BISON Simulation of MARVEL Fuel Performance

Chemical & Fuel Cycle Technologies Division
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BISON Simulation of MARVEL Fuel Performance

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prepared for
U.S. Department of Energy
MARVEL

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ABSTRACT

BISON simulation of MARVEL fuel rod performance was conducted for normal operation. Fuel temperatures, plenum pressures and cumulative damage factors were calculated for five core zones. This report presents the results. BISON simulation for transient cases are planned. When the results are available, this report will be updated.
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1. Introduction

Fuel performance analysis for the design stage of the MARVEL reactor was performed using BISON at Argonne National Laboratory. Los Alamos National Laboratory (LANL) started this task and Argonne took over LANL’s work to complete the simulation. In order to avoid unnecessary redundancy, LANL provided Argonne with input data that were used for the BISON simulation at LANL before Argonne took over [1].

Although models needed for the simulation were mostly available in BISON and collected as input data by LANL, some key fuel properties and performance models needed to be updated for more realistic simulations.

This report describes the model improvements made at Argonne and presents the BISON simulation results for normal operation. This report will be updated when the analyses for transient cases are performed.

2. Input Data and Existing Models used by LANL

The materials properties and models needed for BISON simulations for fuel, reflector and cladding used by LANL are summarized in Table 1–Table 3, respectively.

<table>
<thead>
<tr>
<th>Object</th>
<th>Dependence</th>
<th>Method</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>TC/Cp</td>
<td>temperature</td>
<td>HeatConductionMaterial</td>
<td>data file, fresh fuel data</td>
</tr>
<tr>
<td>LTE</td>
<td>temperature</td>
<td>Compute Instantaneous Thermal Expansion Function Eigenstrain</td>
<td>data file</td>
</tr>
<tr>
<td>Elasticity</td>
<td>none</td>
<td>ComputeIsotropicElasticityTensor</td>
<td>constant</td>
</tr>
<tr>
<td>Plasticity</td>
<td>n/a</td>
<td>n/a</td>
<td>no creep at low burnup</td>
</tr>
<tr>
<td>Density</td>
<td>see LTE</td>
<td>Density</td>
<td>constant</td>
</tr>
<tr>
<td>Burnup</td>
<td>n/a</td>
<td>UPuZrBurnup</td>
<td>hacked</td>
</tr>
<tr>
<td>Swelling</td>
<td>burnup</td>
<td>BurnupDependentEigenstrain</td>
<td>FP+void = 3%/1%FIMA</td>
</tr>
<tr>
<td>FGR</td>
<td>n/a</td>
<td>n/a</td>
<td>low BU, needed</td>
</tr>
<tr>
<td>Hydrogen release</td>
<td>n/a</td>
<td>n/a</td>
<td>needed</td>
</tr>
</tbody>
</table>
Table 2: Reflector Material Properties and Behavior Models for BISON Simulation

<table>
<thead>
<tr>
<th>Object</th>
<th>Dependence</th>
<th>Method</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>TC/Cp</td>
<td>temperature</td>
<td>HeatConductionMaterial</td>
<td>data file</td>
</tr>
<tr>
<td>LTE</td>
<td>none</td>
<td>ComputeThermalExpansionEigenstrain</td>
<td>constant</td>
</tr>
<tr>
<td>Elasticity</td>
<td>n/a</td>
<td>ComputeIsotropicElasticityTensor</td>
<td>constant</td>
</tr>
<tr>
<td>Plasticity</td>
<td>n/a</td>
<td>n/a</td>
<td>Not needed at low burnup</td>
</tr>
<tr>
<td>Density</td>
<td>see LTE</td>
<td>Density</td>
<td>constant</td>
</tr>
<tr>
<td>Swelling</td>
<td>n/a</td>
<td>n/a</td>
<td>Not needed</td>
</tr>
</tbody>
</table>

Table 3: Cladding Material Properties and Behavior Models for BISON Simulation

<table>
<thead>
<tr>
<th>Object</th>
<th>Dependence</th>
<th>Method</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>LTE</td>
<td>temperature</td>
<td>SS316ThermalExpansionEigenstrain</td>
<td>available in BISON</td>
</tr>
<tr>
<td>Elasticity</td>
<td>temperature</td>
<td>SS316ElasticityTensor</td>
<td>available in BISON</td>
</tr>
<tr>
<td>Plasticity</td>
<td>temperature/flux</td>
<td>SS316CreepUpdate</td>
<td>available in BISON</td>
</tr>
<tr>
<td>Density</td>
<td>see LTE</td>
<td>Density</td>
<td>constant</td>
</tr>
<tr>
<td>Swelling</td>
<td>temp/flux</td>
<td>SS316VolumetricSwellingEigenstrain</td>
<td>available in BISON</td>
</tr>
</tbody>
</table>

Preliminary transient simulations, simplified temperature-dependent correlations about fission gas release and hydrogen pressure are also available from LANL [1].

3. Model Improvement

For the MARVEL fuel safety evaluation project, we found that two fuel-related correlations needed to be modified to provide improved fuel performance predictions. These two correlations
are the UZrH fuel thermal conductivity degradation due to irradiation, and the plenum pressure during irradiation due to fission gas release. The approaches are described below.

3.1 UZrH Fuel Thermal Conductivity During Irradiation

In the original BISON simulations performed by LANL [1], a temperature-dependent thermal conductivity model was used. However, the model does not include any dependence on fuel burnup. In reality, fuel depletion introduces a series of microstructural modifications that eventually lead to degradation in thermal conductivity. Within the limited amount of UZrH fuel thermal conductivity degradation data in literature, Terrani et al. [2] performed thermal conductivity measurement for neutron-irradiated UZrH at three different burnup (i.e., 0%, 0.15%, and 0.31%) at various temperatures. The experimental results show considerable drop in thermal conductivity of UZrH at relatively low burnup (see Figure 1).

![Figure 1: Thermal conductivity of irradiated UZrH at different temperatures [2].](image)

Although the uranium loading of this study is different from the MARVEL fuel (40 wt.% versus 30 wt.%), the degradation factor can still be used for the MARVEL fuel. Assuming the degradation factor \( f(T) \) at 0% FIMA is unity, a second order polynomial is used to fit the three burnup data points at each temperature point.

\[
f(T) = 1.0 + C_1(T)Bu + C_2(T)Bu^2
\]

where, \( T \) is temperature, \( Bu \) is burnup, and \( C_1(T) \) and \( C_2(T) \) are the two fitting parameters. Due to the nature of a parabolic curve, \( f(T) \) has a minimum value of \( 1 - \frac{1}{4} \frac{C_1(T)^2}{C_2(T)} \) at \( Bu_{max} = -\frac{1}{2} \frac{C_1(T)}{C_2(T)} \). To prevent recovery of thermal conductivity at relatively high burnup, \( f(T) \) is set at the minimum value beyond \( Bu_{max} \). That is,
\[ f(T) = \begin{cases} 
1.0 + C_1(T)Bu + C_2(T)Bu^2 & 0 \leq Bu \leq -\frac{1}{2} C_1(T)/C_2(T) \\
1 - \frac{1}{4} C_1(T)^2/C_2(T) & Bu > -\frac{1}{2} C_1(T)/C_2(T) 
\end{cases} \] (2)

For the temperature dependence of \( C_1(T) \) and \( C_2(T) \), a linear correlation was found sufficient:

\[
C_1(T) = A_1 T + B_1 \\
C_2(T) = A_2 T + B_2 
\] (3)

After fitting these parameters using the least squares method, the following coefficients were obtained.

**Table 4: Fitting coefficients for fuel thermal conductivity**

<table>
<thead>
<tr>
<th></th>
<th>( A_1 )</th>
<th>( B_1 )</th>
<th>( A_2 )</th>
<th>( B_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.1702</td>
<td>-377.8620</td>
<td>-32.9602</td>
<td>56018</td>
</tr>
</tbody>
</table>

**Figure 2:** Comparison between the model fit and literature data for the degradation factor for two burnup values.

The degradation factor was implemented into BISON using the ParsedMaterial object. Note that both thermal_conductivity and thermal_conductivity_dT need to be scaled.
3.2 Plenum Pressure

In the original BISON simulations performed by LANL, a time-dependent and temperature-dependent correlation for the plenum pressure was used along with a temperature-dependent correlation for hydrogen partial pressure. Improvements have been made to include burnup dependence and temperature dependence functions.

The new correlation is based on a fractional fission gas release correlation reported by Olander [3] as shown in Figure 4.

![Temperature-dependent fractional fission gas release from UZrH](image)

**Figure 4:** Temperature-dependent fractional fission gas release from UZrH [3].

In addition, the intrinsic PlenumPressure UserObject built in BISON was used to calculate the plenum pressure. This UserObject needs a series of Postprocessors as input, including volume of...
the plenum, temperature of the plenum, and material_input. The volume of plenum can be provided by a Volume Postprocessor with a shift that accounts for sodium load. The temperature of the plenum can be obtained using the top end plug inner temperature for conservative evaluation. The material_input contains two components: fission gas and hydrogen.

For the calculation of fission gas release, fission_density is calculated as an AuxVariable “fission_density_aux” by accumulating fission_rate. The combined yield of 0.26 moles for Xe and Kr per fission is used to calculate fission gas production per unit volume. By multiplying with the fractional release factor shown in Figure 4, the amount of released fission gases is calculated. For the hydrogen partial pressure, the correlation used by LANL is adopted. The pressure value was then converted into mole value using the ideal gas law. Based on the fuel pellet volume, the released hydrogen mole value is converted to a Materials property of hydrogen released mole per unit volume “hydrogen_mole_mat”.

Both components are summed up and are integrated using an ElementIntegralMaterialProperty object to generate the material_input value as shown in Figure 5.

```
[./PlenumPressure]
[./plenumPressure]
    broadeny = $(ell_pressure_boundaries)
    initial_pressure = 1e5
    startup_time = 0
    R = 8.3143
    output_initial_moles = initial_moles
    temperature = avc_temp_interior
    volume = gas_volume
    material_input = integrated_fgr
    output = plenum_pressure
[../]
[./]
```

```
[./fgr_mat]
    type = ParsedMaterial
    f_name = fgr_mat
    args = fission_density_aux
    material_property_names = 'fgr_frac hydrogen_mole_mat'
    constant_expressions = '6.02214e23 0.3071'
    constant_names = 'N_A vy'
    block = $(fuel_all)
    function = 'fission_density_aux*vy/MeV*fgr_frac+hydrogen_mole_mat'
    outputs = all
[../]
```

**Figure 5:** A typical input used for implementing plenum pressure.
4. Updated Reactor Core Design Data

4.1 Fuel Rod Design Data

The updated fuel rod design data used for the BISON simulations are given in Table 5.

<table>
<thead>
<tr>
<th>Design parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of fuel rods</td>
<td>37</td>
<td></td>
</tr>
<tr>
<td>Void fuel rods</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>Fuel radius</td>
<td>0.0149</td>
<td>m</td>
</tr>
<tr>
<td>Fuel rod cladding inner radius</td>
<td>0.014986</td>
<td>m</td>
</tr>
<tr>
<td>Fuel rod cladding outer radius</td>
<td>0.015875</td>
<td>m</td>
</tr>
<tr>
<td>Fuel rod outer diameter</td>
<td>0.03175</td>
<td>m</td>
</tr>
<tr>
<td>Active fuel height</td>
<td>0.61</td>
<td>m</td>
</tr>
<tr>
<td>Reflector height (top/bottom)</td>
<td>0.15</td>
<td>m</td>
</tr>
<tr>
<td>Plenum height</td>
<td>0.0254</td>
<td>m</td>
</tr>
<tr>
<td>Gap thickness</td>
<td>8.60E-05</td>
<td>m</td>
</tr>
<tr>
<td>Cladding thickness</td>
<td>8.89E-04</td>
<td>m</td>
</tr>
<tr>
<td>Fuel rod pitch</td>
<td>0.03275</td>
<td>m</td>
</tr>
<tr>
<td>P/D</td>
<td>1.031</td>
<td></td>
</tr>
<tr>
<td>Minimum distance between outer rod surfaces</td>
<td>0.001</td>
<td>m</td>
</tr>
<tr>
<td>Fuel rod area</td>
<td>7.92E-04</td>
<td>m²</td>
</tr>
<tr>
<td>Total fuel rod area</td>
<td>2.93E-02</td>
<td>m²</td>
</tr>
<tr>
<td>Fuel rod perimeter</td>
<td>0.099746</td>
<td>m</td>
</tr>
<tr>
<td>Total fuel rod perimeter</td>
<td>3.690586</td>
<td>m</td>
</tr>
<tr>
<td>Fuel rod heat exchange area</td>
<td>6.08E-02</td>
<td>m²</td>
</tr>
<tr>
<td>Total fuel rod heat exchange area</td>
<td>2.2512574</td>
<td>m²</td>
</tr>
<tr>
<td>Fuel density</td>
<td>7294</td>
<td>Kg/m³</td>
</tr>
<tr>
<td>Uranium content in fuel</td>
<td>40</td>
<td>wt.%</td>
</tr>
</tbody>
</table>

4.2 Fuel Rod Power Data

In this section, the necessary fuel rod power and cladding temperature data for BISON simulation, provided by Carlo and Travis [4], are given.
In the core design, five zones that have different powers are recognized as shown in Figure 6. The zones are labeled as 107 – 110. In the BISON simulations, an imaginary fuel rod is used for each zone that represents the average values for the zone.

Figure 6: Zones in the reactor core [4].
The fuel rod axial power distributions for rods from the five core zones are shown in Figure 7.

![Fig 7: Rod axial power distribution](image)

**Figure 7: Rod axial power distribution [4]**

The radial power distribution in the rod applicable for the rods from the five core zones is shown in Figure 8.

![Fig 8: Radial power distribution in fuel rod](image)

**Figure 8: Radial power distribution in fuel rod [4].**
Fast neutron flux is also used for the BISON simulation as shown in Figure 9.

![Graph of Fast Flux vs Axial Location](image)

**Figure 9:** Fast neutron flux used for the BISON simulation [4].

5. **Bison Simulation Results**

5.1 **Fuel Temperature**

Fuel temperatures for the representing fuel rods from the five zones shown in Figure 6 were simulated. The cladding surface temperatures provided in [4] were used as boundary conditions. The fuel temperatures for the fuel rods from the core zones 107 – 111 are shown in Figure 10 – Figure 14. Cladding surface temperatures (Tod) [4] are also shown for comparison.
Figure 10: Fuel temperatures versus axial position for the fuel rod from the core zone 107 shown in Figure 6. Cladding surface temperatures (Tod) [4] are also shown for comparison.
Figure 11: Fuel temperatures versus axial position for the fuel rod from the core zone 108 shown in Figure 6. Cladding surface temperatures (Tod) [4] are also shown for comparison.
Figure 12: Fuel temperatures versus axial position for the fuel rod from the core zone 109 shown in Figure 6. Cladding surface temperatures (Tod) [4] are also shown for comparison.
Figure 13: Fuel temperatures versus axial position for the fuel rod from the core zone 110 shown in Figure 6. Cladding surface temperatures (Tod) [4] are also shown for comparison.
Figure 14: Fuel temperatures versus axial position for the fuel rod from the core zone 111 shown in Figure 6. Cladding surface temperatures (Tod) [4] are also shown for comparison.

5.2 Plenum Pressure

Plenum pressures are calculated for the fuel rods from the five core zones and shown in Figure 15.
Figure 15: Fuel rod plenum pressures. The as-fabricated pressure was set at 1 atm.

5.3 Cumulative Damage Factor

The cumulative damage factors were calculated and shown in Figure 16.
6. Conclusion

From the BISON simulations for normal operation using the updated fuel rod design and power inputs, the MARVEL fuel rod will perform well without any safety concerns during normal operation.
References

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