

Development of a U-19Pu-10Zr Fuel Performance Benchmark Case Based on the IFR-1 Experiment

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ABSTRACT

Metallic nuclear fuels are subject to research and development for use in advanced reactors. Robust, accurate metallic fuel performance models are important for the design, safety analysis, and licensing of these reactors. However, metallic fuel performance models require additional development; they are not as mature as UO_2 fuel performance models. A benchmark case based on the IFR-1 experiment was developed to better gauge the accuracy of existing models, identify models for high-priority development, and potentially quantify any future improvements made by further model development.

This work collected publicly available information on the IFR-1 experiment and used it to develop the benchmark case. Fuel behavior during the IFR-1 irradiation was simulated by using the fuel performance code BISON, and the predicted results were compared with postirradiation examination data from the IFR-1 experiment. A sensitivity study and tuning studies were performed as a preliminary investigation into the causes of inaccurate temperature and dimensional change predictions.

The benchmark predicted reasonably accurate values for the burnup and fission gas release. There was error in the predicted temperatures, which could be explained by uncertainty in the input parameters and legacy temperatures. BISON over-predicted dimensional changes in the fuel and cladding. The sensitivity study showed that the dimensional changes were most sensitive to the fuel swelling anisotropy and the cladding void swelling model. Future benchmark and model development should focus on cladding swelling behaviors to improve dimensional change predictions.

KEYWORDS: U-Pu-Zr, fuel performance, BISON, sensitivity analysis

1. INTRODUCTION

UO₂ is the dominant nuclear fuel worldwide and is well-established for use in light water reactors, Canada Deuterium Uranium (CANDU) reactors, and Advanced Gas Reactors. Decades of research and development have gone into fuel performance models for this ceramic fuel type. Far less development has been devoted to U-Zr-based metallic fuel performance models [1, 2, 3, 4, 5]. Currently, the US

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6 Department of Energy (DOE) is considering the use of metallic fuel (either U-Zr or U-Pu-Zr) for a possible
7 new test reactor [6, 7], and several private companies are considering metallic fuels in novel reactor
8 designs [8, 9]. Because of these developments, a new focus has been placed on developing accurate fuel
9 performance models to support reactor design, experiment design, and safety qualification for metallic
10 fuels.

11 One way to gauge the accuracy of existing and future metallic fuel performance models is through the
12 use of benchmark cases. Benchmark cases are fuel performance simulations of irradiation experiments
13 that compare the predicted results with the corresponding legacy results. Benchmark cases aid in the
14 development of fuel performance models in several ways. First, they enable the assessments of the
15 accuracy of existing models. Second, any inaccurate predictions can be used to identify models for high-
16 priority development. Third, they can be used to quantify the subsequent improvements made by new or
17 updated models.

18 This work details the development of a benchmark case for 71 wt. % U, 19 wt. % Pu, 10 wt. % Zr (U-19Pu-
19 10Zr) metallic fuel based on the IFR-1 experiment. The IFR-1 experiment was one of seven full-size fuel
20 assemblies irradiated during the Integral Fast Reactor (IFR) program and was the only full-size assembly to
21 include U-Pu-Zr fuel rods [10].

22 The IFR concept was developed by Argonne National Laboratory during the late 1980s and early 1990s
23 [11], and its technology underlies the US Advanced Liquid Metal Reactor program [12] and GE Hitachi's
24 PRISM (Power Reactor Innovative Small Module) reactor [13]. The goal of the program was to update and
25 commercialize the technology used in Experimental Breeder Reactor II (EBR-II), a Na pool-type fast
26 reactor [13]. Most experiments for the IFR were irradiated in EBR-II, but a full-size IFR fuel pin could not
27 be irradiated in EBR-II because the IFR design called for longer fuel pins [10]. Thus, the IFR-1 experiment
28 was irradiated in the Fast Flux Test Facility (FFTF) in Hanford, Washington to identify any long-rod effects
29 not observed in EBR-II fuel rods [14].

30 The FFTF was a loop-type Na-cooled fast-spectrum test reactor that operated between 1982 and 1992. It
31 had a larger test volume than EBR-II and transient testing capabilities [15]. The IFR-1 experiment was
32 irradiated between September 1986 and October 1988 to a target peak burnup of 10 at. %. Researchers
33 were interested in comparing the neutronic and mechanical effects of full-length IFR pins with those seen
34 in EBR-II's shorter test pins.

35 The experiment, including irradiation conditions and postirradiation examination (PIE) results, was
36 documented in three sources: a 1992 conference paper [16], a 2011 Idaho National Laboratory (INL)
37 report [10], and a 2012 peer-reviewed journal article based on the 2011 report [17]. There are some
38 inconsistencies in the data reported in the three sources such as the shape of the axial heat generation
39 distribution. In these cases, one of the original authors of the three sources determined that the 2011
40 report was generally the most complete and reliable [18]. This work includes a comprehensive description
41 of the IFR-1 benchmark case and its implementation in BISON. BISON predictions were compared to
42 legacy measurements [10] and calculations, including burnup, temperatures, fuel and cladding strains, and
43 fission gas release (FGR) fractions. While there are other important values that BISON can predict—such
44 as stresses—these predictions are not included in this work because no corresponding legacy values
45 could be found to gauge the accuracy. Preliminary studies to identify BISON models that could be
46 contributing to inaccurate predictions were also performed. Finally, recommendations are made for
47 further benchmark development and potential areas for additional BISON development.

48 BISON is a fuel performance code maintained by INL and under active development at a variety of
 49 laboratories and universities. As such, the BISON predictions presented in this work are likely to change
 50 over time and have changed since previous versions of the benchmark results were last reported [19].
 51 The work presented here is not meant to validate nor criticize current or future BISON versions. It is
 52 meant as a snapshot of current BISON accuracy and to aid in the future development of the code. All
 53 simulations for this work used a BISON version from June 24, 2020*.

54 2. SUMMARY OF SELECT BISON MODELS

55 A complete description of BISON models and capabilities is beyond the scope of this work but can be
 56 found in the BISON documentation [20, 21]. Only governing equations of the models of interest in this
 57 benchmark case are summarized here. The primary equations governing BISON simulations are
 58 conservation of energy, conservation of mass, and conservation of momentum [21]. Conservation of
 59 energy is described by the heat transport equation,

$$55 \quad \rho C_p \frac{\partial T}{\partial t} - \nabla \cdot (k \nabla T) - e_f \dot{F} = 0, \quad (1)$$

60 where ρ is the density, C_p is the specific heat, T is the temperature, k is the thermal conductivity, e_f is
 61 the average energy produced per fission, and \dot{F} is the fission rate. The conservation equation for a given
 62 species is

$$63 \quad \frac{\partial C}{\partial t} - \nabla \cdot (D \nabla C) + \lambda C - S = 0, \quad (2)$$

64 where C is the concentration, D is the diffusion coefficient, λ is the radioactive decay constant, and S is a
 source term. Conservation of momentum is described by Cauchy's equation,

$$65 \quad \nabla \cdot \sigma + \rho f = 0 \quad (3)$$

66 where σ is the Cauchy stress tensor and f is the body force per unit mass (such as gravity). The primary
 67 solution variable is displacement, which is connected to the stress field via strain through a constitutive
 relationship.

68 Local burnup, $\beta(\vec{x})$, is an important calculated variable correlated to other models such as swelling and
 69 fission gas release. It is based on the local fission rate, $\dot{F}(\vec{x}, t)$, and the initial fuel atom density $N_f^0(\vec{x})$,

$$70 \quad \beta(\vec{x}) = \int \frac{\dot{F}(\vec{x}, t)}{N_f^0(\vec{x})} dt, \quad (4)$$

71 where \vec{x} is the position vector.

72 Equations (1)–(4) are all analytical models. They are derived from relevant physics theories and have been
 73 successfully applied to multiple systems. However, some of the fast-reactor-specific correlations that go
 74 into these equations are empirical relationships. For example, the thermal conductivity of U-Zr-based
 fuels is based on fitting an equation to experimental data. Due to a lack of experimental data with

* git commit 45096d10ec4faeb6e1bba1a1ac99e553f3a18a2a

75 irradiated fuels, the irradiation effects on these equations are often the most uncertain models in BISON
76 U-Zr predictions.

77 Also of interest for this work are the fission gas production and release models for metallic fuels. The
78 amount of fission gas produced is described by the function,

$$G_p(\vec{x}, t) = \int \frac{\dot{F}(\vec{x}, t)\gamma}{N_A} dt, \quad (5)$$

79 where G_p is the amount of fission gas produced in moles, γ is the yield of gas atoms per fission, and N_A is
80 Avogadro's number. The amount of fission gas released, $G_r(\vec{x}, p, t)$, is calculated as

$$G_r(\vec{x}, p, t) = \begin{cases} 0, & p < p_c \\ \alpha_0 G_p(\vec{x}, t), & p = p_c \\ \alpha_0 G_p(\vec{x}, t_c) + \alpha_c \int_{t_c}^t G_p(\vec{x}, t') dt', & p > p_c \end{cases}, \quad (6)$$

81 where p and p_c are the porosity (as determined by the fission gas swelling model) and a critical porosity,
82 respectively, α_0 and α_c are the initial FGR fraction and post-critical FGR fraction, respectively, and t_c is
83 the time at which critical porosity was reached. Equation (5) is an analytical equation, while Equation (6)
84 is a semi-empirical equation. The form of Equation (6) is based on physics theory, but the individual terms
85 such as p_c , α_0 , and α_c can only be determined by fitting the model to match experimental data.

86 These equations govern the predictions of interest in the current work but are not comprehensive and do
87 not capture feedback and nonlinear effects. For example, fission gas production causes pore growth,
88 which increases the stress of the system, directly affecting the displacements and dimensional changes.
89 Pores also degrade thermal conductivity, which in turn causes the temperature in the fuel to increase.
90 That causes additional displacements through thermal expansion and thermal creep. So, Equation (5)
91 affects Equation (3) both directly and indirectly. For more complete descriptions of feedbacks and
92 nonlinear effects, see the BISON documentation [20, 21].

93 3. IFR-1 BENCHMARK CASE

94 Because of the low availability of pin-specific measurements and calculations, this benchmark case was
95 set up as a representative generic U-19Pu-10Zr pin rather than any specific pin. For each of the time-
96 dependent predicted results considered, all available legacy measurements and calculations were
97 included for comparison.

98 3.1. PROBLEM GEOMETRY

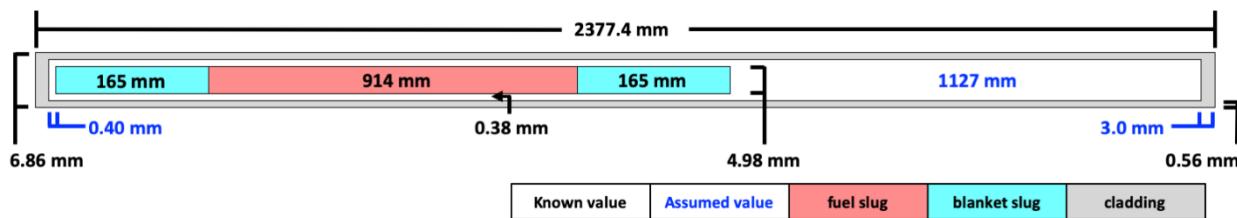
99 The IFR-1 test assembly consisted of 169 fuel pins in a hexagonal assembly. Of the pins, 18 contained U-
100 19Pu-10Zr alloy fuel, 19 contained U-8Pu-10Zr alloy fuel, and the remainder contained U-10Zr alloy fuel.
101 The U enrichment was adjusted for each alloy to maintain the same approximate heat generation rate. All
102 the pins were clad in 20% cold-worked D9 stainless steel [22] and were wrapped in 1.37 mm diameter D9
103 wire that served as a spacer between pins and as a turbulence generator to improve mixing and thermal
104 transport of the Na coolant. However, the wires were not included as part of the simulation mesh.

105 The active fuel column of each pin was made of three slugs with a combined length of 914 mm. These
106 slugs were sandwiched between two 165 mm blanket slugs typical of use in an axial blanket. The blankets

107 were composed of a U-10Zr alloy with depleted U. The radial gap between the slugs and the cladding was
108 filled with Na.

109 The cladding had an external diameter of 6.86 mm and a wall thickness of 0.56 mm. The total cladding
110 length was 2,377.4 mm. The 2011 report [10] stated that at operating temperatures, the fuel/plenum
111 ratio was 1.0. However, the amount of Na was not recorded, so the exact length of the plenum could not
112 be determined. Additionally, no measurements are given for the cladding ends. The top of the cladding
113 had a solid machined section meant for handling the fuel in a hot cell [10]. The bottom end plug
114 configuration included provisions to hold it in place inside the assembly [2, 10].

115 The dimensions used in the benchmark case are shown in Figure 1. The end caps were modeled as flat
116 with a thickness of 3 mm. This approximation does not match the actual end caps but significantly
117 simplifies the mesh. During benchmark development, several thicknesses were tested, and the end cap
118 thicknesses was determined to not significantly impact the predicted results [19]. A small gap of 0.4 mm
119 was also included between the bottom end cap and the bottom blanket slug to prevent computationally
120 expensive contact between the bottom blanket at the cladding. This gap is not necessarily physically
121 accurate, but the approach improves the computational stability and efficiency with negligible impact on
122 the benchmark accuracy.



123
124 *Figure 1. Benchmark case cross-sectional dimensions (not to scale). Black text indicates values from the IFR-1 report*
125 *[10], and blue text indicates values that had to be assumed.*

126 For the BISON simulation, a 2D-RZ axisymmetric mesh was used rather than a full 3D mesh. This was
127 much more computationally efficient and was not expected to impact the predictions because no
128 azimuthal variations were known or modeled. The fuel slug mesh was glued to the blanket meshes,
129 eliminating the need to model contact at the fuel-blanket interfaces.

130 3.2. LINEAR HEAT GENERATION RATE

131 The linear heat generation rate (LHGR) is a primary input into fuel performance simulations. It specifies
132 the energy output of the fuel pin as a function of time and axial position within the fuel. As is commonly
133 done in BISON, the LHGR was treated as a product of two functions: the time dependent average LHGR,
134 $\overline{LHGR}(t)$, and the spatially dependent peaking factor, $p(z)$:

$$LHGR(t, z) = \overline{LHGR}(t)p(z), \quad (7)$$

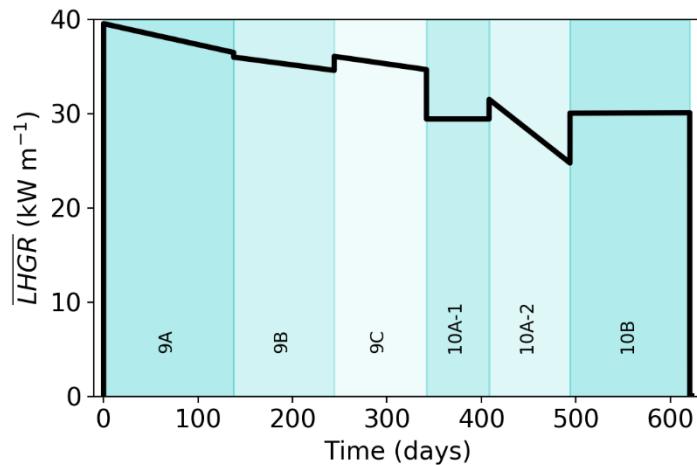
135 where t is the time, and z is the axial position in units of length. Because the peaking factor was meant to
136 reflect deviation from the average, it had the additional constraint:

$$\frac{1}{z_t - z_b} \int_{z_b}^{z_t} p(z) dz = 1, \quad (8)$$

137 where z_b and z_t represent the axial positions of the bottom and top of the active fuel column,
 138 respectively.

139 The IFR-1 experiment ran over the course of six FFTF operating cycles: 9A, 9B, 9C, 10A-1, 10A-2, and 10B.
 140 The INL report included equivalent full-power days (EFPDs) for each operating cycle, as well as the
 141 assembly average LHGR for nearly every beginning of cycle (BOC) and end of cycle (EOC). The only
 142 exception was that no LHGR was recorded for cycle 10A-1 EOC. For convenience, it was assumed that the
 143 10A-1 EOC LHGR matched the 10A-1 BOC LHGR.

144 The power history used in the benchmark case is shown in Figure 2. It began with a coolant inlet
 145 temperature of 298 K and an average LHGR of 0 kW m^{-1} . Over 1 hr, the coolant inlet temperature
 146 increased to 633 K [10], and the average LHGR increased to cycle 9A's BOC average LHGR of 39.6 kW m^{-1} .
 147 The cycle 9A simulation lasted for 138 days to match the legacy EFPD, during which time the average
 148 LHGR was modeled to decrease linearly to the 9A EOC average LHGR of 36.5 kW m^{-1} . After 9A EOC, 1 hr
 149 was added to simulate the transition to 9B BOC average LHGR. The simulation followed this pattern for
 150 the remaining cycles with a constant coolant inlet temperature. Shutdown was simulated over 3 hrs. In
 151 the first hour, the simulated power cycled down to 0.1% of cycle 10B's EOC average LHGR to approximate
 152 decay heat. In the second hour, the simulated coolant inlet temperature was reduced to the experimental
 153 PIE temperature of 305 K [10]. During the third hour, all the parameters were held constant to allow the
 154 simulation to reach equilibrium before PIE measurements were made.



155
 156 *Figure 2. The average LHGR of the IFR-1 benchmark case throughout the six operating cycles.*

157 During the fuel lifetime, the blanket slugs breed fissile isotopes and then begin to fission. However, it is
 158 unclear whether this was accounted for while calculating the average LHGR in the IFR-1 report [10]. For
 159 simplicity, this work assumed it was not. The axial peaking factor in the fuel slug was determined by fitting
 160 a fourth order polynomial to the axial power curve calculated in the report [10]. The polynomial was
 161 integrated over the active fuel column length to calculate the average simulated LHGR at that time. Then,
 162 the polynomial coefficients were divided by the average LHGR to determine the peaking factor

163 polynomial. Isotopic gamma scans of ^{106}Rh from the report were used to approximate the average power
 164 of the blankets. The axial peaking factor was then defined by using the piecewise equation:

$$p(z) = \begin{cases} (m_b z + b_b)bu^*, & 0 \leq z < z_b \\ a_0 + a_1 z_f + a_2 z_f^2 + a_3 z_f^3 + a_4 z_f^4, & z_b \leq z \leq z_t, \\ (m_t z + b_t)bu^*, & z_t < z \leq 1.244 \end{cases} \quad (9)$$

$$z_f = z - z_b,$$

$$bu^* = \frac{bu}{bu_{ref}},$$

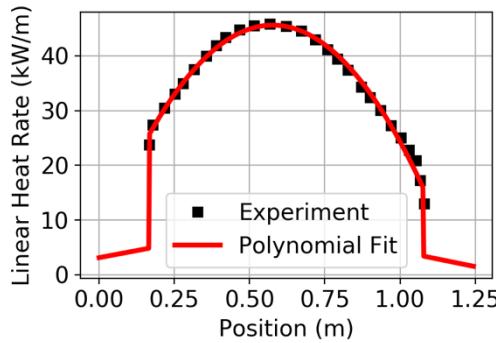
165 where bu is the peak burnup; bu_{ref} is a reference burnup; bu^* is the normalized burnup; z is axial
 166 position; z_b and z_t are the bottom and top positions of the active fuel column, respectively; z_f is the axial
 167 position relative to the fuel column; and the remaining values are fitting coefficients. The fitting
 168 coefficients and reference burnup are given in

169 Table 1. Equation (9) is compared with the report's axial power curve in Figure 3.

170
 171 *Table 1. Constants and fitting parameters for Eq. (9).*

Constant	Value
a_0	0.68687
a_1	2.6352
a_2	-3.20026
a_3	1.35×10^{-5}
a_4	2.69×10^{-5}
b_b	0.084
b_t	0.416
bu_{ref}	5 at. %
m_b	0.279 m^{-1}
m_t	-0.301 m^{-1}
z_b	0.165 m
z_t	1.079 m

172



173
174 *Figure 3. Comparison of the legacy and simulated LHGR profiles at an average LHGR of 37.1 kW m⁻¹ and a peak*
175 *burnup of 5%.*

176 There are three points to consider regarding Eq. (9). First, there was a discrepancy between the axial
177 power profile from the 2011 report used to create Eq. (9) [10] and that reported in the 2012 IFR-1 paper
178 [17]. According to an author of both documents, the 2011 report has the more accurate profile [18].
179 Second, in reality, the axial peaking factor changes with burnup. For this work, it is assumed to be
180 constant because only one profile was calculated during the experiment [10, 17]. Third, Eq.(8) was
181 satisfied only within the active fuel column due to the assumption that the legacy power profile did not
182 include power generated in the blanket. At 10 at. % peak burnup, $LHGR(t, z)$ was 6% higher than
183 $\overline{LHGR}(t)$ due to the blankets.

184 **3.3. ADDITIONAL PARAMETERS**

185 BISON supplied many of the U-10Zr, U-19Pu-10Zr, and D9 material properties internally [20]. However,
186 users must provide others to specify fuel, cladding, and coolant properties. This section lists the material
187 properties used in the IFR-1 benchmark case, except for those called from within BISON. The parameters
188 are sorted by material and tabulated with units and references. Any parameters that required additional
189 derivation or discussion are also explained.

190 Table 2 contains the material parameters for the U-19Pu-10Zr fuel slug. The parameters are for models
191 that include heat transport, thermal expansion, solid mechanics, solid fission product swelling, gaseous
192 fission product swelling, and fuel creep. The anisotropic swelling factor is a value entered as input to
193 control the anisotropy of the predicted fuel swelling. A value of -1 corresponded to 100% axial swelling, a
194 value of 0 was isotropic swelling, and a value of 1 was 100% radial swelling. Metallic fuels swell
195 preferentially in the radial direction, so a value of 0.5 (75% radial swelling) was used [23].

196 *Table 2. Material parameters of the U-19Pu-10Zr fuel slug.*

Parameter	Value	Reference
Anisotropic swelling factor	0.5	[23]
Atom fraction of Pu	0.16	[24]
Atom fraction of Zr	0.226	[24]
Average energy per fission	3.159×10^{-11} J	[10]
Coefficient of thermal expansion	17.3×10^{-6} K ⁻¹	[24]
Initial density	15,800 kg m ⁻³	[24]
Fast flux factor	8.64×10^{14} n J ⁻¹ m ⁻¹	[10, 19]
Thermal expansion reference temperature	295 K	

197

198 The coefficient of thermal expansion (CTE) for U-19Pu-10Zr, as well as CTEs of other materials, had to be
 199 derived. The thermal expansion equation from Janney [24] is nonlinear, but the BISON model used in this
 200 work required a linear thermal expansion equation [20]:

$$\frac{\Delta L}{L_0} = \alpha(T - T_0), \quad (10)$$

201 where L_0 is the reference length at temperature T_0 , T is the current temperature, α is the CTE, and ΔL is
 202 the displacement or change in length. A least-squares approximation was used to linearize the thermal
 203 expansion equation. The slope of the linear equation was used as the CTE, and the reference temperature
 204 was set to the initial temperature of 295 K for all materials to maintain as-manufactured dimensions.

205 The fast flux factor was the ratio of fast neutron flux ($\text{n m}^{-2} \text{ s}^{-1}$) to LHGR (W m^{-1}). It was approximated by
 206 dividing the peak total fast neutron fluence ($15.4 \times 10^{26} \text{ n m}^{-2}$ [10]) by the time integral of $\overline{\text{LHGR}}(t)$ over
 207 the experiment lifetime ($1.78 \times 10^{12} \text{ J m}^{-1}$ [19]) to get $8.64 \times 10^{14} \text{ n J}^{-1} \text{ m}^{-1}$.

208 Table 3 provides the material parameters for the blanket slugs. The anisotropic swelling factor was the
 209 same as for the fuel slug. The density and atom fraction of Zr were different due to the blankets' different
 210 composition. The CTE was linearized using the same method as the fuel slug but by using a nonlinear
 211 thermal expansion equation for U-10Zr [24].

212 *Table 3. Material parameters of the U-10Zr blankets.*

Parameter	Value	Reference
Anisotropic swelling factor	0.5	[23]
Atom fraction of Zr	0.225	[24]
CTE	$16.6 \times 10^{-6} \text{ K}^{-1}$	[24]
Initial density	$16,310 \text{ kg m}^{-3}$	[24]

213

214 BISON developers derived BISON's empirical fission gas swelling and FGR model to match experimental
 215 observations [20]. As such, it had multiple adjustable parameters. The values used in this work are given
 216 in Table 4 and were provided by a BISON developer [25] who calibrated the models to match EBR-II data
 217 from Pahl and Wisner [26].

218 *Table 4. Input parameters of the fission gas swelling and FGR models.*

Parameter	Value	Reference
Bubble number density	$2.09 \times 10^{19} \text{ m}^{-3}$	[25]
Critical porosity	0.17195	[25]
Initial FGR fraction	0.558	[25]
Interconnection initiating porosity	0.125	[25]
Interconnection terminating porosity	0.2185	[25]
Post-critical FGR fraction	0.777	[25]

219

220 Table 5 provides the material parameters for the D9 cladding. All were taken from Hofman et al. [22]. The
 221 CTE was determined in the same way as described for the fuel slug. The Poisson's ratio and Young's

222 modulus were both calculated from the Hofman et al. correlations [22] at an assumed temperature of
223 733 K.

224 *Table 5. Material parameters of the D9 cladding.*

Parameter	Value	Reference
Initial density	$7,761 \text{ kg m}^{-3}$	[22]
CTE	$1.9 \times 10^{-5} \text{ K}^{-1}$	[22]
Poisson's ratio	0.35	[22]
Young's modulus	$1.645 \times 10^{11} \text{ Pa}$	[22]

225
226 The material parameters for liquid Na used in the gap and coolant are given in Table 6. The coolant inlet
227 mass flux was not measured during the experiment. Instead, the FFTF design coolant velocity (7.01 m s^{-1}
228 [15]) was multiplied by the Na density at the coolant inlet temperature of 622 K (866.9 kg m^{-3} [27]).
229 However, the velocity had considerable uncertainty because the design velocity was published in 1980
230 before FFTF began operation. It is unknown whether the velocity was adjusted after the reactor began
231 experimental operation or for individual experiments.

232 *Table 6. Material parameters of the sodium coolant and plenum*

Parameter	Value	Reference
Coolant inlet mass flux	$6,079 \text{ kg m}^{-2} \text{ s}^{-1}$	[15, 27]
Coolant inlet pressure	$1.02 \times 10^6 \text{ Pa}$	[15]
Plenum pressure	84,000 Pa	
Rod pitch ^a	$8.23 \times 10^{-3} \text{ m}$	[10]
Thermal conductivity	$61 \text{ W m}^{-1} \text{ K}^{-1}$	[27]

233 ^aEqual to the pin diameter plus spacing wire diameter

234 The initial plenum pressure was not included in the available IFR-1 reports [10, 16, 17]. As such, a sub-
235 atmospheric pressure representative of the glove box fabrication method used for the IFR-1 pins was
236 assumed. The thermal conductivity was input into BISON as a constant, but Fink and Leibowitz provided it
237 as a function of temperature [27]. The constant value needed to be calculated at a correct sodium
238 temperature, but the predicted temperature profile is partially determined by the thermal conductivity. A
239 simplified mathematical expression of this is $k = f(T)$, $T = g(k)$, where f and g are functions, k is the
240 thermal conductivity, and T is the gap temperature. The thermal conductivity listed in Table 6 was chosen
241 by iteration. A guess T was used to calculate k . Then that value of k was used in a simulation. The gap
242 temperature at cycle 9A BOC was used as a new guess T , and the process was repeated. Subsequent
243 development has added the capability to input thermal conductivity as a function of temperature, so
244 future work can avoid iterations like these.

245 3.4. AVAILABLE DATA FOR COMPARISON

246 One goal of this work was to compare BISON simulation results with legacy measurements and
247 calculations. To do so, it was necessary to determine which data were measured or calculated and which
248 of those data BISON could replicate. Seven legacy measurements and calculations (hereafter referred to
249 as legacy values) that could be directly compared to the BISON predictions were identified:

- 250 1. calculated peak burnup at the end of most cycles,
- 251 2. calculated peak cladding temperature at the beginning and end of each cycle,

252 3. measured coolant outlet temperature during cycle 9A—the only cycle for which the INL report
253 [10] included these measurements,
254 4. measured cladding radial dilation at the time of PIE,
255 5. measured cladding axial elongation at the time of PIE,
256 6. measured fuel axial elongation at the time of PIE, and
257 7. calculated FGR at the time of PIE.

258 The simulation results presented in Sections 4–6 were compared with these legacy values. Other
259 measurements were also taken, such as axial isotopic distributions, radial constituent redistribution, Na
260 penetration, and pin bowing. However, at the time of this work, BISON could not simulate these effects*.
261 There were also quantities that BISON could calculate that were not measured during the experiment,
262 such as stresses in the fuel and cladding and the full fuel temperature profile.

263 **3.5. SIMULATION PROPERTIES**

264 The 2D-RZ simulation mesh was built with BISON’s internal mesh generation system. It consisted of four
265 blocks: the cladding, the fuel column, and two blanket slugs. The fuel column and blanket slugs were
266 attached as shown in Figure 1, but the cladding block did not initially contact the three slugs. The cladding
267 wall included 4 radial elements and 400 axial elements. The fuel slug contained 6 radial and 300 axial
268 elements, and each blanket contained 6 radial and 40 axial elements. A mesh refinement study was
269 performed, and it was concluded that refining the mesh further would not alter the results.

270 Three primary variables were being solved by a system of nonlinear partial differential equations (PDEs):
271 temperature, radial displacement, and axial displacement. Any other variables, such as burnup and FGR,
272 were calculated based on the PDE variables’ values. The initial conditions for the PDE variables were a
273 uniform temperature of 295 K and zero displacements.

274 Boundary conditions for the axial displacement were zero-value Dirichlet conditions at the bottom of the
275 cladding and bottom of the lower blanket slug. The only boundary condition for radial displacement was a
276 zero-value Dirichlet condition at the center line of the fuel and cladding, which was the line of symmetry.
277 Boundary conditions for the temperature included a zero-flux Neuman condition at the center line, more
278 complex functions controlling heat transfer across the gap between the fuel and the cladding, and a
279 coolant flow model that governed heat transport from the cladding to the coolant [20]. The coolant flow
280 model also included feedback that allowed the coolant to increase in temperature and expand as it
281 moved up the fuel pin.

282 As the meshes displaced, BISON used a finite element method (FEM) contact model [20]. However, the
283 treatment of friction as two blocks move against one another can be somewhat complicated in solid
284 mechanics solvers. There were three available options for modeling friction in BISON [20]. The simplest
285 was to not include friction and allow blocks to freely slide against one another. The second option was to
286 use a glued contact model (i.e., mesh points on fuel and cladding surfaces remain connected after
287 achieving contact due to swelling). The third option, which was also the most computationally complex,
288 was to actually model friction forces between the blocks. This required an additional friction coefficient
289 parameter. The primary (i.e., baseline) simulation used the frictionless contact model because it was the
290 most computationally inexpensive. However, the other contact models were also simulated. Their effects
291 are discussed in Section 5.

292 **4. BASELINE SIMULATION**

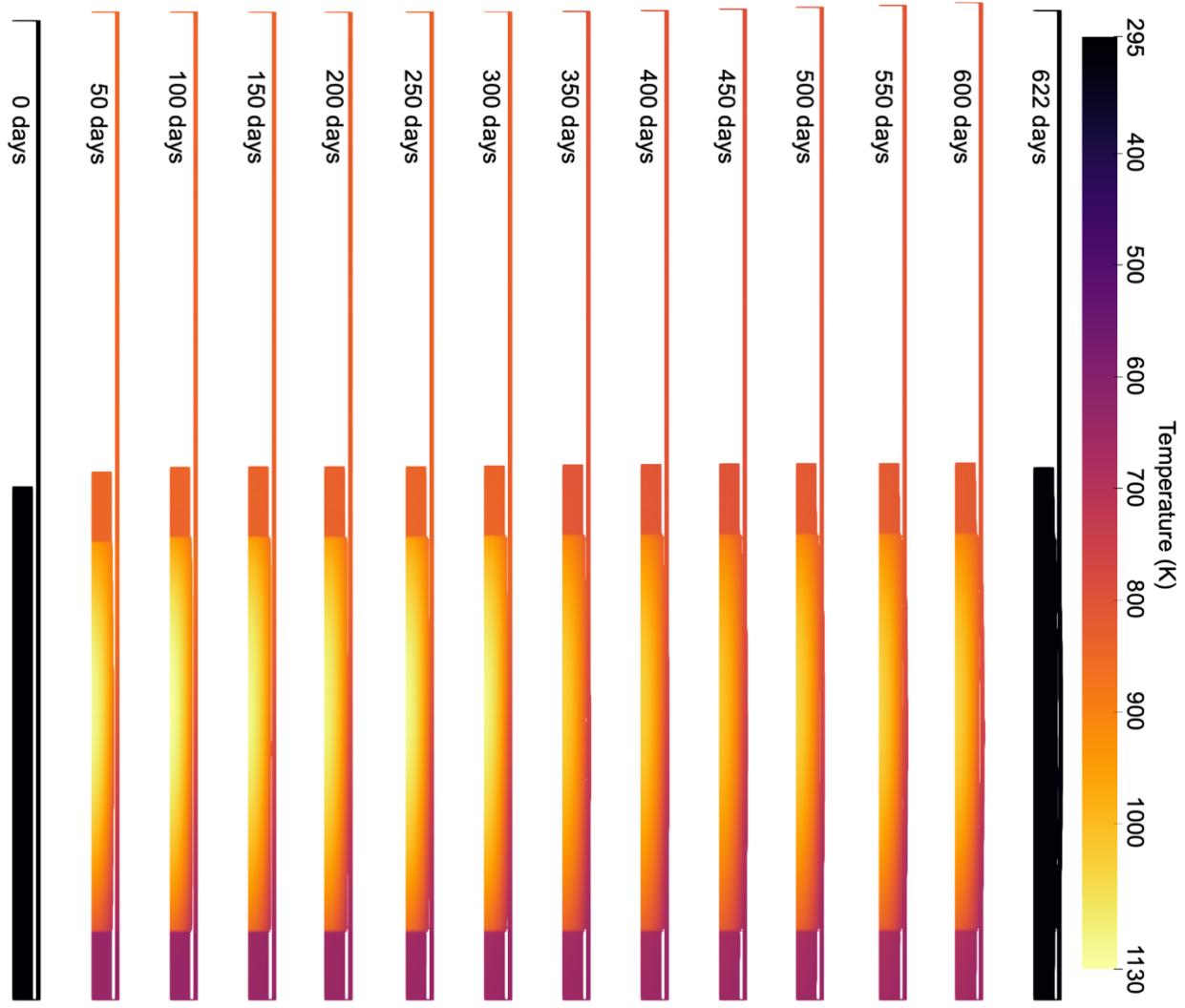
* Constituent redistribution and Na infiltration models were under active development at the time of this work.

293 4.1. SETUP

294 The baseline simulation used all of the parameters listed in Section 3 and the frictionless contact model. It
295 represented the best approximation of the IFR-1 experiment based on the available data. The simulation
296 input file was added to the BISON repository and could be updated in the future as models are improved
297 or if more relevant data are found.

298 4.2. RESULTS

299 Figure 4 shows the FEM mesh at several times during the simulation. The mesh in the figure was
300 compressed by a factor of 20 in the axial direction to facilitate viewing. All three primary variables are
301 shown in the figure. The temperature is represented by the mesh color, and displacements appear as
302 changes to the mesh dimensions. The blankets are not explicitly labeled but can be distinguished as the
303 regions with lower temperatures and displacements above and below the active fuel column. The
304 representations in black for 0 days and 622 days represent simulated dimensions that correspond to the
305 time of as-fabricated measurement and PIE, respectively.



306
 307 *Figure 4. Predicted temperature and displacement results from the baseline BISON simulation. The mesh was*
 308 *compressed by a factor of 20 in the axial direction to make it easier to view. Simulation times are given near the top*
 309 *of each image. Color indicates temperature. Displacements are shown through dimensional changes of the mesh.*

310 Comparisons are made between the predicted results and legacy values in Figure 5. In all seven plots,
 311 predicted results are in red and legacy values are in black. Plot 5(a) shows predicted and legacy peak
 312 burnups throughout the experiment. The simulation agreed very well with the experiment. Plot 5(b)
 313 shows the peak cladding temperatures throughout the experiment. The predicted results were biased
 314 (i.e., had a consistent error) by about 43 K; this difference is discussed later in the paper. Plot 5(c) shows
 315 the predicted coolant outlet temperature through the entire experiment and the measured legacy
 316 coolant outlet temperature during cycle 9A. Once again, the BISON simulation was biased, this time by an
 317 average of 23 K.

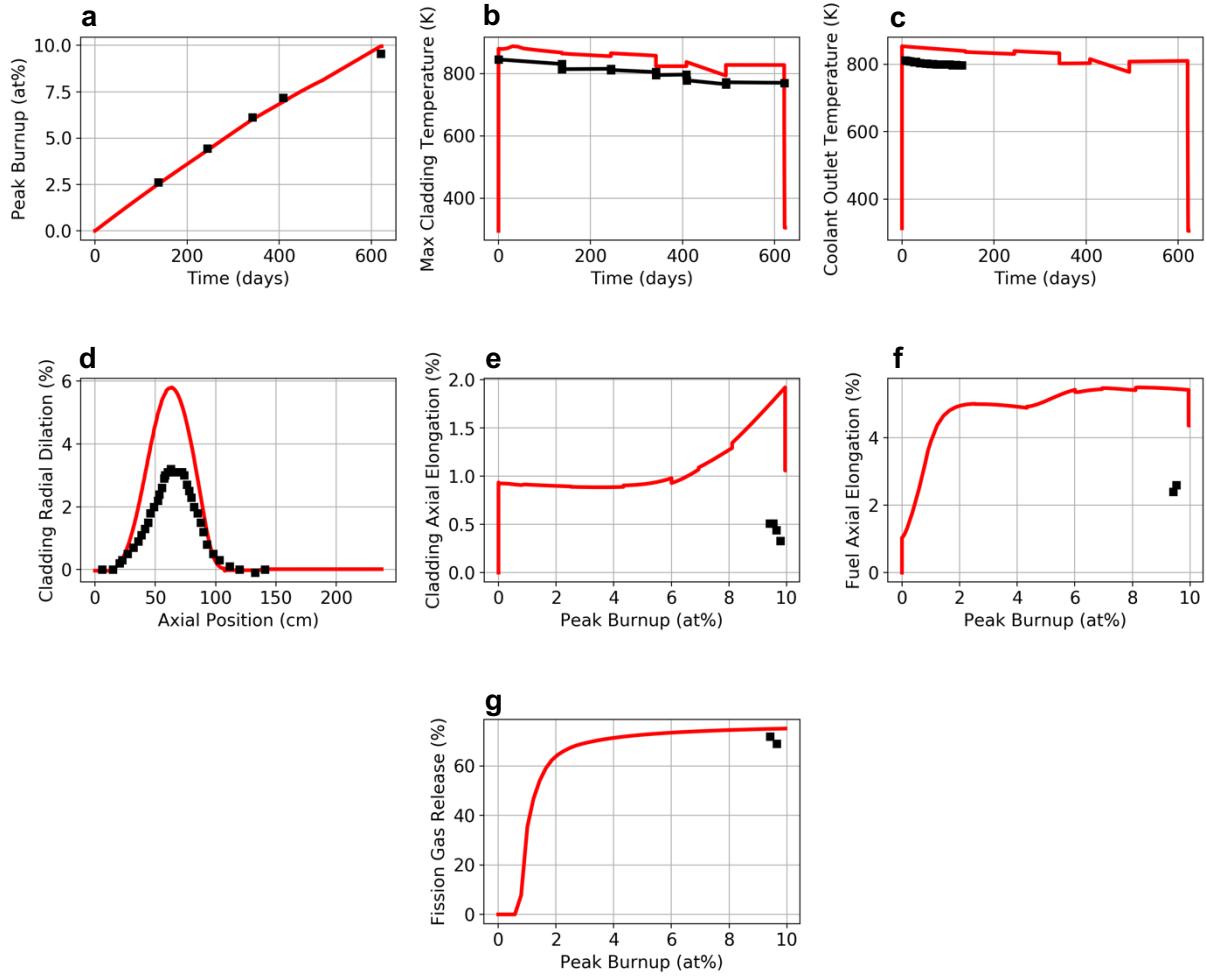
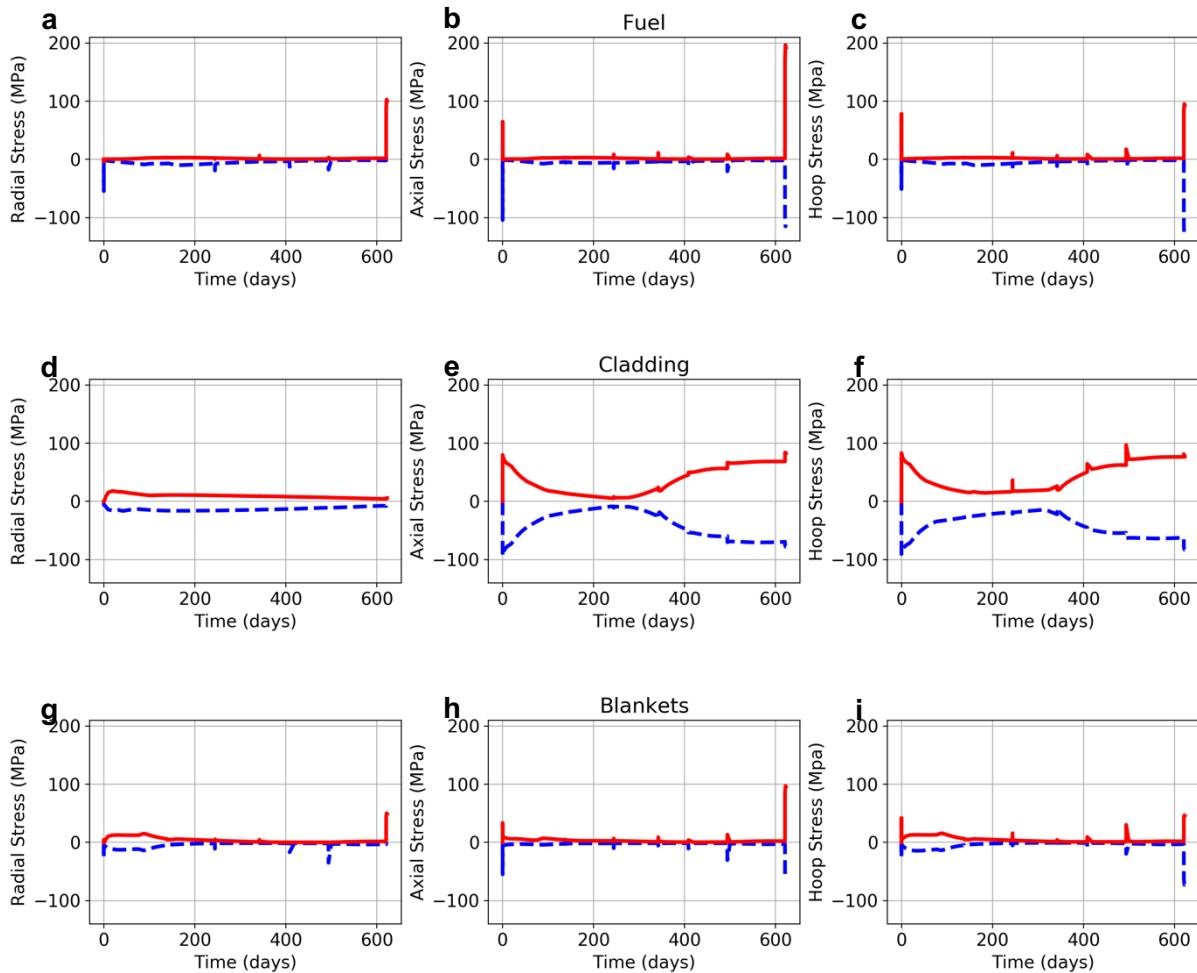


Figure 5. Comparison of BISON baseline predictions (red) and legacy values (black). All available data from U-19Pu-10Zr pins are included. The subplots show a) peak burnup, b) maximum cladding temperature, c) coolant outlet temperature, d) cladding radial dilation at PIE conditions, e) cladding axial elongation, f) fuel axial elongation, g) FGR fraction.

318 Plot 5(d) shows the predicted and legacy PIE cladding radial dilation. The measured peak cladding dilation
 319 was about 3.2%, and the simulation predicted 5.8% dilation. Plot 5(e) shows the cladding axial elongation.
 320 Thermal expansion and contraction during temperature changes can be seen as near-vertical lines at the
 321 beginning and end of the simulation. Predicted results are shown throughout the irradiation lifetime but
 322 were only measured experimentally during PIE at end of life (EOL). The four legacy values fell within the
 323 range of 0.33 to 0.51% elongation, and the simulated cladding axial elongation was 1.06% at EOL PIE
 324 conditions. Plot 5(f) shows the predicted and legacy fuel axial elongation. Once again, the predicted
 325 results are shown throughout the irradiation, and the legacy measurements were taken only at PIE. The
 326 fuel slug elongated 2.5%, and the simulation predicted 4.4% elongation. Plot 5(g) shows the FGR behavior
 327 for which the simulation compared well with PIE results. The legacy values were 69 and 72%, and the
 328 simulated FGR was 75%.

329 BISON-predicted peak stress components are shown in Figure 6 for reference. The subplots show radial,
 330 axial, and hoop stresses in the fuel, cladding, and blankets. The maximum values (tensile stress) are
 331 shown in red while the minimum values (compressive stress) are shown in blue. However, since no legacy

332 values could be found for the stresses in the IFR-1 experiment, the accuracies of these predictions are
 333 unknown.



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Figure 6. BISON baseline predictions of the minimum and maximum radial, axial, and hoop stresses in the fuel, cladding, and blankets. The maximum (tensile) stresses are shown with solid red lines, and the minimum (compressive) stresses are shown with blue dashed lines. The subplots show a) fuel radial stress, b) fuel axial stress, c) fuel hoop stress, d) cladding radial stress, e) cladding axial stress, f) cladding hoop stress, g) blanket radial stress, h) blanket axial stress, i) blanket hoop stress.

334

335 **4.3. DISCUSSION**

336 The predicted burnup and FGR results compared well with the legacy values. The agreement in burnup
 337 results indicates that the power history constructed for this benchmark case was reasonably accurate.
 338 Burnup is a calculated value based on the fuel composition and the total power produced by the pin. The
 339 legacy and simulated values likely used similar calculations, so to get the same results, they must have
 340 had similar compositions and power histories. The agreement in FGR results suggests that the FGR
 341 behavior of FFTF pins was similar to the FGR behavior of EBR-II pins of the same composition and that
 342 EBR-II data might be able to be used to fit functions that are accurate for FFTF pin. However, that cannot
 343 be determined conclusively because the data here represent only a single experiment at a single burnup.

344 Additional comparisons with more data would provide evidence that the burnup model was
345 interchangeable between reactors.

346 The cladding and coolant outlet temperatures of the simulation were biased. The cladding temperature
347 was not directly measured during the experiment. According to the IFR-1 report [10], the peak cladding
348 temperature was approximated by adding 40 K to the measured coolant outlet temperature. However,
349 the temperatures listed in the IFR-1 report actually vary by about 32 K. The reason for this discrepancy
350 was unclear. Given the uncertainties in the legacy cladding temperature and the coolant inlet mass flux
351 parameter, these results might be reasonable. The potential impact of these inconsistencies is examined
352 in Section 6.4 by applying sensitivity analysis to investigate the effects of coolant mass flux on the
353 predicted temperatures.

354 The three measured dimensional changes all saw significant differences between the BISON simulation
355 and the legacy measurements. BISON consistently predicted more dilation and elongation than the
356 experiment measured, indicating that BISON over-predicted axial and radial swelling. However, these
357 measurements were results of the integrated effects of many phenomena and properties. Swelling,
358 creep, FGR, friction, fuel-cladding chemical interactions (FCCI), and solid mechanics all influenced these
359 values. Determining the specific source of the discrepancies would require considerable effort.

360 The BISON simulation was adjusted to test the effects of friction and FCCI. The results are presented in
361 Section 5. Then, a sensitivity study was used to determine the effects of individual models. Those results
362 are presented in Section 6.

363 5. FUEL AND CLADDING INTERACTION SIMULATIONS

364 The simulation in Section 4 used a frictionless contact model because it is the most computationally
365 efficient. However, there are two other BISON contact models that can be used to account for the blocks'
366 movements against one another: glued contact and frictional contact. The glued contact model behaved
367 similar to one of the effects of FCCI, fuel and cladding bonding, which can cause the fuel to permanently
368 bond to the cladding. Note that while the BISON glued contact model is a mechanical model, fuel and
369 cladding bonding is a chemical effect, not a mechanical one, so the model can only be used as a rough
370 approximation. The frictional model used a friction coefficient to add resistance to shear motion between
371 the fuel and cladding. The baseline simulation was adjusted for simulations by using each of these
372 models. The predicted results are given in this section.

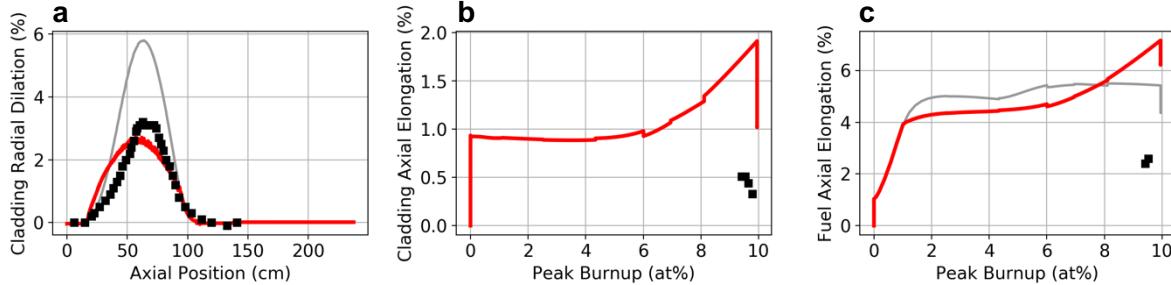
373 5.1. SETUP

374 Switching between the frictionless and glued models in BISON is a simple process that only required
375 changing one line of the input file. However, implementing the friction model was more complex. BISON
376 used an Augmented Lagrangian model for frictional contact [20], which required more iterations to solve.
377 It also requires the addition of a unitless friction coefficient. For UO₂, a friction coefficient of 0.3 or 0.4
378 was typically applied [20]. For metallic fuels, the value was unknown, so four values were used for
379 parametric evaluation: 0.5, 1.0, 1.5, and 2.0.

380 5.2. RESULTS

381 The comparisons of the dimensional changes that used glued contact against legacy data are shown in
382 Figure 7. The burnup, temperatures, and FGR were identical to the baseline case and are not shown in
383 the figure. Once again, predicted results are in red and legacy data are in black. Plot 6(a) compares the
384 cladding radial dilation. The glued simulation predicted 2.7% dilation, slightly lower than the actual
385 dilation of 3.2%. Glued contact improved the BISON prediction. Plot 6(b) compares the cladding axial

386 elongation. This is only marginally different from the baseline case with a final predicted elongation of
 387 1.02%. Plot 6(c) compares the fuel axial elongation. In this case, the predicted results worsened. BISON
 388 predicted that the fuel would elongate 6.2%—significantly more than the legacy 2.5% and the baseline
 389 4.4%.



390 *Figure 7. Comparison of the dimensional changes predicted by BISON that use glued contact (red), the baseline
 391 predictions (gray), and the legacy results (black). Subplot a) shows the cladding radial dilation. Subplot b) shows
 392 the cladding axial elongation. Subplot c) shows the fuel axial elongation.*

393 The predicted results from the friction simulations with all four friction coefficient values were identical to
 394 the frictionless baseline simulation. Their predictions are not shown here.

395 5.3. DISCUSSION

396 Initially, glued contact reduced the fuel elongation. At 1.1% peak burnup and 4% elongation
 397 (corresponding to the time of fuel-cladding contact in the simulation), Plot 6(c) shows that the elongation
 398 in the glued case plateaued at a noticeably lower value compared to the baseline case. By 4% peak
 399 burnup, it only reached 4.4% elongation, but at the same burnup, the baseline case had reached 4.9%
 400 elongation. However, after 6% burnup fuel elongation of the glued case began accelerated. This
 401 correlates to the onset of cladding axial elongation, as shown in both plots 5(e) and 7(b).

402 The similar increase rates between cladding and fuel elongation at the same burnups suggests that the
 403 cladding void swelling-induced elongation caused additional fuel elongation. This is possible because the
 404 cladding is much stiffer than the fuel and the two are “glued” together in the simulation space. The more
 405 elongated fuel put less radial mechanical stress on the cladding, compared to the baseline case, which
 406 would explain the smaller cladding dilation results shown in plot 7(a).

407 In previously reported IFR-1 BISON simulations [19], the baseline case under-predicted cladding dilation,
 408 predicted no cladding elongation, and over-predicted fuel elongation. In that work, adding friction
 409 improved the predicted dimensional changes. In this work, the baseline case over-predicted all three
 410 measurements, although the fuel elongation was more accurate than in the previous work. An
 411 examination of the BISON source code found that the D9 swelling and creep models had been recently
 412 updated and now predict more dilation and elongation. This appears to have resulted in a simulated
 413 contact pressure that was insufficient for friction to govern the simulated dilation and elongation
 414 behaviors. Therefore, the baseline case was the most physically accurate and computationally efficient
 415 contact model at this time.

416 6. SENSITIVITY STUDIES AND SIMULATION TUNING

415 Since the use of alternative contact models (i.e., friction and glued contact) did not improve BISON's
416 predictions on cladding and fuel elongations compared to legacy results, a study was performed to
417 examine several of the physics models. A main effects study based on orthogonal array sampling [28, 29]
418 was performed to identify the models to which the dimensional changes were most sensitive.

419 Once models that could be contributing to the errors were identified, the question turned to whether the
420 errors could be contributed to poor calibration of the models and/or errors in legacy measurements, or if
421 the models themselves were inaccurate. As a preliminary investigation, the benchmark was tuned in two
422 cases. In the first case, parameters chosen based on the main effects study were used to try to improve
423 the dimensional changes. If the benchmark can be successfully tuned, then a more comprehensive study
424 can be used to improve BISON metallic fuel predictions. If, however, the benchmark cannot be tuned, it is
425 evidence that the models are not accurately reflecting the physics. In the second case, the coolant mass
426 flux was tuned to improve the predicted temperature profile. If that can be successfully tuned, it may
427 suggest that the model calibration and/or uncertainty in the BISON inputs were the cause of the error.

428 It is not recommended to use the tuned parameter values in other BISON simulations because there was
429 no physical basis for changing the values nor is there evidence that the tuned values would improve the
430 predicted results of other simulations.

431 6.1. MAIN EFFECT STUDY SETUP

432 Four models that affected fuel and cladding dilation and elongation were chosen for variation: fuel
433 swelling, FGR, cladding swelling, and cladding creep. In the case of fuel swelling, cladding swelling, and
434 cladding creep, multipliers were applied to the models' values to reduce or enhance their effects. For the
435 sake of consistency, every multiplier used the same three values: 0.9, 1.0, and 1.1. The FGR model had six
436 parameters (Table 4). The post-critical FGR fraction was varied because it controlled the FGR model at
437 high burnup, which was the only condition with legacy data to compare against. It was varied by $\pm 10\%$ of
438 its original value to approximate the same relative variations as the multipliers. The fuel anisotropy factor
439 was also varied to have values of 0.35, 0.5, and 0.65. These corresponded to $75\% \pm 7.5\%$ of the swelling
440 that occurs in the radial direction.

441 This resulted in five varied parameters with three values each. One simulation ran by using each unique
442 combination of values, resulting in $3^5 = 243$ simulations. The seven response functions were then
443 measured for each simulation. For each unique input parameter value, the predictions for the 81
444 simulations that used that unique value were averaged so that the change from that individual parameter
445 could be measured across its three values.

446 6.2. MAIN EFFECT STUDY RESULTS

447 Figure 8 shows the complete main effect study results. The individual predictions are shown in gray, and
448 the averages are shown in red. None of the model parameters had any effect on the burnup or coolant
449 outlet temperature predictions, so those results are not included. Figure 8(a) shows the predictions for
450 the highest cladding temperature reached over the entire simulation. The fuel swelling multiplier had the
451 largest effect, but the anisotropy factor also had an effect.

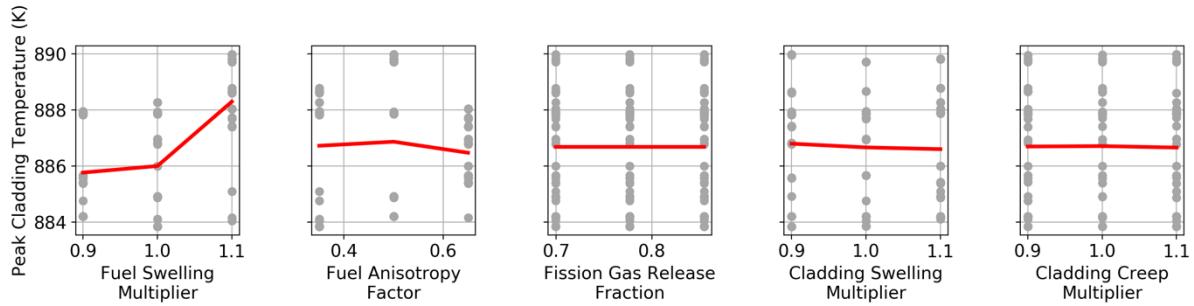


Figure 8(a). Model effects on peak cladding temperature. The range of temperatures only varied by 6 K, but the parameter with the largest effect was the fuel swelling multiplier.

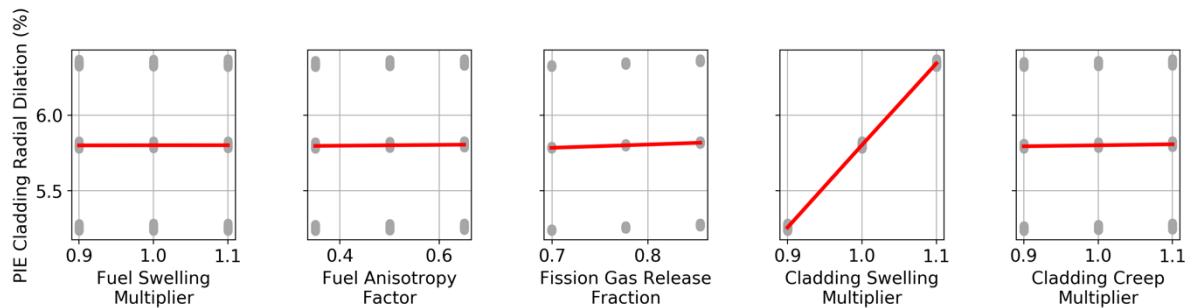


Figure 8(b). Model effects on cladding dilation. The cladding swelling multiplier was the only parameter to have an effect.

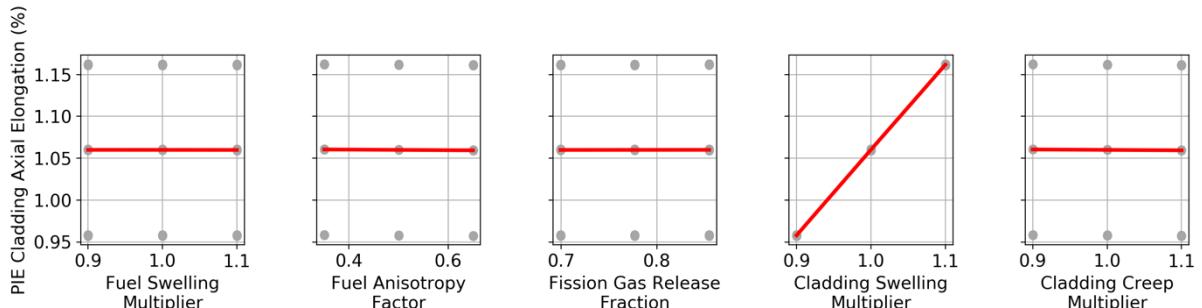


Figure 8(c). Model effects on cladding elongation. The cladding swelling multiplier was the only parameter to have an effect.

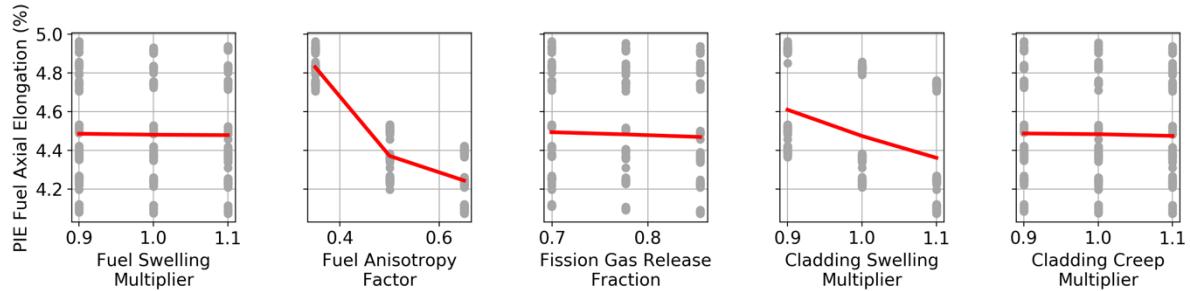


Figure 8(d). Model effects on fuel elongation. Several parameters affected it, but the fuel anisotropy factor had the largest effect.

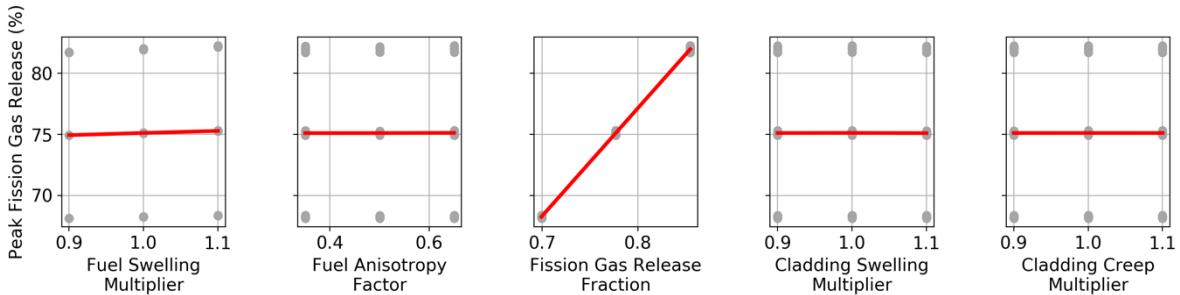


Figure 8(e). Model effects on FGR. The FGR fraction was the only parameter to have any effect.

453 Figure 8(b) shows the predictions of the study on cladding radial dilation at PIE. The cladding swelling
 454 multiplier was the only parameter to affect it. This indicates that for this set of conditions, BISON does not
 455 simulate appreciable fuel cladding mechanical interactions (FCMI) or stress induced in the cladding by
 456 fuel swelling. Figure 8(c) shows the predictions of cladding axial elongation. Once again, the cladding
 457 swelling multiplier was the only parameter to have an effect. Figure 8(d) shows the parameter effects on
 458 fuel axial elongation. The cladding swelling multiplier and fuel anisotropy factors had effects, although the
 459 cladding axial swelling effect on fuel elongation is not clearly supported by experimental observation, as
 460 discussed in Section 5.3. Finally, Figure 8(e) shows the effects on FGR. Only the FGR fraction had any
 461 effect.

462 The cladding swelling multiplier affected all three calculated dimensional changes and none of the other
 463 predictions, making it an excellent candidate for tuning the simulation. However, it alone could not tune
 464 all three calculated dimensional changes because it had a positive correlation to cladding dilation and
 465 elongation but a negative correlation to fuel elongation. Decreasing the cladding swelling multiplier
 466 would decrease cladding dilation and elongation but increase fuel elongation. Therefore, the fuel
 467 anisotropy factor was also tuned.

468 6.3. DIMENSIONAL PARAMETER TUNING SETUP

469 Two parameters were tuned to improve three result values: peak cladding dilation at EOL PIE, peak
 470 cladding elongation at EOL PIE, and peak fuel elongation at EOL PIE. Let \vec{e} represent the 3×1 vector of
 471 differences between these three values and the averages of the available legacy values, \vec{x} represent the 2
 472 $\times 1$ vector of input values (cladding swelling multiplier and fuel anisotropy factor), and \vec{y} represent the
 473 input values with a constant:

$$\vec{y} = \begin{bmatrix} \vec{x} \\ 1 \end{bmatrix}. \quad (11)$$

474 Then assume a linear relationship:

$$\vec{\epsilon} = A\vec{y}, \quad (12)$$

475 where A is the 3×3 coefficient matrix. The coefficient matrix can be found by using three linearly
 476 independent input vectors $Y = [\vec{y}_1, \vec{y}_2, \vec{y}_3]$ and their corresponding error vectors $E = [\vec{\epsilon}_1, \vec{\epsilon}_2, \vec{\epsilon}_3]$, so that:

$$E = AY \Leftrightarrow A = EY^{-1}. \quad (13)$$

477 Now define a solution vector $\vec{\xi}$, so that:

$$\vec{0} \approx A \begin{bmatrix} \vec{\xi} \\ 1 \end{bmatrix}. \quad (14)$$

478 To solve for the solution vector, break A into two components, $A = [B \quad \vec{a}]$, where \vec{a} is a 3×1 vector
 479 made from the third column of A , and B is a 3×2 matrix made from the first two columns. Rearrange to
 480 get:

$$\vec{0} \approx B\vec{\xi} + \vec{a} \Leftrightarrow -\vec{a} \approx B\vec{\xi}. \quad (15)$$

481 $\vec{\xi}$ can be found by using the least-squares method:

$$\vec{\xi} = -(B^T B)^{-1} B^T \vec{a}. \quad (16)$$

482 The simulation inputs were tuned by following this procedure, beginning with the baseline simulation and
 483 two guesses. The input and error vectors were updated with each simulation, resulting in a new tuned
 484 value. Depending on how the vectors were updated, the path could vary slightly but eventually reach the
 485 same values. However, the tuning process called for an anisotropy factor larger than what BISON allowed,
 486 so the maximum allowable value was used. The optimized cladding swelling multiplier and anisotropy
 487 factor were 0.5 and 1.0, respectively.

488 6.4. DIMENSIONAL PARAMETER TUNING RESULTS

489 The predicted results of the tuned simulation are shown in Figure 9. Burnup, temperatures, and FGR were
 490 unchanged compared with the baseline case, so only the dimensional changes are shown. Plot 8(a) shows
 491 the cladding dilation, which was nearly a perfect match to the entire legacy profile—not just the peak
 492 legacy value to which it was tuned. It reached a peak dilation of 3.0%. Plot 8(b) shows the cladding
 493 elongation. It decreased significantly to 0.54%. Plot 8(c) shows the fuel elongation. This result worsened
 494 compared with the baseline simulation. The fuel grew 5.5%, which was considerably higher than the
 495 measured elongation.

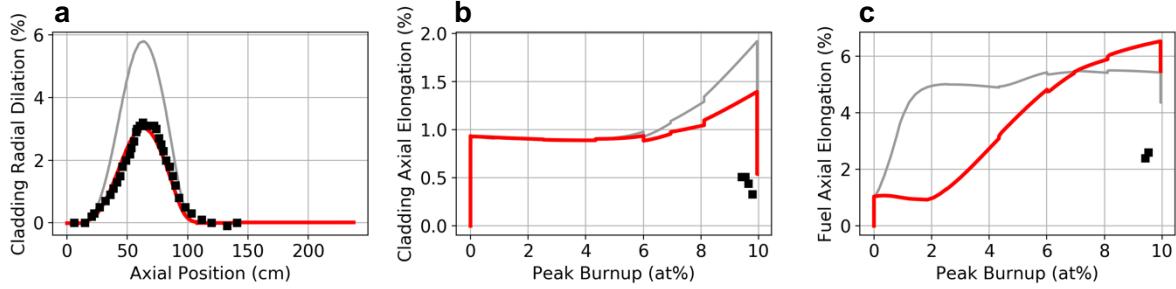


Figure 9. Dimensional changes comparison of dimensional-tuned BISON simulation (red), baseline BISON simulation (gray), and legacy values (black). Subplot a) shows the cladding radial dilation, subplot b) shows the cladding axial elongation, and subplot c) shows the fuel axial elongation.

496 6.5. TEMPERATURE PARAMETER TUNING SETUP

497 In addition to tuning the dimensional change predictions, a separate simulation was used to tune the
 498 temperature profile predictions. Because only one parameter was changed to vary one result, the
 499 method was somewhat simpler than the aforementioned dimensional tuning. Let ΔT be the average
 500 difference between the legacy peak cladding temperature and the simulation predicted peak cladding
 501 temperature and let \dot{m} be the coolant inlet mass flux. Then, assume a linear relationship:

$$502 \Delta T = c_0 \dot{m} + c_1, \quad (17)$$

503 where c_0 and c_1 are constants. The constants are found by solving the equation for two coolant inlet
 504 mass flux, temperature difference pairs. Then, set the new mass flux to $-c_1/c_0$.

505 The coolant inlet mass flux was chosen for tuning because of the aforementioned unreliability of the
 506 referenced value. It was adjusted over several iterations to reduce the average error between the legacy
 507 and simulated peak cladding temperature. The tuned mass flux was $7,960 \text{ kg m}^{-2} \text{ s}^{-1}$, which was 31%
 higher than the baseline case.

508 6.6. TEMPERATURE PARAMETER TUNING RESULTS

509 Figure 10 shows the predicted results of the tuned temperature simulations with the increased coolant
 510 inlet mass flux. The baseline predictions and measured values are also shown. Plot 9(a) shows the burnup,
 511 which did not vary significantly from the baseline simulation. Plot 9(b) shows the peak cladding
 512 temperature, and plot 9(c) shows the coolant outlet temperature. The average temperature differences
 513 between the simulation and the experiment were 5 K for the cladding and 1 K for the coolant. Plot 9(d)
 514 shows the cladding radial dilations. The reduction in the predicted temperature reduced the dilation
 515 compared with the baseline. Likewise, plot 9(e) shows that the cladding axial elongation was somewhat
 516 improved compared with the baseline simulation. Plot 9(f) shows the fuel axial elongation. The fuel was
 517 slightly more elongated compared with the baseline prediction. The FGR fraction is shown in plot 9(g).
 518 Like plot 9(a), it did not deviate from the baseline prediction.

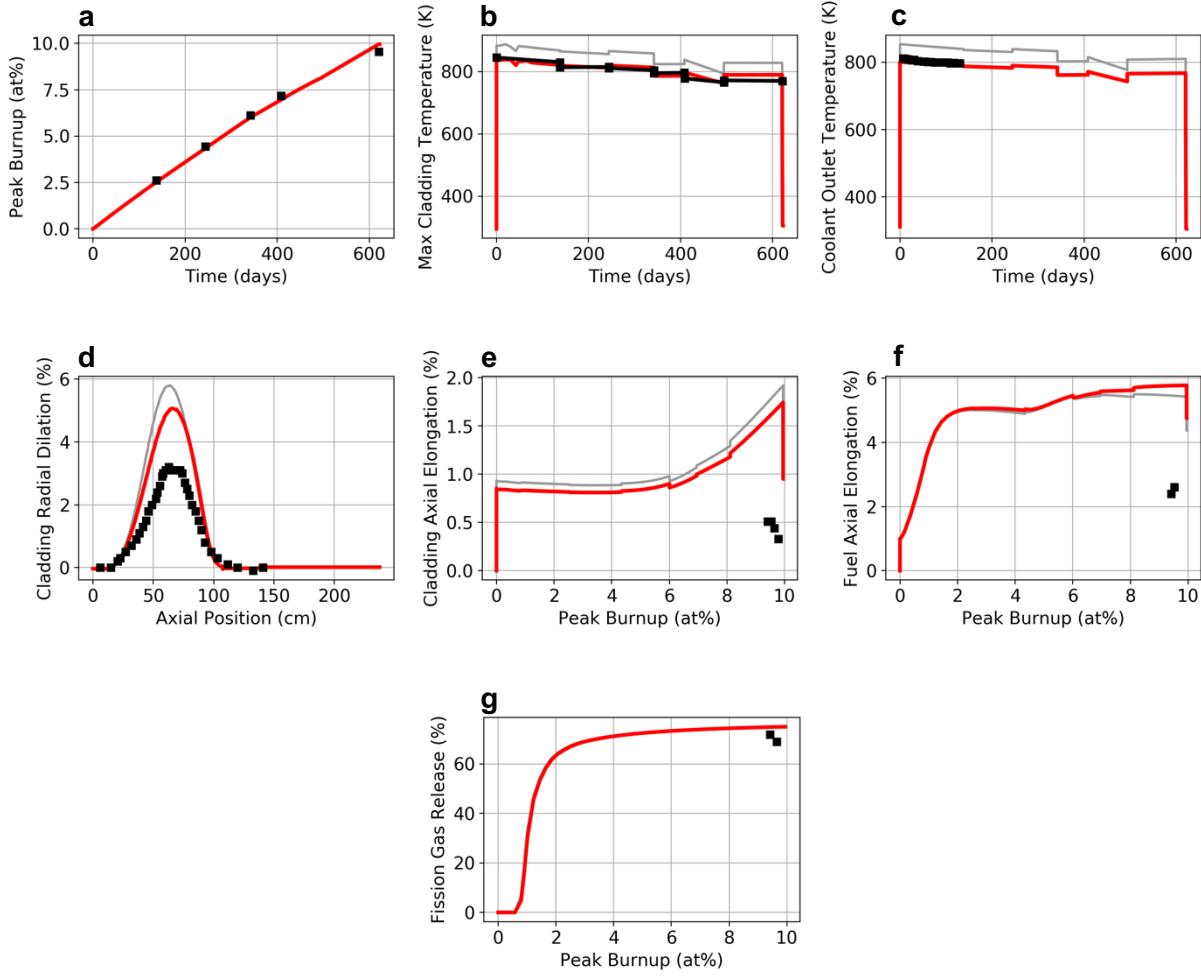


Figure 10. Comparison of temperature-tuned BISON simulation (red), baseline simulation (gray), and legacy values (black). Subplot a) shows the peak burnup was not affected. Subplots b) and c) show the maximum cladding temperature and coolant outlet temperature, respectively. Subplot d) shows the cladding radial dilation. Subplot e) shows the cladding axial elongation. Subplot f) shows the fuel axial elongation. Subplot g) shows the FGR fraction.

519

520 6.7. DISCUSSION

521 Possibly the most unexpected result of this sensitivity analysis and tuning studies was the effect of
 522 cladding dimensional changes on fuel dimensional changes. Figure 8(d) shows that the fuel swelling
 523 multiplier had only a negligible impact on the fuel axial elongation compared with the impact of the
 524 cladding swelling multiplier. This suggests that the cladding dimensions control the extents to which the
 525 fuel swells axially and radially. Once the fuel contacted the cladding, its radial dilation was constricted, so
 526 it began to swell axially. For this to be the case, the fuel must be too soft to deform the cladding. The
 527 tuned simulation predictions in Figure 9(a) show this very clearly. Despite 100% of the fuel swelling
 528 occurring in the radial direction, the fuel grew axially 5.5% because the reduced cladding dilation further
 529 constricted the fuel. This is also consistent with the glued contact simulation showed in Figure 7 in which
 530 cladding forced the fuel to stretch as it swelled. If this is the case, then the anisotropy factor cannot be

531 measured experimentally after fuel-cladding contact occurs. It should only be measured by using low-
532 burnup, pre-contact fuel.

533 The main effects study found that the fuel and cladding swelling models controlled the marginal fuel and
534 cladding dilation and elongation behaviors more than creep and fission gas models. However, tuning the
535 swelling models could not correct the simulation error. To correct the error in cladding and fuel dilation
536 and elongation, it might be necessary to develop a more mechanistic model.

537 The predicted results of tuning according to temperature show that the over-predicted simulation
538 temperature can be completely explained as a result of uncertainty in the model input parameters. This
539 does not prove that inaccurate input parameters were the cause of the temperature discrepancy. To do
540 that, a more certain value of the coolant inlet velocity must be found or determined. However, it was
541 enough to conclude that the temperature profiles were reasonably accurate.

542 Additionally, correcting for the temperature improved the cladding dilation and elongation predictions.
543 However, like the mechanical tuning simulation, improving the cladding prediction worsened the
544 predicted fuel axial growth.

545 7. CONCLUSIONS

546 A benchmark case was designed and configured to simulate the IFR-1 experiment in the FFTF reactor. The
547 benchmark was simulated by using BISON and was compared with IFR-1 legacy values and calculations.
548 The burnup and FGR predictions compared well against legacy results. The simulated temperatures were
549 somewhat higher than the previously measured and calculated experiment temperatures, but they were
550 as accurate as could be expected given the uncertainty of the coolant inlet velocity (and hence mass flux),
551 the LHGR, and other input parameters. BISON over-predicted the dimensional changes of the fuel and
552 cladding. A sensitivity study was performed to determine which physical models could have been
553 responsible for this, and the dimensional changes were found to be the most sensitive to the cladding
554 swelling model and fuel swelling anisotropy. However, improvements in these two models alone would
555 not correct the predictions, as indicated by an attempt to tune the simulation by using these parameters
556 that resulted in increased axial elongation in the fuel.

557 The fuel swelling was limited by mechanical contact with the cladding. After fuel contacted the cladding,
558 swelling was forced to occur in the axial direction irrespective of the degree of swelling anisotropy in the
559 fuel. Therefore, any future attempts to measure the fuel swelling anisotropy should use low burnup fuel
560 that has not come into contact with the cladding.

561 Future simulation and benchmarking work should incorporate additional irradiation experiments to
562 compare simulations predictions with an expanded range of operating conditions, cladding and fuel
563 materials, and measurements. These should especially focus on more complete dimensional change data
564 to help pinpoint the behaviors that are causing the benchmark cases to have inaccurate swelling
565 predictions. Future development on fuel and cladding interaction models, especially cladding swelling and
566 FCCI, would be beneficial. As models are developed or improved, their effects can be measured by
567 running this benchmark case again with the updated models. Future experiments should focus on low-
568 burnup swelling anisotropy, friction, and bonding between the fuel and cladding, and they should always
569 record the experimental coolant inlet flow rate.

570

571

572 **ACKNOWLEDGMENTS**

573 This work was funded by the DOE Office of Nuclear Energy (NE) Versatile Test Reactor (VTR) Project. The
574 reported work resulted from studies that support a VTR conceptual design, cost, and schedule estimates
575 for DOE-NE to make a decision of procurement. As such, it is preliminary.

576 The authors thank Stephen Novascone, Al Casagrande, and Adam Zabriskie of the INL BISON development
577 team and Alexander Lindsay of the INL MOOSE development team for their valuable input in BISON fuel
578 performance models in metallic fuels. The authors also thank Doug Porter for sharing his knowledge and
579 experience with metallic fuels in general and the IFR-1 experiment in particular.

580 **DATA AVAILABILITY**

581 Simulation results can be made available upon request. BISON is export controlled with access granted on
582 an individual basis. To apply for BISON access, visit <https://bison.inl.gov>. The input file for the baseline
583 version of the IFR-1 benchmark case is distributed with the BISON code as a metallic fuel assessment
584 case.

585 **AUTHOR IMPACT STATEMENT**

586 Ian Greenquist led the development of the IFR-1 benchmark case and wrote the manuscript text. Kaylee
587 Cunningham developed the initial version of the IFR-1 benchmark case. Jianwei Hu helped with BISON
588 model development and parameter selection. Jeffrey Powers led the benchmark development work at
589 Oak Ridge National Laboratory (ORNL) and provided important technical feedback and manuscript
590 editing. Doug Crawford led the fuel design team engaged with this work and provided technical editing.

591 **DISCLAIMERS**

592 The authors have no competing interests. Portions of this research have been previously published in an
593 ORNL technical memo [19].

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