can be used to simulate fuel microstructure evolution (e.g., void swelling, fission gas bubble formation, species redistribution) during irradiation. MARMOT was recently coupled to BISON to provide multiscale analysis of nuclear fuel.

A detailed description of BISON, including application to both LWR and TRISO fuels forms and demonstration of concurrent coupling to MARMOT, was recently published.[5] A brief overview of the models currently available in BISON is provided below.

2.2 Oxide Fuel Material and Behavioral Models

Two empirical models are available in BISON to compute thermal conductivity and its dependence on temperature, porosity, and burnup. In the first, the temperature-dependence of unirradiated material is defined using the equation suggested by Fink[6]. This relationship is then modified to account for the effects of irradiation, porosity and burnup using a series of multipliers, as outlined in detail by Lucuta et al.[7] The second is the model from MATPRO[8], which is based on an equation proposed by Ohira and Itagaki[9].

Volumetric swelling as a result of both solid and gaseous fission products is included using empirical relations from MATPRO[8]. Solid fission product swelling is expressed as a simple linear function of burnup. Gaseous fission product welling is prescribed as a function of both burnup and temperature. Fuel densification is computed using the ESCORE[10] empirical model.

A model for combined secondary thermal creep and irradiation creep of UO_2 is available, with the creep rate modeled as a function of time, temperature, effective stress, density, grain size, fission rate, and oxygen-to-metal ratio (O/M). The constitutive relation is taken from the MATPRO[8] FCREEP material model.

Pellet fracture can be modeled using a simple empirical relocation model and/or a smeared cracking model. The relocation model is from ESCORE[10] and prescribes the increase in fuel diameter as a function of the linear heating rate and burnup. The smeared cracking model follows the approach outlined by Rashid[11], where cracking is simulated by adjusting the elastic constants at material points. This is in contrast to a discrete cracking model, where topographic changes are made to the finite element mesh.

Fission gas production and release is computed using the Forsberg-Massih[12] two-stage model, evaluated at each finite-element integration point in the fuel. The first stage of the Forsberg-Massih model computes fission gas diffusion to grain boundaries, based on an analytical solution to the diffusion equation in spherical coordinates. An effective diffusion coefficient is used, which accounts for gas resolution and trapping within the fuel grain. The gas diffusion coefficient developed by Turnbull et al.[13] is employed. In the second stage, time-dependent boundary conditions are used to determine grain boundary gas accumulation, resolution, saturation, and release parameters. Release from the grain boundaries is controlled using a grain boundary saturation criterion. For the current implementation, the fuel grains are assumed to be constant in diameter, thus grain growth and grain-boundary sweeping effects are not considered.

2.3 Cladding Material and Behavioral Models

Focusing initially on Zircaloy as a clad material, models have been implemented in BISON for thermal and irradiation creep, irradiation growth and combined creep and instantaneous plasticity.

Secondary thermal creep is described using a traditional power-law formulation described by Hayes and Kassner[14], with the creep rate specified as a function of effective stress and temperature. Irradiation-induced creep is based on an empirical model developed by Hoppe[15] that relates the creep rate to the current fast neutron flux and stress. A model for primary creep of zirconium alloys has not yet been implemented.

Cladding elongation as a result of radiation-induced growth is included using the ESCORE[10] empirical model, where the irradiation growth strain is specified as a function of the fast neutron fluence.

A constitutive model is also available for combined instantaneous plasticity and time-dependent creep. Creep is modeled using the thermal and irradiation creep constitutive equations described above. Time-independent plasticity is modeled assuming J2 plasticity based on a simple linear strain-hardening curve.

2.4 Gap and Plenum Models

Gap heat transfer is modeled by summing the gap gas conductance, the increased conductance due to solid-solid contact, and the conductance due to radiant heat transfer. This model is typically applied between the fuel and clad, but can also be used to simulate heat transfer between individual pellets or between a pellet and end cap.

The gap gas conductance is described using the well-known form published by Ross and Stoute[16], where the conductance is specified as a function of the gap width and the roughnesses and jump distances of the two surfaces. The conductivity of the gas mixture is computed using the mixture rule from MATPRO[8], which permits mixtures of seven gases (helium, argon, krypton, xenon, hydrogen, nitrogen, and water vapor). The increased conductance due to solid-solid contact is described using the empirical model suggested by Olander[17], where the conductance is specified as a function of the thermal conductivities of the solid materials in contact, the contact pressure, the average gas film thickness, and the Meyer hardness of the softer material. The conductance due to radiant heat transfer is approximated using a diffusion approximation.

Mechanical contact is computed using a traditional node/face approach. To date, BISON supports only frictionless and tied contact. Friction between the pellets and clad is important, and will be implemented in the future. Finite element contact is notoriously difficult to make efficient and robust in three dimensions, thus effort is underway to improve the contact algorithm.

The pressure in the gap and plenum is computed based on the ideal gas law. The moles of gas, the temperature, and the cavity volume are free to change with time. The gas mass is the original amount plus any fission gas released. The temperature is currently taken as the average temperature of the pellet exterior and cladding interior surfaces, though any other measure of temperature could be used. The cavity volume is computed based on the evolving pellet and clad geometry.

3. APPLICATIONS

As mentioned above, BISON was under active development during the full duration of the FUMEX-III exercise and the ability to simulate integral fuel rod tests only became possible near the end of the project. Application to the FUMEX-III priority cases was therefore limited the single Riso3-GE7 experiment, which includes measurements of rod outer diameter following pellet clad mechanical interaction (PCMI) resulting from a power ramp late in fuel life.

Results from the BISON fission gas model were also compared to a priority case from the earlier FUMEX-II project. A brief description of this early comparison will be included for completeness.

3.1 Fission Gas Release

A frequent test of Fission Gas Release models involves a comparison to the Vitanza or Halden threshold. Vitanza et al.2[2], collected data for a large number of UO_2 fuel rods in the low release range (typically 0.5 to 2% FGR) and correlated the data in terms of fuel centerline temperature versus burnup. A fit to this widely scattered data is known as the Vitanza threshold, and is often used both to evaluate and calibrate FGR models.

The BISON fission gas release model was tested using a single LWR UO_2 fuel pellet, assuming uniform constant power. Since fission gas release is affected by a large number of input parameters, a limited parametric study was conducted. Table 1 lists the required input data for the Forsberg-Massih model and gives typical values as reported by Denis and Piotrkowski.[18] Simulations using these data will be referred to as the reference case in results to follow. The three parameters varied here include the hydrostatic pressure in the pellet, the resolution rate from intergranular bubbles, and the fractional coverage of grain boundaries at saturation. For each parametric case considered, the Vitanza curve is included for comparison.

Table 1. Reference input parameters for the Forsberg-Massih fission gas release model and Turnbull diffusion coefficient.[18]

Fuel grain radius (m)	10.0×10^{-6}
Resolution rate from intergranular bubbles (s^{-1})	1.55×10^{-5}
Resolution layer depth (m)	1.0×10^{-8}
Grain boundary bubble radius (m)	0.5×10^{-6}
Nonspherical bubble shape factor	0.287
Bubble surface tension (J/m^2)	0.626
Fractional coverage of grain boundary at saturation	0.5
External hydrostatic pressure (Pa)	10.0×10^{6}
Fraction of gas released at saturation	1.0
Fractional yield of fission gas atoms per fission	0.3017
Atomic volume (m^3)	4.09×10^{-29}
Sink strength of interstituals (m^{-2})	$1.0e^{15}$
Number of sites for which recombination is inevitable	2.0
Damage rate (defects/fission)	2.44×10^{4}

As a first parametric case, all parameters were held fixed except the hydrostatic pressure, which was varied from 0 to 20 MPa in 5-MPa increments. The results are summarized in Figure 1, which plots the fuel centerline temperature versus burnup when 1% FGR is predicted. Symbols indicate individual simulations at various axial power levels; the Vitanza experimental curve is included. An increase in hydrostatic pressure significantly shifts the onset of gas release to higher burnups. The results demonstrate the substantial role played by the hydrostatic pressure and provide clear evidence of the need for accurate solid mechanics models for the fuel, including fracture effects if the fuel is susceptible to cracking.

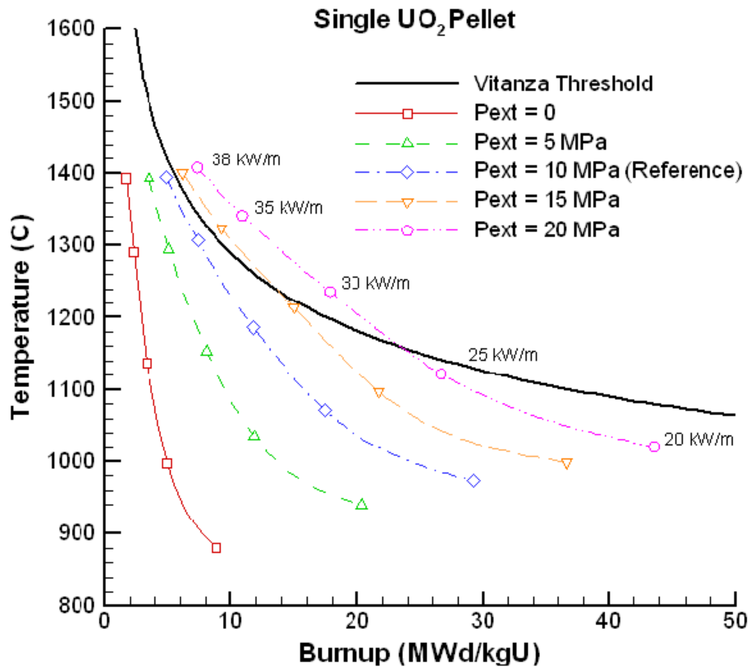

Figure 1. Effect of hydrostatic pressure on centerline temperature versus burnup, for 1% average fission gas release. The Vitanza threshold is included for comparison.

In the second parametric case, all parameters were held at reference conditions, except the resolution rate from intergranular bubbles, which was varied from 0 to the reference value of 1.55×10^{-5} s^{-1}. The results are summarized in Figure 2. The resolution rate has a significant effect, becoming more pronounced at higher burnups.

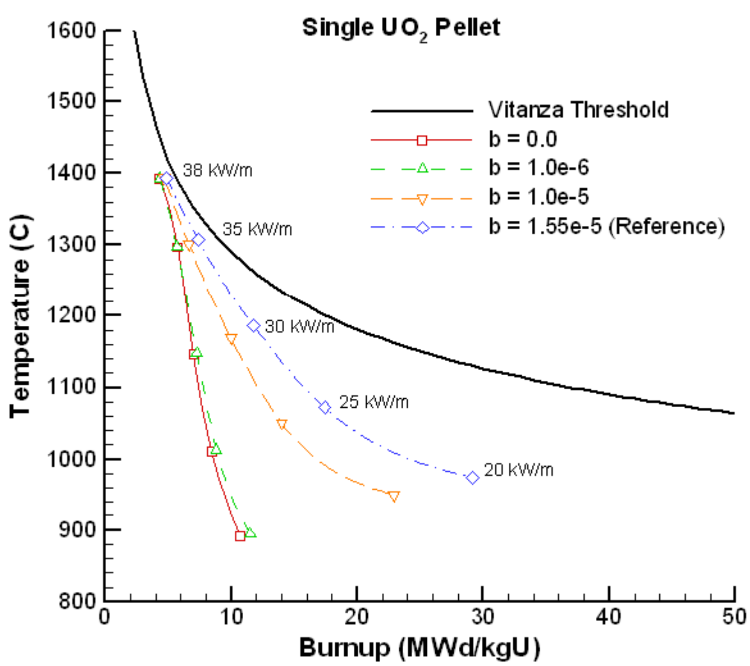

Figure 2. Effect of resolution rate from intergranular bubbles on centerline temperature versus burnup, for 1% average fission gas release. The Vitanza threshold is included for comparison.

In the final parametric case considered, all parameters were held at reference conditions except V_c—the fractional coverage of the grain boundary at saturation—which was assumed to be either 0.5 (reference value) or 0.85. The results, summarized in Figure 3, indicate a strong sensitivity to V_c, again, most predominantly at higher burnups.

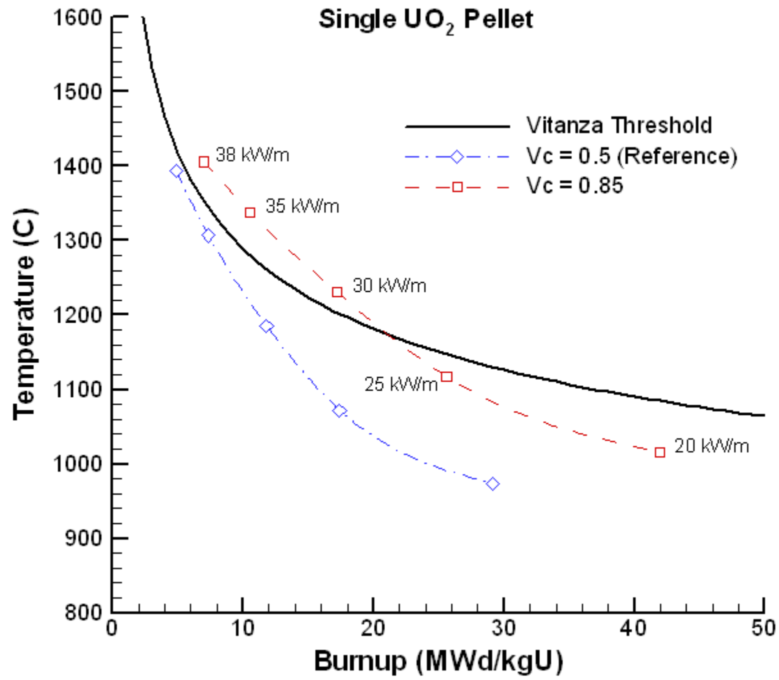

Figure 3. Effect of grain boundary fractional coverage on centerline temperature vs. burnup, for 1% average fission gas release. The Vitanza threshold is included for comparison.

3.2 Riso3-GE7 Ramp Test

3.2.1 Test description

Test GE7 is a bump test that was carried out during the third Riso Transient Fission Gas Release Project in 1989[19]. The fuel pin was supplied by General Electric Company and was neither punctured nor opened for refabrication prior to the test. The test pin (ZX115) was the lower middle segment of four approximately 0.975 m long segments assembled to a stringer. The fuel pellets were flat ended and chamfered, enriched to 3% UO_2, with an average grain size of approximately 12 µm. The cladding was stress relieved Zircaloy-2 with a bonded zirconium liner. The fuel segment was base irradiated in the Quad Cities-1 BWR over four reactor cycles. Figure 4 shows a history of the linear heat generation rate in test pin ZX115 during the base irradiation.

The bump irradiation was performed in a water-cooled rig under BWR conditions. The power history during the bump, shown in Fig. 5, included a 6 hour conditioning period at approximately 23 kW/m, a power ramp over the next approximately 15 minutes, and then a 4 hour hold. The peak power at the end of the hold period was 35.5 kW/m. Note that the tabular power data supplied with the test documentation indicated a 2 kW/m power rise during the final hold period, as shown in Fig. 5. This differs from the power history plotted in Figure 5.1 of Reference 19, where the power is shown to be constant during this final period.

The measured axial power distribution at peak power, taken from Reference 19, is shown in Fig. 6. A strong profile exists in the test, with a peak axial factor of 1.48.

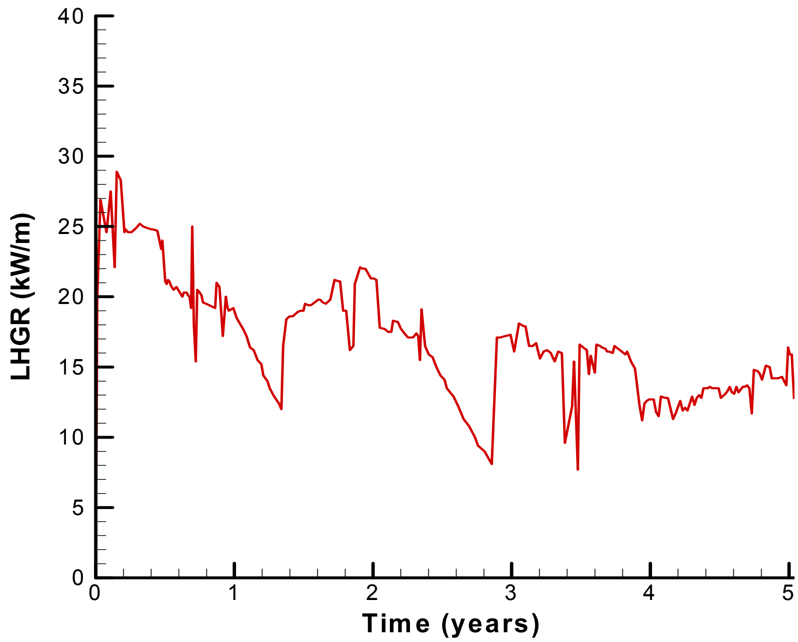

Figure 4. Base irradiation average power history for test pin ZX115.

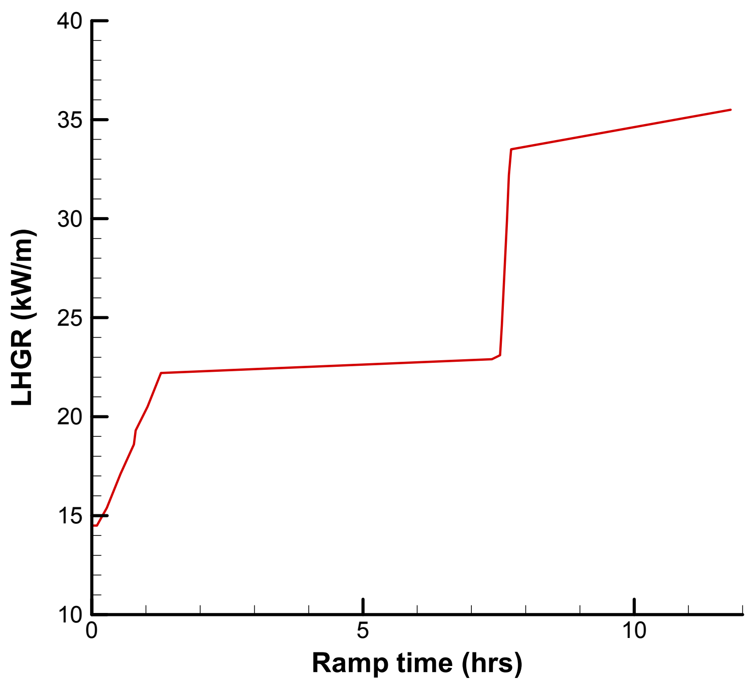

Figure 5. Average power history during power bump.

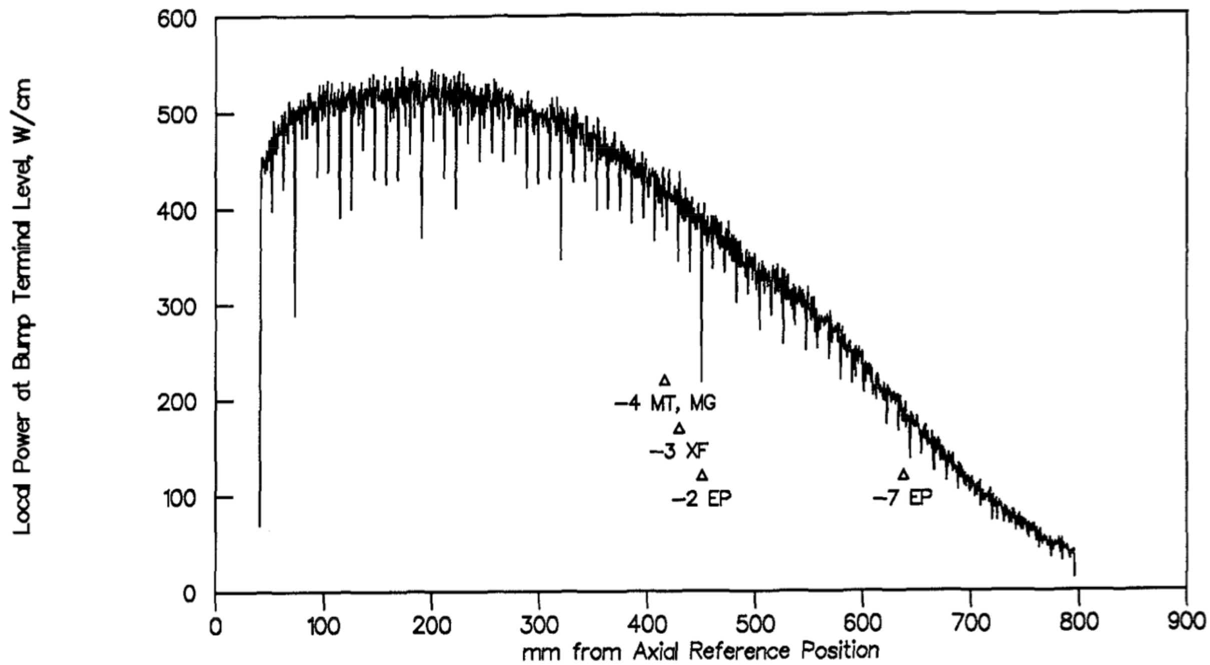

Figure 6. Axial power distribution at peak power.

3.2.2 Model description

A fully-coupled thermomechanical analysis was performed during both the base irradiation and bump test. The rod segment was modeled assuming 2D axisymmetry, based on the geometry specified in Reference 19. For simplicity, the pellet stack was simulated as a single smeared fuel column. The liner was assumed to have the same material properties as the clad. Cladding oxidation was not considered. Mechanical contact between the fuel and clad was assumed to be frictionless.

The coolant pressure was ramped to 7.24 MPa early in the base irradiation, and then held constant through the end of the power bump. The clad outer wall temperature was fixed at 564 K. Helium was the rod fill gas, having an initial pressure of 0.29 MPa.

Fuel thermal properties were prescribed using the Fink-Lucuta formulation. Fuel thermal and irradiation creep and fission product swelling were included. Fuel fracture was simulated using the empirical relocation model.

The nonlinear material response of the cladding was simulated using the combined thermal and irradiation creep and instantaneous plasticity model. This model is required to capture the very slow creep behavior during the base irradiation, and rapid plastic response during the power bump. The effects of irradiation growth were included.

Assuming fresh fuel, the base irradiation was simulated based on the power history of Figure 4. The axial power profile during the base irradiation was relatively flat, varying over the range of 0.96 to 1.027. The fast neutron flux in the clad was supplied via input using experimental data supplied with the experiment. The power history of Fig. 5, combined with the axial power distribution of Fig.6, defined the power during the bump test.

The BISON input file for this simulation is given in Appendix 1.

3.2.3 Results

A comparison of the predicted and measured rod outer diameter is shown in Fig. 7. The dashed line is the as-manufactured rod diameter, prior to irradiation. The experimental data, shown as symbols, indicate the measured average rod diameter at both the end and middle fuel pellet locations, giving an indication of rod ridging due to pellet hourglassing. The solid line is the predicted rod diameter following the power bump.

Note that contact release is not fully implemented in BISON thus once the fuel and clad surfaces are in contact, they can slide relative to each other, but are not permitted to separate. This is a temporary limitation, with contact release an area of active code development. The issue here, however, is that to obtain a prediction of the final rod diameter, it was not possible to simply reduce the power and cool the rod at the end of the power bump, since thermal contraction of fuel would artificially pull the clad inward. Thus, to obtain the prediction in Fig. 7, the final rod diameter was simply computed from the original diameter by applying the total plastic strains at the end of the bump test. For 2D axisymmetry, the hoop strain can be closely approximated as the radial displacement divided by the original radius, thus the rod final diameter was computed as $D = D_o + 2u_x = D_o(1 + \varepsilon_\theta)$ where D_o is the original rod diameter, u_x is the radial displacement, and ε_θ is the total inelastic hoop strain.

Due to the large axial power profile during the power bump, the upper portion of the rod remained relatively cool and did not undergo plastic deformation as a result of the bump. The final rod diameter in this region is thus a function of clad creep during the base irradiation. BISON appears to over-predict the clad creep-down, giving a rod diameter approximately 10 μm less than measured. The prediction, however, is reasonable.

Permanent clad deformation during the bump is observed over roughly the bottom two thirds of the rod. BISON predicts the shape of this deformation nicely, but under-predicts the magnitude.

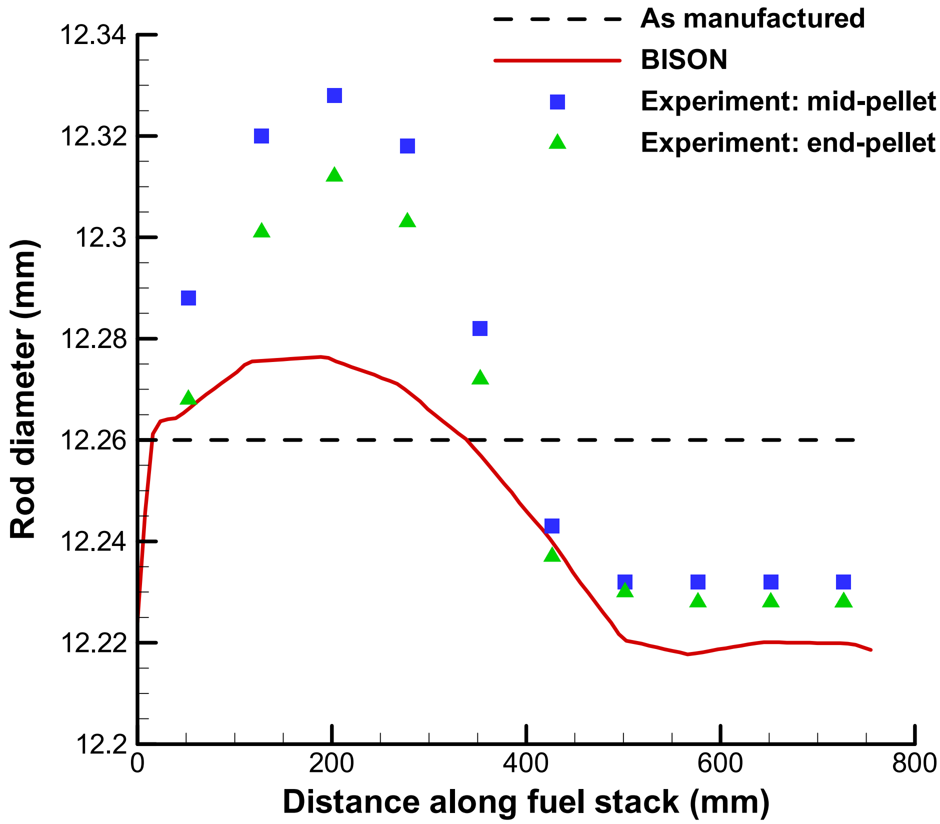

Figure 7. Comparison of the predicted and measured rod outer diameter.

3.3 Computer Platforms and Software Version

BISON is designed to run on a variety of UNIX-based computer platforms. All the simulations described in this study were run on a 12-CPU MAC workstation (Mac OS X-10.6.5 operating system), typically using eight processors. 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.

Simulations described in this report were run using BISON at revision number 9642.

4. CONCLUSIONS

FUMEX-III was the first of the IAEA sponsored fuel modeling Coordinated Research Projects in which the INL participated. During the same time period, the INL initiated development of a new multidimensional (2D and 3D) multiphysics nuclear fuel performance code called BISON. Interactions with international fuel modeling researchers via FUMEX-III played a significant and important role in the BISON evolution, particularly influencing the selection of material and behavioral models which are now included in the code.

BISON's ability to model integral fuel rod behavior did not mature until 2011, thus the only FUMEX-III case considered was the Riso3-GE7 experiment, which includes measurements of rod outer diameter following pellet clad mechanical interaction (PCMI) resulting from a power ramp late in fuel life. BISON comparisons to the Riso3-GE7 final rod diameter measurements are quite reasonable.

The INL is very interested in participation in the next Fuel Modeling Coordinated Research Project and would like to see the project initiated as soon as possible.

5. REFERENCES

[1] J. Killeen, E. Sartori and T. Tverberg, "FUMEX-III: A New IAEA Coordinated Research Project on Fuel Modeling at Extended Burnup", Proceedings of Top Fuel 2009, Paper 2176, Paris, France, September 6-10, 2009.

[2] C. Vitanza, E. Kolstad, and U. Graziani, "Fission Gas Release from UO_2 Pellet Fuel at High Burnup," *Proceedings of American Nuclear Society Topical Meeting on Light Water Reactor Fuel Performance, Portland, OR, April 29 to May 3, 1979*, p. 361.

[3] D. Gaston, C. Newman, G. Hansen, and D. Lebrun-Grandie, "MOOSE: A Parallel Computational Framework for Coupled Systems of Nonlinear Equations," *Nuclear Engineering and Design,* Vol. 239, p. 1768, 2009.

[4] M.R. Tonks, D. Gaston, P.C. Millett, D. Andrs, P. Talbot, "An Object-Oriented Finite Element Framework for Multiphysics Phase Field Simulations," *Computational Material Science*, Vol. 51, pp. 20-29, 2012.

[5] R. L. Williamson, J.D. Hales, S.R. Novascone, M.R. Tonks, D.R. Gaston, C.J. Permann, D. Andrs, R.C. Martineau, "Multidimensional Multiphysics Simulation of Nuclear Fuel Behavior," *Journal of Nuclear Materials,* Vol. 423, pp. 149-163, 2012.

[6] J. K. Fink, "Thermophysical Properties of Uranium Dioxide," *Journal of Nuclear Materials*, Vol. 279, p. 1, 2000.

[7] P. G. Lucuta, H. Matzke, and I. J. Hastings, "A Pragmatic Approach to Modeling Thermal Conductivity of Irradiated UO_2 Fuel: Review and Recommendations," *Journal of Nuclear Materials*, Vol. 232, p. 166, 1996.

[8] C. M. Allison, et al., SCDAP/RELAP5/MOD3.1 Code Manual Volume IV: MATPRO, Idaho National Engineering Laboratory Technical Report, NUREG/CR-6150, 1993.

[9] K. Ohira, N. Itagaki, "Thermal Conductivity Measurements of High Burnup UO2 Pellet and a Benchmark Calculation of Fuel Center Temperature," in: Proceedings of the American Nuclear Society Meeting on Light Water Reactor Fuel Performance, Portland, Oregon, March 2–6, 1997, p. 541.

[10] Y. Rashid, R. Dunham, and R. Montgomery, Fuel Analysis and Licensing Code: FALCON MOD01, EPRI Report 1011308, December 2004.

[11] Y.R. Rashid, "Mathematical Modeling and Analysis of Fuel Rods," *Nuclear Engineering and Design*, Vol. 29, pp. 22–32, 1974.

[12] K. Forsberg and A. R. Massih, "Diffusion Theory of Fission Gas Migration in Irradiated Nuclear Fuel UO_2," *Journal of Nuclear Materials,* Vol. 135, p. 140, 1985.

[13] J. A. Turnbull, R. White, and C. Wise, The Diffusion Coefficient for Fission Gas Atoms in UO_2, IAEA-TC-659/3.5 (1987) pp. 174-181.

[14] T. A. Hayes and M. E. Kassner, "Creep of Zirconium and Zirconium Alloys," *Metallurgical and Materials Transactions,* Vol. 37A, p. 2389, 2006.

[15] N. E. Hoope, "Engineering Model for Zircaloy Creep and Growth," Proceedings of the ANS-ENS International Topical Meeting on LWR Fuel Performance, Avignon, France, April 21-24, 1991.

[16] A. M. Ross and R. L. Stoute, Heat Transfer Coefficient Between UO_2 and Zircaloy-2, Atomic Energy of Canada Technical Report, AECL-1552, 1962.

[17] D. R. Olander, Fundamental Aspects of Nuclear Reactor Fuel Elements, National Technical Information Service, Springfield, Virginia, 1978, Chapters 10 and 16.

[18] A. Denis and R. Piotrkowski, "Simulation of Fission Gas Release," *Journal of Nuclear Materials,* Vol. 229, p. 149, 1996.

[19] The Third Riso Fission Gas Project Bump Test GE7 (ZX115), Technical Report RISO-FGP3-GE7, September 1990.

Appendix 1

Input file for Riso3-GE7 Bump Test

```
 [GlobalParams]
  density = 10431.0
  disp_x = disp_x
  disp_y = disp_y
  order = FIRST
  family = LAGRANGE
  energy_per_fission = 3.2e-11
[]

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

# Set problem dimension (2d-rz here) and import mesh file
[Mesh]
  file = pelletcladsmearedmedium1_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
  [../]

  [./burnup]
    block = 2
  [../]

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

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

  [./stress_xx]      # stress aux variables are defined for output
    order = CONSTANT
    family = MONOMIAL
  [../]
```

```
  [./stress_yy]
    order = CONSTANT
    family = MONOMIAL
  [../]
  [./stress_zz]
    order = CONSTANT
    family = MONOMIAL
  [../]
  [./vonmises]
    order = CONSTANT
    family = MONOMIAL
  [../]
   [./creep_strain_hoop]
    order = CONSTANT
    family = MONOMIAL
  [../]
  [./elastic_strain_hoop]
    order = CONSTANT
    family = MONOMIAL
  [../]
  [./plastic_strain_hoop]
    order = CONSTANT
    family = MONOMIAL
  [../]
  [./plastic_strain_radial]
    order = CONSTANT
    family = MONOMIAL
  [../]
  [./plastic_strain_axial]
    order = CONSTANT
    family = MONOMIAL
  [../]
[]

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

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

  [./axial_peaking_factors]      # reads and interpolates an input file containing the axial power profile vs time
    type = PiecewiseBilinear
    yourFileName = powerfactor72.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'
    y = '0 1'
```

```
  [../]

  [./fast_neutron_flux_function]
    type = PiecewiseLinearFile
    yourFileName = FastNeutronFlux.csv
    format = columns
  [../]

  [./q]
    type = Composite
    functions = 'power_history axial_peaking_factors'    # W/m
  [../]

[]

# 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
[Kernels]

[
  [./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_history            # using the power function defined above
    function2 = axial_peaking_factors     # using the axial power profile function defined above
    pellet_diameter = 0.01041
```

```
  pellet_inner_diameter = 0
  f_volume_reduction = 1
[../]

[./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
[../]

[./fast_neutron_flux]
  type = FastNeutronFluxAux
  variable = fast_neutron_flux
  block = 1
  factor = 1
  function = fast_neutron_flux_function
[../]

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

[./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_hoop]
  type = MaterialTensorAux
```

```
    tensor = creep_strain
    variable = creep_strain_hoop
    index = 2
    execute_on = timestep
  [../]
  [./elastic_strain_hoop]
    type = MaterialTensorAux
    tensor = elastic_strain
    variable = elastic_strain_hoop
    index = 2
    execute_on = timestep
  [../]
  [./plastic_strain_hoop]
    type = MaterialTensorAux
    tensor = plastic_strain
    variable = plastic_strain_hoop
    index = 2
    execute_on = timestep
  [../]
  [./plastic_strain_radial]
    type = MaterialTensorAux
    tensor = plastic_strain
    variable = plastic_strain_radial
    index = 0
    execute_on = timestep
  [../]
  [./plastic_strain_axial]
    type = MaterialTensorAux
    tensor = plastic_strain
    variable = plastic_strain_axial
    index = 1
    execute_on = timestep
  [../]
[]

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

# 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
  [../]
[]
```

```
# 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 = DirichletBC
    variable = temp
    boundary = ' 1 2 3'
    value = 564
[../]

  [./Pressure]
#  apply coolant pressure on clad outer walls
    [./coolantPressure]
      boundary = '1 2 3'
      factor = 7.24e6
      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 = 0.29e6
      startup_time = 1.0e4
      R = 8.3143
      output_initial_moles = initial_moles       # coupling to post processor to get inital 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
    [../]
```

```
  [../]

[ ]

# Define material behavior models and input material property data
[Materials]
  [./fuel_thermal]                    # temperature and burnup dependent thermal properties of UO2 (bison kernel)
    type = ThermalUO2
    block = 2
    temp = temp
    burnup = burnup
  [../]

  [./fuel_elasticity_and_creep]
    type = CreepUO2
    block = 2
    disp_r = disp_x
    disp_z = disp_y
    temp = temp
    fission_rate = fission_rate
#    cracking_stress = 130e6
#    max_cracks = 1
#    active_crack_planes = 2
    youngs_modulus = 2.e11
    poissons_ratio = .345
    thermal_expansion = 10e-6
#    grain_radius = 6.0e-6
    grain_radius = 10.0e-6              # set larger than 6 microns (see ForMas) to impove convergence
    oxy_to_metal_ratio = 2.0
    max_its = 10
    output_iteration_info = false
  [../]

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

  [./fuel_relocation]
    type = RelocationUO2
    block = 2
    burnup = burnup
    diameter = 0.01041                  # fuel pellet diamter in meters
    gap  = 220.e-6                      # diametral gap in meters
    q = q
    burnup_relocation_stop = 0.03       # turn off relocation just before contact
  [../]

  [./clad_thermal]                      # general thermal property input (elk kernel)
    type = HeatConductionMaterial
    block = 1
    thermal_conductivity = 16.0
    specific_heat = 330.0
    density = 6551.0
```

```
  [../]

  [./clad_solid_mechanics]             # thermoelasticity, plasticity, and thermal and irradiation creep for Zr4
    type = ThermalIrradiationCreepPlasZr4
    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
    yield_stress = 230e6
    hardening_constant = 2.5e9
    a_coef = 3.14e24
    n_exponent = 5
    activation_energy = 2.7e5
    c0_coef = 9.881e-28
    c1_exponent = 0.85
    c2_exponent = 1.0
    thermal_expansion = 5.0e-6
    relative_tolerance =1e-7
    max_its = 100
    output_iteration_info = false
  [../]

  [./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 = 6.0e-6             # prescribed grain size is 11.3-12.8 microns
    external_pressure = 10.0e6
    calibration_factor = 6.5
  [../]
[]

[Executioner]
  type = AdaptiveTransient

  # PETSC options
  petsc_options = '-snes_mf_operator -ksp_monitor'
  petsc_options_iname = '-snes_type -snes_ls -ksp_gmres_restart -pc_type -pc_hypre_type -
pc_hypre_boomeramg_max_iter'
  petsc_options_value = 'ls        basic    201              hypre    boomeramg      4'

  # 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 = 161801196
  num_steps = 5000

  time_t =  '  0  161759796  161785896'
  time_dt = '200        100        100'
  dtmax = 2e6
  dtmin = 1
  optimal_iterations = 6
  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 = 9
     variable = temp
   [../]

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

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

  [./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
  [../]

  [./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
  [../]

  [./average_fission_rate]
    type = AverageFissionRate
    rod_ave_lin_pow = power_history
    fuel_outer_radius = 5.205e-3
    fuel_inner_radius = 0.0
  [../]

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

# Define output file(s)
[Output]
  file_base = out_3-22-2012
```

```
  interval = 1
  output_initial = true
  exodus = true
  perf_log = true
[]
```