Fuel Performance of Multi-Layered Zirconium and Silicon Carbide Based Accident Tolerant Fuel Claddings

by

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Abstract

The Accident Tolerant Fuel (ATF) program is focused on extending the time for fuel failure during postulated severe accidents compared to the standard UO$_2$-Zr alloy fuel system. This thesis investigates the feasibility of four different cladding concepts, two of which are zirconium-alloy based and two are SiC-based. The Zirconium-alloy based claddings are 1) Zr4-Chromium coated cladding and 2) Zr4-FeCrAl coated cladding with a molybdenum interlayer (Zr4-Mo/FeCrAl). The SiC-based claddings are 3) composite SiC coated with chromium (SiC/SiC-Cr) and 4) Three layered SiC cladding consisting of inner and outer monolith with a composite layer sandwiched in between (mSiC-SiC/SiC-mSiC). The coated claddings were kept to a 50µm of coating thicknesses, deducted from the base layer thicknesses. The claddings were studied, using the multi-physics fuel performance tool MOOSE/BISON, under steady-state PWR operating conditions as well as two transients: power ramp and loss-of-coolant accident (LOCA). The major finding is that the chromium coated concepts proved to be the most promising in both Zr4 and SiC based claddings. The three layered SiC cladding showed a high probability of failure during normal operation and transient conditions, while the Zr4-Mo/FeCrAl cladding showed high plastic strains in the molybdenum layer making its possibilities of survival questionable. On the other hand, the Zr4-Cr and SiC/SiC-Cr concepts showed acceptable plastic strains for the chromium coatings, with the SiC/SiC-Cr being more advantageous during LOCA scenarios. Both concepts warrant further experimental investigation as well as modelling of beyond design-basis accidents.

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Title: Assistant Professor of Nuclear Science and Engineering
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1 Introduction

The Fukushima accident in 2011, triggered by a massive 9.0 magnitude earthquake followed by a tsunami, had a devastating effect on the status and prospects of nuclear power worldwide. Alarmed by the incident and the following large release of radioactive material to the atmosphere and the surrounding land and ocean [1], Japan authorities required a shutdown of its nuclear capacity [2]. Longer term effects included Japan’s later announcement of plans to reduce dependency on nuclear power and to revise their Basic Energy Plan [2]. In addition, Germany and Switzerland have announced plans to phase-out nuclear energy in the foreseeable future [3].

As a result of the accident, a renewed interest was generated to address the shortcomings of the traditional zirconium-based (so-called “Zircaloy”) claddings under accident conditions. Current light water reactors (LWRs) use a fuel system composed of uranium dioxide (UO\(_2\)) pellets, zirconium-alloy cladding and a helium filled pellet-cladding gap. The choice of zirconium alloys as the primary cladding material is due to its low neutron absorption, good corrosion resistance and structural integrity under operating conditions [4]. However, under design-basis accidents (DBAs) and beyond DBAs, zirconium alloys can rapidly lose their integrity due to its interaction/oxidation in high-temperature steam [5]. This lead to a large research effort to mitigate and possibly eliminate high temperature oxidation of the currently used fuel system in LWRs. The proposed solutions are called accident tolerant fuels (ATFs) [6].

ATFs are fuels, which in comparison with the standard UO\(_2\)-Zr system, can tolerate loss of active cooling in the core for a considerably longer time period (depending on the LWR system and accident scenario) while maintaining or improving the fuel performance during normal operations [7]. These improved properties are mainly focused on reducing the oxidation rate and hydrogen (or other combustible gases) production at high temperatures. Additional, targeted improvements include increasing the cladding melting point and its strength at high temperature in comparison to current Zircaloy cladding. Improvements to the fuel are also under investigation, especially in the areas of improved fission gas retention and higher temperature margin to fuel melt. Among current ATF concepts, multi-layered Zirconium-based composite and thin walled FeCrAl claddings are considered to be near-term options [6], [8].
The focus of this thesis is to investigate some of the prominent ATF cladding system concepts using thermo-mechanical modelling under both steady-state and transient conditions. The aim of this initial investigation is to provide enough results to be able to compare the performance of each concept with regards to a standard Zirconium alloy cladding. The most promising concepts could be then further investigated experimentally to test their performance and possible performance enhancement under simulated accident conditions. Further experimentation would also provide more data for feedback into the modelling/simulation codes, as data is one of the essential limitations to developing physical/realistic models i.e. more experiments would also help develop better models in the future. However, as experiments are rather cost and time intensive, it is essential to limit it to promising ATF concepts. Therefore, simulations/modelling can help focus the experimental effort and provide an informed judgement of the expected best promising concepts.

1.1 Background & Motivation

Nuclear power is considered a key resource in mitigation and managing of climate change and will have an important role in efforts to “decarbonize the production of electricity” [9]. UO$_2$-Zr alloys are currently considered the standard fuel system for LWRs. The fuel system has been optimized over decades of research and development, offering reliable, economic and safe operation under normal operating conditions. This continuous optimization has resulted in failure rates of fuel rods on the order of few ppm per year [10]. In the US alone, LWRs with UO$_2$-Zr alloy fuel provide 70% of the country’s clean energy[7]. However, as stated earlier, the current deployed fuel system has its limitations when subjected to DBAs and beyond DBAs. This section will discuss the current limitations of the current UO$_2$-Zr alloy fuel system and explain the motivation or necessity of studying alternative ATFs currently under research and development.

The limitations of the UO$_2$-Zr alloy fuel system is better understood by examining its accident performance. Two standard cases are considered as a metric of performance, loss-of-coolant accidents (LOCAs) and reactivity insertion accidents (RIAs). Starting with LOCA, the current US regulatory requirements uses many limiting metrics including a maximum peak clad temperature (PCT) of 1204 °C and an equivalent cladding reacted (ECR) limited of 17% of initial cladding thickness [11]. These limits are based on the assumption of zirconium alloy cladding. Beyond these limits the cladding will be highly susceptible to
embrittlement and failure upon quench. The embrittlement is mainly caused by the excessive dissolution of oxygen in the cladding and the effect of absorbed hydrogen on the oxidation rate [12]. The effect of oxygen dissolution is better explained by looking at Figure 1, which shows a Zircaloy-2 specimen oxidized for 2h at 1200 °C and quenched. The specimen has three different layers, an oxide layer on the surface, an oxygen stabilized α-Zr(O) layer followed by a β-Zr phase, which constitutes the only source of ductility in the three layers. Further oxygen dissolution exacerbated by the increased solubility above 1200°C, would result in the loss of structural integrity of the cladding.

![Figure 1: Cross section of an oxidized Zircaloy-2 sample; adapted from [5].](image)

In addition, at higher temperatures, further embrittlement occurs due to the absorption of hydrogen produced by the Zr-cladding reaction with high temperature steam. The presence of hydrogen in the cladding increases the extent of oxygen solubility and lowers the cladding creep resistance [13], [14]. Therefore, new regulatory criteria, DG-1263, have been proposed to account for the combined detrimental effect of the presence of both oxygen and hydrogen in the cladding [5], [12], [15] as shown in Figure 2.

With respect to RIAs, the regulatory limit is designed to limit the energy deposition during a transient. The failure mechanism under RIA is dependent on burnup, where at lower burnups (<40 MWd/kgU) the limiting event is the post-departure from nucleate boiling (DNB); at higher burnups, the closure of the pellet-clad gap due to swelling and the
adsorption of hydrogen into the cladding that causes embrittlement, caused a shift in the failure mechanism to be dominated by pellet-clad mechanical interaction (PCMI) [16]. The regulatory limit for RIAs set as function of hydrogen content is shown in Figure 3.

Figure 2: Current and proposed regulatory limits on cladding oxidations; adapted from [5].

Figure 3: Current and proposed regulatory limit on energy deposition during RIA [5].
It is noticeable that for both a LOCA and an RIA, the hydrogen content has an adverse effect on performance. Hydrogen is mainly produced by the Zr-alloy cladding oxidation in water. Therefore, an improvement in oxidation kinetics is a necessity to improve the performance of such claddings under both steady state and transient conditions. A major part of the development and optimization efforts for Zr-alloy claddings has been focused on the reducing oxidation kinetics. Figure 4 shows the oxide thickness across the years for the same burnup; oxide thicknesses in 2010 is 10 times lower than thicknesses found prior to 1990. However, the oxidation kinetics and hydrogen pickup at high temperatures (>1000°C) of all these alloys are similar.

Figure 4: Cladding oxide thickness versus burnup accross the years; adapted from [5].

The limitations of the currently employed UO₂-Zr alloy fuels provides the motivation for this thesis to study alternatives that would provide better performance, especially under transient conditions. To re-iterate, the purpose of ATFs is to provide alternatives that “can tolerate the loss of active cooling in the reactor core for a considerably longer time period while maintain or improving the fuel performance during normal operations, operational transits as well as design-basis and beyond design-basis events” [7].
1.2 Thesis Objective and Outline

This thesis aims to examine multiple proposed ATF concepts and determine whether any of the concepts fit the previously quoted description for ATFs or not. The thesis will start by examining the performance of these concepts in comparison to the UO$_2$-Zr system under steady-state conditions. Once proven to be successful under normal operation, the concepts will be further examined under DBA scenarios. The goal is to find a fuel system that would offer more reliable, safer performance compared to the UO$_2$-Zr alloy system.

The thesis will start by providing a brief description of the methodology in Chapter 2 as well as a list of different ATF concepts to be investigated. Chapter 3 presents a compilation of all material properties added to the MOOSE/BISON framework [17], [18] as part of this work, in order to be able carry out the simulations. Material properties already implemented in BISON, for example Zircaloy-4 properties, are not listed in the chapter for brevity and the interested reader is referred to the BISON manual [19]. An analysis of the performance of the proposed ATF claddings starts with Chapter 4, which shows the results of steady-state simulations using a representative PWR power profile. Chapter 5 shows the results for power ramps, while Chapter 6 concludes with the results section by showing loss-of-coolant accident (LOCA) performance simulations. Chapter 7 concludes with a summary of the main findings of the thesis and offers a path forward for investigating ATFs.
2 Methodology

The multi-physics fuel performance tool BISON [18] is used for the thermo-mechanical modelling of the different fuel concepts throughout this thesis. BISON is a finite element-based nuclear fuel performance code built on the MOOSE framework [17], which is a finite element-base framework capable of solving systems of coupled non-linear equations. The BISON code is capable of solving the fully coupled thermo-mechanics and diffusion equations up to 3D geometries. The code has implemented fuel models that can capture temperature and burnup dependent material properties, such as swelling, fuel densification, thermal and mechanical properties, fission gas production and release, and irradiation and thermal creep. Several cladding material properties are included as well, such as Zr6Al-2/4 and FeCrAl. The included properties are augmented by this work with the inclusion of additional materials including Chromium, Molybdenum and Silicon Carbide. These material properties are coded, using object oriented C++, into the program and are described in Chapter 4. As the BISON code is proprietary of Idaho National Laboratory and under US department of energy export control restrictions, the source code for these added materials are not included in thesis. However, the properties in Chapter 4 are enough to re-create the simulations in case the reader has access to BISON.

2.1 ATF Concepts

The thesis will focus on two types of claddings, Zirc-4 based claddings and SiC based claddings. Unless explicitly stated, the claddings and coating thicknesses in the simulations are limited to the prescribed dimensions in the following section.

2.1.1 Zircaloy-4 Based Claddings:

Two different Zircaloy-4 based ATF concepts will be studied: (1) chromium coated Zirc-4 cladding (Zr4-Cr) and (2) FeCrAl coated Zirc-4 cladding with an interlayer of molybdenum (Zr4-Mo/FeCrAl). The thickness of the coatings is kept to a total of 50µm, which is deducted from the base Zr4 thickness as shown in Figure 5.
2.1.2 SiC Based Claddings:

Two SiC-based claddings are studied as well, a chromium coated composite HNLS concept (HNLS-Cr) and a three layered monolithic/composite/monolithic (SiC-3layers) concept. The thicknesses are shown in Figure 6.

![Figure 5: Different Zr4-based claddings and proposed coating thicknesses.](image)

![Figure 6: Different SiC-based claddings and proposed coating thicknesses.](image)

The simulations discussed in chapters 4-6 will divide the results for the two types of Zr4-based and SiC-based and will compare each's performance against a reference Zr4 cladding. A total of 4 ATF coatings as well as the reference case are modelled throughout the thesis. These will be subjected to steady state simulations followed by power ramps and finally LOCA simulations to give an insight into the most promising ones.
3 Material and Behavior Models

3.1 FeCrAl

3.1.1 Isotropic Plasticity

An isotropic plasticity model for FeCrAl can also be used with the combined creep and plasticity model available within MOOSE. This model calculates the yield stress as a function of temperature and fluence.

3.1.1.1. Yield Strength:

As part of this thesis, we are interested in comparing low/high chromium containing FeCrAl alloys. Therefore, we will use Fe-12Cr-4.4Al and Fe-18Cr-2.9Al as our two reference cases [20], which correspond to alloy B125Y and B183Y-2 respectively [21]. Data is extracted from figure 5 in [21], and is tabulated in Table 1.

Table 1: Yield stress of two model FeCrAl alloys as function of temperature.

<table>
<thead>
<tr>
<th>Alloy</th>
<th>Temperature (°C)</th>
<th>Yield Stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>B125Ys</td>
<td>22</td>
<td>600</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>540</td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>580</td>
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<td>480</td>
<td>260</td>
</tr>
<tr>
<td></td>
<td>560</td>
<td>110</td>
</tr>
<tr>
<td>B183Y-2</td>
<td>22</td>
<td>525</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>490</td>
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<td>220</td>
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<tr>
<td></td>
<td>560</td>
<td>100</td>
</tr>
</tbody>
</table>

The following correlations were used for each alloy:

\[
\sigma_{\text{yield,B125Y}} = (3.013 \times 10^{-8}T^4 - 7.1862 \times 10^{-5}T^3 + 0.0594T^2 - 20.6751T + 3143.839) \text{ MPa}
\] (1)
R² = 0.9944; T is in Kelvin.

\[ \sigma_{\text{yield,B183Y-2}} = (6.405 \times 10^{-9}T^4 - 1.7185 \times 10^{-5}T^3 + 0.0148T^2 - 5.4818T + 1247.0455) \text{ MPa} \]  \hspace{1cm} (2)

R² = 0.9918; T is in Kelvin.

3.1.1.2. Irradiation hardening:

Neutron Irradiation data for these two alloys has been reported up to 7.73x10²⁵ for an equivalent of ~7.0 dpa at a target temperature of 320 °C[20]. Actual temperatures ranged from 320-382 °C. The hardening effect is summarized in Table 2.

Table 2: Irradiated tensile data for two FeCrAl alloys

<table>
<thead>
<tr>
<th>Alloy</th>
<th>Irradiation Temperature (°C)</th>
<th>Neutron Fluence (n/m²)</th>
<th>Test Temperature (°C)</th>
<th>0.2 % Yield strength</th>
<th>Hardening factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>B125Y</td>
<td>Unirradiated</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>355</td>
<td>9.25 \times 10^{24}</td>
<td>24</td>
<td>576</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>382</td>
<td>1.95 \times 10^{25}</td>
<td>24</td>
<td>676</td>
<td>1.1736</td>
</tr>
<tr>
<td></td>
<td>320</td>
<td>7.73 \times 10^{25}</td>
<td>24</td>
<td>775</td>
<td>1.3455</td>
</tr>
<tr>
<td>B183Y-2</td>
<td>Unirradiated</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>355</td>
<td>9.25 \times 10^{24}</td>
<td>24</td>
<td>519</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>382</td>
<td>1.95 \times 10^{25}</td>
<td>24</td>
<td>801</td>
<td>1.5434</td>
</tr>
<tr>
<td></td>
<td>320</td>
<td>7.73 \times 10^{25}</td>
<td>24</td>
<td>842</td>
<td>1.6224</td>
</tr>
</tbody>
</table>

Since the irradiation temperature differs for each fluence due to experimental conditions, the hardening factor-fluence correlation is slightly limited as more data is required at equivalent temperatures and at higher irradiation temperature as well to have a complete formulation for fluence-temperature effect on hardening. Therefore, for our purposes, a straight line fitting for the above data is used as an average for the influence of the hardening effect and the following correlations are obtained:

\[ \sigma_{\text{Irradiated,B125Y}} = \sigma_{\text{yield,B125Y}} \times \text{IRRfactor} \]
\[ = \sigma_{\text{yield,B125Y}} \times (4.8738 \times 10^{-27} \phi + 1) \text{ MPa} \]  \hspace{1cm} (3)

* For fitted correlations, we use the coefficient of determination, R², which measures the percent of variation in the dependent variable that can be explained by the regression i.e. R² is a measure of the goodness of the fit, ranging from 0 to 1, with higher being better.
\( \sigma_{\text{yield,B125Y}} \) is obtained from Eqn. (1); \( \phi \) is in n/m².

\[
\sigma_{\text{Ir,irradiated,B183Y-2}} = \sigma_{\text{yield,B183Y-2}} \times \text{Ir} \text{factor}
\]

\[
= \sigma_{\text{yield,B183Y-2}} \times (9.9641 \times 10^{-27} \phi + 1) \text{ MPa}
\]

\( \sigma_{\text{yield,B183Y-2}} \) is obtained from Eqn.(2); \( \phi \) is in n/m².

### 3.1.2 Oxidation and Corrosion

The oxidation of FeCrAl follows parabolic oxidation kinetics [22]. The parabolic rate constant \( (k_p) \) is fitted to an Arrhenius relationship:

\[
k_p = k_0 \exp(-E_a/RT) \quad (g^2 \cdot cm^{-4} \cdot s^{-1})
\]

Where \( k_0 \) is a constant, \( E_a \) is the activation energy, \( R \) is the gas constant and \( T \) is temperature in Kelvin. The weight gain by oxide formation is then calculated by:

\[
w_g = k_p^{1/2} \cdot t^{1/2} \quad (g \cdot cm^{-2})
\]

Robb et al [23] suggested a correction multiplier for the parabolic rate constant proposed by earlier by Pint et al. [22]. Based on the corrected model, the following correlation is used to calculate weight gain for FeCrAl:

\[
(w_g)^2 = \left[ 11.5 \exp \left( \frac{41,376}{T} \right) \right] \cdot t \quad (g \cdot cm^{-2})^2
\]

Taking the square root of equation (7):

\[
w_g = \left[ 3.391 \cdot \exp \left( \frac{20,688}{T} \right) \right] \cdot t^{1/2} \quad (g \cdot cm^{-2})
\]

A conversion factor of \( 5.35 \times 10^3 \mu m \cdot (cm^2 \cdot g^{-1}) \) is adopted from Jonsson et al. [24] to convert the weight gain to oxide thickness for FeCrAl.

### 3.2 Chromium

Pure chromium properties are not commonly studied, as it is usually used as an alloying element for Cr-based alloys. This section cites compiled properties for chromium and the limitations of the data.
3.2.1 Thermal Properties:

Thermal properties were obtained for commercially available pure chromium Ducropure (trademark of Metallwerke Plansee AG, Austria) [25].

3.2.1.1. Specific Heat:

Specific heat ($C_p$) between 300 and 1300K is expressed as [25]:

$$C_p(T) = (-1.278 \times 10^{-7} T^3 + 3.388 \times 10^{-4} T^2 - 0.092934 T + 483.201) \text{J.kg}^{-1}\text{K}^{-1} \quad (9)$$

$T$ is in Kelvin.

3.2.1.2. Thermal Conductivity:

Thermal Conductivity (between 300 and 1300 K) [25]:

$$\lambda(T) = (-2.06676 \times 10^{-8} T^3 + 4.84508 \times 10^{-5} T^2 - 0.0636326 T$$

$$+ 101.754) \text{W.K}^{-1}\text{m}^{-1} \quad (10)$$

$T$ is in Kelvin.

3.2.2 Mechanical Properties

Mechanical properties for chromium includes elastic modulus, poisons ratio, and coefficient of thermal expansion.

3.2.2.1. Elastic Modulus:

The Elastic Modulus as a function of Temperature $E(T)$ (between 300 and 1500K) is tabulated in Table 3 [26]. The data can be fitted to the following polynomial:

$$E(T) = (-2.50126440919815 \times 10^{-5} T^2 - 0.0098566538 T + 264.1122700281) \text{GPa} \quad (11)$$

$T$ is in Kelvin. The coefficient of determination $R^2 = 0.9934$. This fitted relationship is used throughout the thesis.

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Elastic Modulus (10^6 psi)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>36.66</td>
</tr>
<tr>
<td>50</td>
<td>37.31</td>
</tr>
<tr>
<td>100</td>
<td>37.47</td>
</tr>
<tr>
<td>150</td>
<td>37.35</td>
</tr>
<tr>
<td>200</td>
<td>37.15</td>
</tr>
<tr>
<td>250</td>
<td>36.88</td>
</tr>
</tbody>
</table>
### 3.2.2.2. Poisson’s ratio:

The Poisson ratio can be approximately considered as a constant [27]:

\[ v = 0.22 \]  \hspace{1cm} (12)

### 3.2.2.3. Coefficient of Thermal Expansion:

The thermal expansion coefficient (between 300 and 1300 K) is [25]:

\[ \alpha(T) = \left(1.27483 \times 10^{-10}T^3 + 5.40955 \times 10^{-7}T^2 + 0.00148495T + 7.86733\right) \times 10^{-6}K^{-1} \]  \hspace{1cm} (13)

### 3.2.3 Thermal Creep

The thermal creep rate of chromium can be calculated using a Norton creep law:

\[ \dot{\epsilon} = A \exp\left(-\frac{Q}{RT}\right) \sigma^n \]  \hspace{1cm} (14)

where \( \dot{\epsilon} \) is the creep rate (s\(^{-1}\)), \( \sigma \) the effective stress (Pa) and \( T \) (K) is the temperature, \( A \) is the pre-exponential coefficient of creep, \( Q \) is the activation energy for creep, \( R \) is the...
universal constant and \( n \) is the creep exponent \([28]\). Table 4 lists these parameters for Chromium:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A ) [Pa(^{-1})S(^{-1})]</td>
<td>( 3.2555 \times 10^{-40} )</td>
</tr>
<tr>
<td>( Q ) [J.mol(^{-1})]</td>
<td>36805.4</td>
</tr>
<tr>
<td>( R ) [J.mol(^{-1})K(^{-1})]</td>
<td>8.3145</td>
</tr>
<tr>
<td>( n )</td>
<td>6.2</td>
</tr>
</tbody>
</table>

### 3.2.4 Isotropic Plasticity

The isotropic plasticity model for chromium can be used with the combined creep and plasticity model available within MOOSE. This model calculates the yield stress as a function of temperature and fluence.

#### 3.2.4.1. Yield Strength:

The yield strength can be expressed as proof stress at 0.2% plastic deformation (between 300 and 1300 K) \([25]\):

\[
\sigma_{0.2} = (-8.24413 \times 10^{-7} T^3 + 0.00185557 T^2 - 1.39399 T + 513.166) \text{MPa} \tag{15}
\]

\( T \) is in Kelvin.

#### 3.2.4.2. Irradiation hardening:

Irradiation tests on pure chromium are extremely limited. A search for data on neutron irradiation of pure chromium only yielded one paper published in the 60s \([29]\). Although extremely limited, it gives us a first order approximation of the effect of neutron irradiation on chromium. Table 5 shows data obtained from Figure 1 in the referred paper at 200°C \([29]\).

<table>
<thead>
<tr>
<th>Fluence [n/m(^2)]</th>
<th>Yield Strength [10(^3) lbf/in(^2)]</th>
<th>Hardening Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>21</td>
<td>1</td>
</tr>
<tr>
<td>( 2 \times 10^{23} )</td>
<td>26</td>
<td>1.238095</td>
</tr>
</tbody>
</table>

As the source is old and limited to fast neutron fluence (>1 MeV), we cannot use the hardening factor directly as it would give rise to 119x at an end of life fluence of \(~1 \times 10^{26}\) n/m\(^2\). Therefore, examining results for other metals, such as FeCrAl in section 3.1.1.2 and
chromium hardening under fast fluence, a rough estimate can be made that Cr will harden by at least 1.5x at end of cycle. Therefore, pending more experimental data, we use the following correlation:

$$\text{Irr}_{\text{factor}} = 5 \times 10^{-27} \phi + 1$$  \hspace{1cm} (16)

Where $\phi$ is the fluence in n/m$^2$. Equation (15) for yield strength can now be modified as follows:

$$\sigma_{\text{Irradiated}} = \sigma_{0.2} \times \text{Irr}_{\text{factor}} = \sigma_{0.2}(5 \times 10^{-27} \phi + 1) \text{ MPa}$$  \hspace{1cm} (17)

3.2.5 Oxidation and Corrosion

At PWR steady state conditions, tests conducted by AREVA at 360°C with simulated PWR chemistry, showed negligible weight gain in the order of 1mg/dm$^2$ after 180 days of exposure [30]. Therefore, corrosion at PWR steady state conditions will not be included in this work.

As for oxidation behavior at high temperatures (>1000 °C), data is currently very limited as experimental efforts are still ongoing. Brachet et al [31] conducted one-sided steam oxidation test at 1200°C. Their experiments showed the weight gain for the Cr-coated M5 to be ~15-20 times less than the uncoated material. Hyun-Gil Kim et al. [32] also conducted high temperature oxidation of Cr at 1200°C and showed a 20-fold decrease in weight gain in comparison to uncoated Zr4. For the purpose of simplification and due to data limitations, we will simply modify the parabolic rate law for zirconium with a reduction factor of 15 times in weight gain, and adopt that model for high temperature Cr oxidation. For the temperature range 673-1800K, the Leistikov [33] correlation is used in bison [19]; modification gives us:

$$w'_{K} = 2.33 \times 10^{-3} \cdot \exp \left( \frac{20,962}{T} \right) \cdot t \quad (g.cm^{-2})^2$$  \hspace{1cm} (18)

Where $w'_{K}$ is the weight gain in (g.cm$^{-2}$), t is time in seconds and T is the temperature in Kelvins. Taking the square root of equation (20):

$$w'_{K} = 4.83 \times 10^{-2} \cdot \exp \left( \frac{10,481}{T} \right) \cdot t^{1/2} \quad (g.cm^{-2})$$  \hspace{1cm} (19)

A conversion factor of $2.22 \times 10^3 \mu m.(cm^2.g^{-1})$ is adopted from Lillerud et al [34] to convert the weight gain to oxide thickness for chromium.
3.3 Molybdenum

3.3.1 Thermal Properties

Thermal properties for molybdenum include temperature dependent thermal conductivity and heat capacity.

3.3.1.1. Specific Heat:

The specific heat for pure molybdenum is tabulated in [35]:

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>Specific heat (J·kg⁻¹K⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>400</td>
<td>258</td>
</tr>
<tr>
<td>700</td>
<td>247</td>
</tr>
<tr>
<td>1000</td>
<td>290</td>
</tr>
<tr>
<td>1500</td>
<td>326</td>
</tr>
<tr>
<td>2000</td>
<td>347</td>
</tr>
<tr>
<td>2400</td>
<td>415</td>
</tr>
<tr>
<td>2800</td>
<td>458</td>
</tr>
</tbody>
</table>

This is fitted to the following correlation:

\[ C_p(T) = 241 + 1.81 \times 10^{-2}T + 2.13 \times 10^{-5}T^2 \text{ (J·kg}^{-1}\text{K}^{-1}) \]  

\( R^2 = 0.978; \) T is in Kelvin.

3.3.1.2. Thermal Conductivity:

Thermal conductivity is values is tabulated in Table 7 [35]:

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>Thermal expansion (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>400</td>
<td>133</td>
</tr>
<tr>
<td>700</td>
<td>122.5</td>
</tr>
<tr>
<td>1000</td>
<td>112</td>
</tr>
<tr>
<td>1500</td>
<td>94</td>
</tr>
<tr>
<td>2000</td>
<td>78</td>
</tr>
<tr>
<td>2500</td>
<td>70</td>
</tr>
<tr>
<td>3000</td>
<td>67</td>
</tr>
</tbody>
</table>

The following correlation is obtained:

\[ \lambda(T) = 7.5841 \times 10^{-6}T^2 - 0.0524T + 154.6085 \text{ (Wm}^{-1}\text{K}^{-1}) \]

3.3.2 Mechanical Properties

Mechanical properties for Molybdenum include elastic modulus, poisons ratio, and coefficient of thermal expansion.
3.3.2.1. Elastic Modulus

Elastic modulus values are obtained from [35] and tabulated in Table 8:

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>Elastic Modulus (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>330</td>
</tr>
<tr>
<td>900</td>
<td>297</td>
</tr>
<tr>
<td>1500</td>
<td>270</td>
</tr>
<tr>
<td>2000</td>
<td>242</td>
</tr>
<tr>
<td>2500</td>
<td>200</td>
</tr>
</tbody>
</table>

The following correlation is obtained:

$$E(T) = -8.2007 \times 10^{-6}T^2 - 0.0341T + 338.9251 \text{ (GPa)}$$ (22)

With $R^2=0.9952$.

3.3.2.2. Poisson’s ratio:

The Poisson ratio can be approximately considered as a constant [35]:

$$\nu = 0.356$$ (23)

3.3.2.3. Coefficient of Thermal expansion

Thermal expansion coefficient can be obtained from thermal expansion values tabulated in Table 9 [35]:

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>Thermal expansion (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>0</td>
</tr>
<tr>
<td>700</td>
<td>0.2</td>
</tr>
<tr>
<td>1000</td>
<td>0.46</td>
</tr>
<tr>
<td>1600</td>
<td>0.83</td>
</tr>
<tr>
<td>2100</td>
<td>1.27</td>
</tr>
<tr>
<td>2500</td>
<td>1.7</td>
</tr>
<tr>
<td>2900</td>
<td>2.22</td>
</tr>
</tbody>
</table>

$$\frac{\Delta L}{L} = \alpha_L \Delta T$$ (24)

Using the linear thermal expansion relationship, Eqn. (24), we can obtain the following correlation for thermal expansion:
\[ \alpha(T) = -1.7551 \times 10^{-18}T^4 + 1.3635 \times 10^{-14}T^3 - 3.7184 \times 10^{-11}T^2 + 4.2649 \times 10^{-8}T - 1.0858 \times 10^{-5} \text{ (m.m}^{-1}) \]  

With \( R^2 = 0.99886 \).

### 3.3.3 Thermal Creep

Molybdenum, a refractory metal, has a melting temperature of 2895 K [36] and possesses excellent creep resistance[37]. Creep studies of Molybdenum have been mainly limited to high temperature applications 1600-2000 K [37], [38]. The following power-law creep relationship is suggested for the temperature range of 1600-2100K [37]:

\[ \dot{\epsilon} = A \exp \left( -\frac{Q}{RT} \right) \sigma^n \]  

(26)

where \( \dot{\epsilon} \) is the creep rate (s\(^{-1}\)), \( \sigma \) the effective stress (Pa), T (K) is the temperature, A is the pre-exponential coefficient of creep, Q is the activation energy for creep, R is the universal constant and n is the creep exponent. Table 10 lists the values of these parameters for Molybdenum:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A [s(^{-1})]</td>
<td>0.28</td>
</tr>
<tr>
<td>Q [J.mol(^{-1})]</td>
<td>275 \times 10^3</td>
</tr>
<tr>
<td>R [J.mol(^{-1})K(^{-1})]</td>
<td>8.3145</td>
</tr>
<tr>
<td>n</td>
<td>2.27</td>
</tr>
</tbody>
</table>

### 3.3.4 Isotropic Swelling

Irradiation induced swelling is expected in Molybdenum. Previous studies by Garner and Stubbins [39] showed void swelling limited to 4% over a range of irradiation temperatures (420-722 °C). Recent studies performed at Oak Ridge National Laboratory by Cockeram et al. [40] showed similar behavior. However, at 300°C, which is close to the PWR operating temperature, irradiation of molybdenum “produces negligible swelling that is counteracted by the small increases in density due to the formation of transmutation products so that the net result is a small amount of densification at higher doses” [40]. Figure 7 shows the expected temperature-dependent swelling behavior.
Figure 7: Temperature dependence for maximum swelling values determined from highest fluence for the irradiation of ODS, LCAC, and TZM molybdenum. Adapted from [40].

The fluence-temperature effect on swelling is rather complex in molybdenum as shown by data obtained for wrought Low Carbon Arc Cast material (LCAC) in Table 11.

Table 11: Summary of measured swelling for different irradiations.

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Fluence (x10^{24} n/m^2)</th>
<th>Swelling (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>10.5</td>
<td>0.38</td>
</tr>
<tr>
<td></td>
<td>232</td>
<td>0.1</td>
</tr>
<tr>
<td>600</td>
<td>16.2</td>
<td>0.41</td>
</tr>
<tr>
<td></td>
<td>27</td>
<td>0.63</td>
</tr>
<tr>
<td></td>
<td>246</td>
<td>1.93</td>
</tr>
<tr>
<td>900</td>
<td>18</td>
<td>0.95</td>
</tr>
<tr>
<td></td>
<td>44.5</td>
<td>0.54</td>
</tr>
<tr>
<td></td>
<td>61.3</td>
<td>0.63</td>
</tr>
<tr>
<td></td>
<td>246</td>
<td>1.46</td>
</tr>
<tr>
<td></td>
<td>247</td>
<td>0.66</td>
</tr>
</tbody>
</table>

Developing a correlation for temperature-fluence effect on swelling using such limited data is implausible. However, for the sake of simplicity and initial analysis, we can use a straight line fit for swelling at 600°C and add a temperature correction factor from Figure 7. This gives the following volumetric swelling correlation:

\[
\epsilon = (8.10361 \times 10^{-29} \phi)(-8.923 \times 10^{-6} T^2 + 0.0161 T - 6.2254) \tag{27}
\]

Where \( \phi \) is the fluence in n/m^2 and \( T \) is temperature in K.
3.3.5 Isotropic Plasticity

The isotropic plasticity model for molybdenum can also be used with the combined creep and plasticity model available within MOOSE. This model calculates the yield stress as a function of temperature and fluence.

3.3.5.1. Yield Strength:

The 0.2% yield strength for LCAC molybdenum is tabulated in Table 12 [41]. This data can be used to obtain a correlation for molybdenum in Eqn. (28).

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>0.2% Yield Stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>22</td>
<td>751.9</td>
</tr>
<tr>
<td>150</td>
<td>538.9</td>
</tr>
<tr>
<td>300</td>
<td>505.4</td>
</tr>
<tr>
<td>600</td>
<td>475.6</td>
</tr>
<tr>
<td>700</td>
<td>464</td>
</tr>
<tr>
<td>800</td>
<td>402.3</td>
</tr>
<tr>
<td>1000</td>
<td>280.3</td>
</tr>
<tr>
<td>1093</td>
<td>110.3</td>
</tr>
</tbody>
</table>

\[ \sigma_{0.2} = (-2.1022 \times 10^{-6}T^3 + 0.0051T^2 - 4.1102T + 1558.9189) \text{MPa} \] (28)

\( R^2 = 0.9872 \) and \( T \) is in Kelvin.

3.3.5.2. Irradiation hardening:

Neutron irradiation for LCAC molybdenum has been conducted up to \( 2.47 \times 10^{26} \text{n/m}^2 \) or \( \approx 13.1 \text{ dpa} \) [41]. Specimens were irradiated at different temperatures and the tensile strength was obtained post-irradiation at different temperatures as well. The irradiation data is listed in Table 13. We will use the data to obtain average hardening for each irradiation temperature. Taking the average for each irradiation temperature and the average fluence \( (2.42 \times 10^{26} \text{n/m}^2) \), we can obtain a first order correlation for irradiation hardening as a function of fluence and temperature between 294 and 936 °C.

\[ \sigma_{\text{Irradiated}} = \sigma_{0.2} \times \text{Irr\_factor} \]
\[ = \sigma_{0.2}[(4.8606 \times 10^{-8}T^3 - 0.00013T^2 + 0.1159T - 30.7059) \times (4.1379 \times 10^{-27}\phi + 1)] \text{MPa} \] (29)

\( \sigma_{0.2} \) is obtained from Eqn. (28); \( T \) is in Kelvins and \( \phi \) is in \text{n/m}^2.
Table 13: Irradiated tensile date for LCAC molybdenum sheet [41]. Hardening factor is calculated using unirradiated yield strength at the same test temperature from Table 12.

<table>
<thead>
<tr>
<th>Irradiation Temperature (°C)</th>
<th>Neutron Fluence (n/m²)</th>
<th>Test Temperature (°C)</th>
<th>0.2 % Yield strength</th>
<th>Hardening factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>294</td>
<td>232 × 10²⁴</td>
<td>22</td>
<td>1244.5</td>
<td>1.6551</td>
</tr>
<tr>
<td>294</td>
<td>232 × 10²⁴</td>
<td>600</td>
<td>1190.8</td>
<td>2.5038</td>
</tr>
<tr>
<td>294</td>
<td>232 × 10²⁴</td>
<td>700</td>
<td>944.6</td>
<td>2.0358</td>
</tr>
<tr>
<td>294</td>
<td>232 × 10²⁴</td>
<td>800</td>
<td>638.5</td>
<td>1.5871</td>
</tr>
<tr>
<td><strong>Average</strong></td>
<td></td>
<td></td>
<td><strong>1.9455</strong></td>
<td></td>
</tr>
<tr>
<td>560</td>
<td>246 × 10²⁴</td>
<td>22</td>
<td>1386.6</td>
<td>1.8441</td>
</tr>
<tr>
<td>560</td>
<td>246 × 10²⁴</td>
<td>150</td>
<td>1475.5</td>
<td>2.7380</td>
</tr>
<tr>
<td><strong>Average</strong></td>
<td></td>
<td></td>
<td><strong>2.2912</strong></td>
<td></td>
</tr>
<tr>
<td>784</td>
<td>246 × 10²⁴</td>
<td>300</td>
<td>559.9</td>
<td>1.1078</td>
</tr>
<tr>
<td>784</td>
<td>246 × 10²⁴</td>
<td>600</td>
<td>463.3</td>
<td>0.9741</td>
</tr>
<tr>
<td><strong>Average</strong></td>
<td></td>
<td></td>
<td><strong>1.0410</strong></td>
<td></td>
</tr>
<tr>
<td>936</td>
<td>247 × 10²⁴</td>
<td>22</td>
<td>692.3</td>
<td>0.9207</td>
</tr>
<tr>
<td>936</td>
<td>247 × 10²⁴</td>
<td>1000</td>
<td>399.9</td>
<td>1.4267</td>
</tr>
<tr>
<td><strong>Average</strong></td>
<td></td>
<td></td>
<td><strong>1.1737</strong></td>
<td></td>
</tr>
</tbody>
</table>

3.4 Silicon Carbide

In this section, we will list thermal and mechanical properties of monolithic CVD (Chemical Vapor Deposition) SiC and SiC/SiC CVI (Chemical Vapor Infiltrated) ceramic matrix composite (CMC), which are both used in ATF concepts studied. Properties are adopted mainly from [42].

3.4.1 Thermal Properties

3.4.1.1. Specific Heat:

The specific heat for both monolithic and composite are very similar [43] and can be expressed as [44] over the temperature range 200-2400 K:

\[
C_p(T) = 925.62 + 0.3772 \, T - 7.9259 \times 10^{-5} \, T^2 - \frac{3.1946 \times 10^7}{T^2} \quad \text{(J.kg}^{-1}\text{K}^{-1})
\]  (30)

3.4.1.2. Thermal Conductivity:

Thermal conductivity for SiC is affected by neutron irradiation [43]. We will start first by listing unirradiated behavior and follow by discussing irradiation effects on conductivity. Unirradiated thermal conductivity is obtained from the following correlations [42], [44], [45]:

\[
35
The effect of irradiation on conductivity is pronounced as seen in . It can be described by the defect thermal resistivity model proposed by Snead et al [46]:

\[
K_{irr}^{-1} = K_0^{-1} + K_{rd}^{-1}
\]  

Where \( K_{irr}^{-1} \) and \( K_0^{-1} \) are radiated and unirradiated thermal resistivity. \( K_{rd}^{-1} \) is thermal resistivity from irradiation and can be expressed as [43], [44]:

a) SiC/SiC

\[
K_{rd}^{-1} = 15.11 \times S \text{ (Wm}^{-1}\text{K}^{-1})^{-1}
\]  

b) mSiC

\[
K_{rd}^{-1} = 6.08 \times S \text{ (Wm}^{-1}\text{K}^{-1})^{-1}
\]

Where \( S \) is the volumetric swelling strain \((\Delta V/V_0)\), which is described in the following section.

Figure 8: Degradation in room-temperature thermal conductivity for CVD SiC; adapted from [44].
3.4.2 Mechanical Properties

3.4.2.1. Elastic Modulus & Poisson’s ratio

The elastic moduli exhibits a minor decrease with swelling [43], while Poisson’s ratio is taken as a constant.

| Table 14: Elastic modulus and Poisson’s ratio for SiC |
|--------------------------------|--------|--------|
| Elastic modulus (GPa) [44], [47] | 296    | 460    |
| Poisson’s ratio [43], [44]      | 0.18   | 0.21   |

3.4.2.2. Coefficient of Thermal expansion

The thermal expansion coefficient for both composite and monolithic SiC can be calculated using the following correlation [43]:

\[
\alpha(T) = (3.83 \times 10^{-9}T^3 - 1.22 \times 10^{-5}T^2 + 0.0144T - 0.777) \times 10^{-6} \text{ (m.m}^{-1})
\]  (36)

T is in kelvins.

3.4.3 Volumetric Swelling

Irradiation induced swelling in CVD SiC is described with the following equation from Katoh et al. [48]:

\[
\dot{S} = k_s \gamma^{-1/3} \exp \left( -\frac{\gamma}{\gamma_{sc}} \right)
\]  (37)

Where \( \dot{S} \) is the swelling rate, \( k_s \) is the rate constant for swelling, \( \gamma \) is the fast fluence (in dpa) and \( \gamma_{sc} \) is the characteristic fluence (in dpa) for swelling saturation by the negative feedback mechanism. The rate constant and characteristic saturation fluence can be described for the temperature range (473-1073K) as follows:

\[
k_s(T) = 0.10612 - 1.5904 \times 10^{-4}T + 6.0631 \times 10^{-8}T^2 \quad (38)
\]

\[
\gamma_{sc}(T) = 0.51801 - 2.7651 \times 10^{-3}T + 9.4807 \times 10^{-6}T^2 - 1.3095 \times 10^{-8}T^3 + 6.7221 \times 10^{-12}T^4 \quad (39)
\]

T is in Kelvin. To convert fluence (n/m²) into(dpa), a conversion factor of \( 10^{25} \text{n/m}^2 (>0.1 \text{MeV}) \) per dpa is used[43]. For the purpose of this thesis, the composite SiC/SiC and monolithic are
assumed to have the same swelling behavior as published data suggests no significance difference in behavior [43].

Although equation (39) has been shown to recreate experimental observations of neutron-induced swelling in SiC, it has been argued by Mieloszyk [49] to have two flaws when implemented: First, it doesn’t explicitly converge towards a saturation swelling. Second, it gets erratic when integrated at low doses. For these aforementioned reasons, we adopt his numerical implementation to describe SiC swelling. The reader is referred to section 7.2.2 in Mieloszyk’s thesis [49] for detailed explanation of this implementation. The model is shown to predict expected swelling of SiC under variable temperature and dose history as shown in Figure 9.

![Figure 9: Temperature and dose history and resultant swelling. Saturation swelling is plotted as well. Adapted from [49]](image-url)
3.4.4 Pseudo-plasticity

The inter-woven nature of composite SiC/SiC allows it to deform in a pseudo-plastic manner, giving it improved fracture toughness. Otherwise, SiC in general is treated as a purely linear-elastic material up to failure. The stress-strain behavior of SiC/SiC begins with a linear-elastic region up to the initiation of matrix cracking and then continues to deform non-linearly due to continuous matrix cracking and fiber sliding [50], [51]. To account for this behavior a modified stress-strain curve is adopted as shown in Figure 10. \((\varepsilon_p, \sigma_p)\) are the proportional limit strain and stress respectively, where \((\varepsilon_u, \sigma_u)\) refer to the ultimate tensile limit. These values are listed in Table 15 [47]. The stress-strain behavior is not significantly affected by either temperature up to 1000°C [52] or irradiation conditions in LWRs[42], [43]; thus their effects are disregarded in this study.

<table>
<thead>
<tr>
<th>SiC/SiC</th>
<th>Proportional limit stress ((\sigma_p))</th>
<th>163 MPa</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Strain at PLS ((\varepsilon_p))</td>
<td>0.056 %</td>
</tr>
<tr>
<td></td>
<td>Ultimate tensile strength ((\sigma_u))</td>
<td>404 MPa</td>
</tr>
<tr>
<td></td>
<td>Strain at UTS ((\varepsilon_u))</td>
<td>0.494%</td>
</tr>
</tbody>
</table>

Figure 10: Example modified Stress-Strain behavior for SiC/SiC. Adapted from [42].
For modeling implementation, this behavior can be represented by linking the young’s modulus to mechanical strain using the following correlations:

\[
E = \begin{cases} 
296 \times 10^9 \text{ Pa} & \epsilon \leq \epsilon_p = 0.056\% \\
\left(5.5023 \times 10^{10} \epsilon + 1.3219 \times 10^8\right)/\epsilon & \epsilon > \epsilon_p = 0.056\%
\end{cases}
\]  (40)

3.4.5 Failure

Failure of SiC is statistical due to its brittle nature. It can be described using the Weibull model [53]:

\[
P_f(\sigma) = 1 - \exp\left(-\left(\frac{\sigma - \sigma_c}{\sigma_0}\right)^m \frac{V}{V_0}\right)
\]  (41)

Where \(\sigma\) is the stress, \(\sigma_0\) is the characteristic strength, \(\sigma_c\) is the stress which below no failure occurs, \(m\) is the Weibull modulus, \(V\) is the volume of the specimen and \(V_0\) is the reference volume. The equation can be further simplified by assuming \((\sigma_c = 0)\) and \((V = V_0)\). This reduces to:

\[
P_f(\sigma) = 1 - \exp\left(-\left(\frac{\sigma}{\sigma_0}\right)^m\right)
\]  (42)

\(\sigma_0\) and \(m\) are empirical parameters that are fitted experimentally. Table 16 lists values used for predicting failure for monolithic and composite SiC [53].

<table>
<thead>
<tr>
<th>Table 16: Weibull failure model parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weibull Characteristic Strength ((\sigma_0))</td>
</tr>
<tr>
<td>-----------------------------------------------</td>
</tr>
<tr>
<td>Weibull Modulus ((m))</td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>
4 Steady-State Simulations

4.1 Overview
The steady state simulations were designed to simulate representative US commercial PWR power plant operation [54], with a total average fuel rod burnup of approximately 60 MWd/kgU. The simulations included full-shutdown for all cases, to give an accurate representation of the cladding behavior and to account for shutdown contribution to some phenomena, such as PCMI and swelling. For all the plots the solid line represents the right y-axis and the dashed line represents the left (secondary) y-axis.

4.2 Test Description

4.2.1 Rod Design Specifications
The rod used is a 2D axisymmetric fuel rodlet with discrete fuel pellets. The rodlet is expected to produce similar behavior as the full length rod [55]. Details of the fuel rod geometry and specifications are summarized in Table 17. The cladding thicknesses were summarized in Section 2.1.

Table 17: Steady state case Test rod specifications

<table>
<thead>
<tr>
<th>Fuel Rod</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel stack height</td>
<td>cm</td>
<td>15</td>
</tr>
<tr>
<td>Nominal Plenum height</td>
<td>cm</td>
<td>0.75348</td>
</tr>
<tr>
<td>Number of pellets per rod</td>
<td></td>
<td>15</td>
</tr>
<tr>
<td>Fill gas composition</td>
<td></td>
<td>He</td>
</tr>
<tr>
<td>Fill gas pressure</td>
<td>MPa</td>
<td>4.2</td>
</tr>
<tr>
<td>Fuel</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Material</td>
<td></td>
<td>UO$_2$</td>
</tr>
<tr>
<td>Enrichment</td>
<td>%</td>
<td>5</td>
</tr>
<tr>
<td>Density</td>
<td>%</td>
<td>95</td>
</tr>
<tr>
<td>Outer diameter</td>
<td>mm</td>
<td>8.1919</td>
</tr>
<tr>
<td>Pellet geometry</td>
<td></td>
<td>Dished</td>
</tr>
<tr>
<td>Grain diameter</td>
<td>µm</td>
<td>5</td>
</tr>
<tr>
<td>Pellet Dishing</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Dish diameter</td>
<td>mm</td>
<td>21.2</td>
</tr>
<tr>
<td>Dish depth</td>
<td>mm</td>
<td>0.287</td>
</tr>
<tr>
<td>Chamfer width</td>
<td>mm</td>
<td>0.5</td>
</tr>
<tr>
<td>Chamfer depth</td>
<td>mm</td>
<td>0.16</td>
</tr>
</tbody>
</table>
4.2.2 Operating Conditions and Irradiation History

The power history for the steady state case is shown in Figure 11, with axial peaking factors shown in Figure 12. Other reactor operation parameters are tabulated in Table 18.

![Graph showing power history over time](https://via.placeholder.com/150)

**Figure 11: BISON input power history for the steady state case**

<table>
<thead>
<tr>
<th>Operational input parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coolant inlet temperature</td>
<td>C 293</td>
</tr>
<tr>
<td>Coolant pressure</td>
<td>MPa 15.5</td>
</tr>
<tr>
<td>Fast neutron flux</td>
<td>n/(cm².s) 4.022 x 10¹³</td>
</tr>
</tbody>
</table>

*Table 18: Operational input parameters*
4.2.3 Geometry and Mesh

A 2-dimensional axisymmetric quadratic mesh was used for the simulations. The fuel pellets were modeled using discrete meshes. Both the fuel and cladding used fine meshes, each fuel pellet had 30 radial elements and 30 axial elements. The cladding had 4 radial elements and the number of axial elements were adjusted to simulate approximately square elements for the cladding as shown in Figure 13. The simulation for the reference Zircaloy-4 case had a total of 9,612 elements.
4.2.4 Material and Behavioral Models

4.2.4.1. Fuel

The following BISON material models were used for the UO₂ fuel [19]:

- **CreepUO₂**: A model for combined secondary thermal creep and irradiation creep of UO₂ fuel, with the creep rate as a function of time, temperature, effective stress, density, grain size, fission rate, and oxygen to metal ratio. Young’s modulus, Poisson’s ratio and the coefficient of thermal expansion can each be specified using MATPRO correlations.
- **ThermalFuel**: NFIR correlation; burnup and temperature dependent thermal properties.
- **RelocationUO₂**: relocation strains, relocation activation threshold power set to 5 kW/m.
- **Sifgrs**: Coupled fission gas release and swelling model.
- **VswellingUO₂**: Calculating swelling in fuel due to both solid and gaseous fission products, based on empirical relations from MATPRO.

4.2.4.2. Cladding

The following BISON material models were used for the Zircaloy-4 cladding [19]:

- **Constant thermal conductivity of 16 W/m-K.**
- **MechZry**: Elastic modulus and thermal expansion are based on MATPRO correlations. Thermal and irradiation creep are modeled using the Limback model. Irradiation growth is based on Franklin’s correlations [56].
- **CombinedCreepPlasticity**: models the deformation under both creep and instantaneous plasticity.
- **ZryPlasticity**: Plasticity model for Zircaloy based on PNNL stress/strain correlations for Zircaloy [57].
4.3 Results:

4.3.1 Zr-based fuel systems:

The simulation results for Zr-based fuel systems are shown in Figures 14-18. The two Zr4-based fuels, Zr4-Mo/FeCrAl and Zr4-Cr, showed comparable performance to the reference Zr4 cladding under steady-state operation. Plenum pressures and fission gas released is slightly lower for the coated claddings as seen in Figure 14. The major difference is the lower inward creep for the coated claddings, due to the higher stiffness of the coatings as well as lower thermal creep relative to Zircaloy-4. This results in lower inward cladding displacement and delayed contact as illustrated in Figure 15. The delayed gap closure results in a slight difference in centerline fuel temperature for the first ~500 days of operation as shown in Figure 16; the temperatures become similar after contact is achieved for all three claddings as the metals have comparable thermal conductivity. As seen in Figure 17, the coated claddings show slightly lower but comparable stresses in the base Zr4 layer in each of the cases resulting in stresses lower than plastic yield strain for Zr4. As for the coatings, their stresses and effective plastic strains are plotted in Figure 18. All the coatings yield upon initial heating from room temperature, due to thermal mismatch with the base Zr4 layer. The coatings further yield to 1.3%, 0.3% and 0.1% plastic strain for chromium, molybdenum and FeCrAl layers respectively. These expected plastic strains suggest that further experimental investigation of the claddings at these temperatures to test their integrity during operations is warranted. For Zr4-Cr, chromium is expected to survive elongations of 40% before fracture at 300°C [25] and thus is expected to survive the much lower 1.3% plastic strains resulting here. As for the Zr4-Mo/FeCrAl, the limiting factor would be molybdenum which, depending on test temperature, shows total elongations of only 0.03-0.2% at 13.1 dpa radiation damage [41]. This could be mitigated by the utilization of ODS Molybdenum which has higher yield strength under irradiation [58]. However, for the moment, these resulting plastic strains puts the Zr4-Mo/FeCrAl at question and warrants further investigation.
Figure 14: Plenum pressure and FGR for the Zr4 based fuels

Figure 15: Average radial displacement and contact pressure for the Zr4 based fuels
Figure 16: Centerline fuel temperature for the Zr4-based fuels

Figure 17: Von Mises stresses in the base Zr4 cladding for the three Zr4-based fuels
4.3.2 SiC-based fuel systems:

This section will present the calculated performance of the two SiC-based ATFs in comparison to the reference Zr-4 cladding. Figures 19-25 show the simulation results. The reference Zr-4 case settings modeled are slightly different from the one in the Zr4-based ATF in section 4.3.1; pellet-clad interaction occurred with the SiC cladding, using the same BISON setting from the Zr4-based ATF section. PCI occurred due to a significant increase in fuel temperature due to a lack of cladding creep down and lower cladding thermal conductivity compared to Zr4. However, PCI could be also an artifact of the fuel swelling model implemented in bison, as pellet-clad contact is not expected to occur with SiC based cladding based on predictions of the FRAPCON fuel performance code [59]. In order to simplify matters and focus on the cladding behavior, we changed the fuel thermal conductivity to 1.3 times the implemented standard fuel conductivity in BISON. This can be thought of as enhancing the fuel conductivity using additives such as BeO, previously investigated to address the high fuel temperatures reached with SiC cladding[60]. The idea is that pellet-clad contact should be avoided for SiC-based fuels and designed out. The enhancement of the fuel conductivity by 1.3x resulted in much lower contact stresses for the
SiC fuels. The reference case for Zr4 in this section also has the enhanced fuel thermal conductivity for an unbiased comparison; thus the fuel centerline temperatures are expected to be lower than the Zr4-ref case in the Zr-based fuel systems in section 4.3.1. Aside from the enhanced fuel conductivity, everything else is kept the same in the simulations. The two concepts are referred to as 1) SiC/SiC-Cr and 2) SiC-3layers.

Looking at the results for the steady-state simulations, we can see that plenum pressures and fission gas release is higher for the SiC-based fuels, with SiC-3layers being higher than SiC/SiC-Cr as seen in Figure 19. This can be understood looking at the calculated centerline fuel temperatures in Figure 21, where SiC-3layers shows the highest temperature followed by SiC/SiC-Cr; this is mainly due to the higher thickness of the 3-layers cladding combined with the low thermal conductivity of SiC. The higher temperatures result in more fission gas release and higher plenum pressures as well. As for the claddings radial displacement, the SiC-based claddings do not creep inwards like the Zr4 reference case but rather keep displacing outwards due to the increasing plenum pressure. Therefore, contact is delayed for the SiC-based claddings but still occurs. This could be the result of increased swelling of the UO$_2$ fuel due to higher fuel temperature in the SiC-based fuels (~200 degrees difference for Zr4 reference). As for the stresses, Figure 22 shows the resulting maximum principal stresses for all SiC layers. The SiC-3layers cladding has generally higher stresses than the SiC/SiC-Cr, with the inner monolith layer having the highest stress. These high stresses make the SiC-3layers questionable in its current configuration, as it is expected to fail as seen in Figure 23, where the inner monolith layer is certain to fail ($P(f) = 1$). The SiC/SiC-Cr generally has lower failure probability except for the second shutdown where it reaches ($P(f) = ~0.5$). The higher stress could be the result of pellet-clad contact occurring between the first and second shutdown. There is a possibility that this pellet-clad interaction could be designed out by optimizing the gap thickness and cladding dimensions, and thus the SiC/SiC-Cr is deemed promising for further investigation. As for the Chromium coating, it is expected to yield up to an effective plastic strain of $\sim$2.4% which is higher but still comparable to the Zr4-Cr fuel earlier. It is expected that the Cr layer would be able to survive steady-state operation under these conditions.
Figure 19: Plenum pressure and FGR for the SiC-based fuels versus reference Zr4

Figure 20: Average radial displacement and contact pressure for the SiC-based fuels
Figure 21: Centerline Fuel temperatures for the SiC-based fuels versus reference Zr4

Figure 22: Maximum principal stresses of all SiC layers in the two SiC-based fuels and Von Mises stress of reference Zr4
Figure 23: Failure probability for SiC layers in SiC-based fuels under steady state operation

Figure 24: Stress and effective plastic strain of the Cr coating in the SiC/SiC-Cr
Figure 25: Average swelling in different SiC layers for the two SiC-based fuels
5 Transient Simulations: Ramp Test

5.1 Overview

The ramp test of choice is based on the French OSIRIS J12-5 test [61]. The purpose is to study the PCMI resistance of the proposed ATFs. The experimental test is based on a segmented PWR rod that has been base-irradiated then re-fabricated and ramp-tested in the French Alternative Energies and Atomic Energy Commission (CEA) OSIRIS reactor.

5.2 Test Description

5.2.1 Rod Design Specifications

The rod simulated is a 2D axisymmetric fuel rodlet with discrete fuel pellets. Details of the fuel rod geometry and specifications are summarized in Table 19. The coatings are kept at the same thicknesses and are deducted from the base Zr cladding thickness.

<table>
<thead>
<tr>
<th>Table 19: Steady state case Test rod specifications</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Fuel Rod</strong></td>
</tr>
<tr>
<td>Overall length mm 522.4</td>
</tr>
<tr>
<td>Fuel stack height mm 432.95</td>
</tr>
<tr>
<td>Nominal Plenum height mm 89.44</td>
</tr>
<tr>
<td>Number of pellets per rod 32</td>
</tr>
<tr>
<td>Fill gas composition He</td>
</tr>
<tr>
<td>Fill gas pressure MPa 2.6</td>
</tr>
<tr>
<td><strong>Fuel</strong></td>
</tr>
<tr>
<td>Material UO₂</td>
</tr>
<tr>
<td>Enrichment % 4.5</td>
</tr>
<tr>
<td>Density % 95.73</td>
</tr>
<tr>
<td>Outer diameter mm 8.192</td>
</tr>
<tr>
<td>Pellet geometry Dished</td>
</tr>
<tr>
<td>Grain diameter μm 10</td>
</tr>
<tr>
<td><strong>Pellet Dishing (no chamfers)</strong></td>
</tr>
<tr>
<td>Dish diameter mm 6</td>
</tr>
<tr>
<td>Dish depth mm 0.32</td>
</tr>
<tr>
<td><strong>Cladding</strong></td>
</tr>
<tr>
<td>Outer diameter mm 9.5</td>
</tr>
<tr>
<td>Inner diameter mm 8.36</td>
</tr>
<tr>
<td>Wall thickness mm 0.57</td>
</tr>
</tbody>
</table>
5.2.2 Operating Conditions and Irradiation History

Experimentally, the segmented Zr-4 rod was irradiated to a burnup of 23.852 MWd/kgU in the Electricity of France (EDF) Graveline 5 PWR. After base-irradiation the rod-segment was re-fabricated with new end plugs, while retaining the fuel column and internal fill gas. The re-fabricated rod was then ramp-tested; first, the rod was reconditioned at 21 kW/m for 762 minutes, then the power was ramped at a rate of 9 kW/min up to 39.5 kW/m, where it was held for 739 minutes. The base-irradiation power history is shown in Figure 26 and ramp test power history is shown in Figure 27. The external clad temperature was estimated as a function of time as shown in Figure 28 and Figure 29. The axial peaking factor is kept flat at 1.0 for the base-irradiation run; peaking factors for the ramp test is shown in Figure 30.

Figure 26: BISON input power history for OSIRIS J12 in the Gravelines 5 PWR
Figure 27: BISON input power history for OSIRIS J12 power ramp test

Figure 28: External cladding temperature for OSIRIS J12 base-irradiation
Figure 29: External cladding temperature for OSIRIS J12 power ramp

Figure 30: BISON input fast neutron flux axial peaking factors for OSIRIS J12 ramp test
5.2.3 Geometry and Mesh

A 2-dimensional axisymmetric quadratic mesh was used for these simulations. The fuel pellets were modeled using discrete meshes. Both the fuel and cladding used medium-sized meshes, each fuel pellet had 11 radial elements and 3 axial elements. The cladding had 4 radial elements and the number of axial elements were adjusted to simulate approximately square elements for the cladding as shown in Figure 31. The simulation for the reference zirc-4 case had a total of 6,704 elements.

![Figure 31: Section of BISON mesh for the PCI reference zirc-4 case, scale is in meters.](image)

5.2.4 Material and Behavioral Models

5.2.4.1. Fuel

The UO$_2$ fuel is modeled as an elastic solid with nonlinear mechanical behavior. Young’s modulus is set to 200 GPa, Poisson’s ratio of 0.345 and a coefficient of thermal expansion is set to $10^{-6}$. The following BISON material models were used as well for the fuel [19]:

- ThermalFuel: NFIR correlation; burnup and temperature dependent thermal properties.
- RelocationUO$_2$: relocation strains, relocation activation threshold power set to 5 kW/m.
- Sifgrs: Coupled fission gas release and swelling model.
• VswellingUO_2: Calculating swelling in fuel due to both solid and gaseous fission products, based on empirical relations from MATPRO.

5.2.4.2. Cladding

The following BISON material models were used for the Zirc-4 cladding [19]:

• Constant thermal conductivity of 16 W/m-K is used.
• MechZry: Elastic modulus and thermal expansion are based on MATPRO correlations. Thermal and irradiation creep are modeled using the Limback model. Irradiation growth is based on Franklin’s correlations [56].
• CombinedCreepPlasticity: models the deformation under both creep and instantaneous plasticity.
• ZryPlasticity: Plasticity model for Zircaloy based on PNNL stress/strain correlations for Zircaloy [57].

5.3 Results

5.3.1 Zr-based fuel systems:
The results of the simulations are shown in figures 32-36. The power ramp simulations show similar trends to the steady-state ones earlier; similar plenum pressure, fission gas release, centerline fuel temperatures for the two Zr4-based claddings in comparison to the reference case. Pellet-clad contact is again reduced for the two coated claddings as seen in Figure 33, due to lower inward creep, resulting in lower contact pressures. The base Zr4 layer stress is almost reduced to half in the coated claddings in comparison to the reference case as shown in Figure 35. This is mainly due to the lower pellet-clad contact pressure. As for the coatings, the stresses resulting from the power ramp are not high enough to cause any significant increase in plastic strains in comparison pre-power ramp steady state levels as seen in Figure 36. This keeps the calculated effective plastic strains to ~1%, ~0.3% and 0.1% for the chromium, molybdenum and FeCrAl layer respectively. Therefore, it is expected that power ramps that might occur in the fuels having burnups up to ~30 MWd/kgU would have no significant impact on the coated Zr4-based cladding performance. In chapter 6, we look at LOCA simulations to test the claddings under more extreme transients.
Figure 32: Plenum pressure and FGR of Zr4-based fuels under power ramp

Figure 33: Average radial displacements and contact pressure of Zr4-based fuels under power ramp
Figure 34: Centerline fuel temperature of Zr4-based fuels under a power ramp

Figure 35: Stresses in the base Zr4 layer for the Zr4-based fuels under a power ramp
5.3.2 SiC-based fuel systems:

The results of this simulations are shown in Figures 37-43. The 1.3x thermal conductivity enhancement factor was used for the fuel as in section 4.3.2. Looking at Figure 37, we can see higher calculated plenum pressures and fission gas release for the SiC-based fuels in comparison to the reference Zr4 case. This is expected due to the almost ~400 degrees difference in centerline fuel temperatures as seen in Figure 39. However, in this simulation pellet-clad contact did not occur for the SiC-based claddings as seen in Figure 38; this is expected as SiC-based claddings do not creep inwards like the Zr4 reference, but rather displace outwards due to the increasing plenum pressure. However, even without contact, the resulting stresses in the SiC layers are still high for the SiC-3layers cladding as seen Figure 40. This gives rise to the possible failure of the inner monolith (P(f)=~0.2) as seen in Figure 41, agreeing with earlier results in section 4.3.2. On the other hand, the SiC-Cr cladding still looks promising with a negligible failure probability and no increase in the Cr coating plastic strain due to the power ramp. The plastic strain hovers at around 1% at this point. Therefore, the power ramp simulations further confirm the earlier results from steady state simulations, that the SiC-3layers fuel is questionable and SiC-Cr is promising.
Figure 37: Plenum pressure and FGR of SiC-based fuels under power ramp

Figure 38: Average radial displacements and contact pressure for SiC based fuels under power ramp
Figure 39: Centerline fuel temperature of SiC-based fuels under power ramp

Figure 40: Stresses of different layer in SiC-based fuels under power ramp
Figure 41: Failure probabilities of different layer in SiC-based fuels under power ramp

Figure 42: Von Mises Stress and effective plastic strain of the Cr coating for SiC/SiC-Cr under power ramp
Figure 43: Average swelling in different SiC layers under power ramp
6 Transient Simulations: LOCA

6.1 Overview

To conclude the testing of the fuel concepts for steady-state operation and major design based accidents (DBA), LOCA fuel analysis simulations were carried out for the proposed ATF fuel concepts. To mirror experimental conditions, we chose the MT-4 test conducted by the National Research Universal (NRU) reactor at Chalk river National Laboratory in Canada by Pacific Northwest Laboratory [62], [63]. The tests were conducted under the LOCA simulation program sponsored by the US Nuclear Regulatory Commission (NRC). The experiments used full-length fuel rods, with test conditions designed to simulate adiabatic heat-up, re-flood and quench phases of a large-break LOCA.

6.2 Test Description

The rod used is a 2D axisymmetric fuel rodlet with smeared fuel column. Details of the fuel rod geometry and specifications are summarized in Table 20. The coating are kept at the same thicknesses and are deducted from the base Zr cladding thickness.

Table 20: LOCA case Test rod specifications

<table>
<thead>
<tr>
<th>Fuel Rod</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Overall length</td>
<td>mm</td>
</tr>
<tr>
<td>Fuel stack height</td>
<td>mm</td>
</tr>
<tr>
<td>Nominal Plenum height</td>
<td>mm</td>
</tr>
<tr>
<td>Number of pellets per rod</td>
<td></td>
</tr>
<tr>
<td>Fill gas composition</td>
<td></td>
</tr>
<tr>
<td>Fill gas pressure</td>
<td>MPa</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Fuel</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Material</td>
<td>UO₂</td>
</tr>
<tr>
<td>Enrichment</td>
<td>%</td>
</tr>
<tr>
<td>Density</td>
<td>%</td>
</tr>
<tr>
<td>Outer diameter</td>
<td>mm</td>
</tr>
<tr>
<td>Pellet geometry</td>
<td></td>
</tr>
<tr>
<td>Grain diameter</td>
<td>μm</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cladding</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Outer diameter</td>
<td>mm</td>
</tr>
<tr>
<td>Inner diameter</td>
<td>mm</td>
</tr>
<tr>
<td>Wall thickness</td>
<td>mm</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Fuel Rod</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Overall length</td>
<td>mm 3880</td>
</tr>
<tr>
<td>Fuel stack height</td>
<td>mm 3660</td>
</tr>
<tr>
<td>Nominal Plenum height</td>
<td>mm 200</td>
</tr>
<tr>
<td>Number of pellets per rod</td>
<td>1</td>
</tr>
<tr>
<td>Fill gas composition</td>
<td>He</td>
</tr>
<tr>
<td>Fill gas pressure</td>
<td>MPa 4.62</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Fuel</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Material</td>
<td>UO₂</td>
</tr>
<tr>
<td>Enrichment</td>
<td>% 2.93</td>
</tr>
<tr>
<td>Density</td>
<td>% 95</td>
</tr>
<tr>
<td>Outer diameter</td>
<td>mm 8.26</td>
</tr>
<tr>
<td>Pellet geometry</td>
<td>Smeared</td>
</tr>
<tr>
<td>Grain diameter</td>
<td>μm 7.8</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cladding</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Outer diameter</td>
<td>mm 9.63</td>
</tr>
<tr>
<td>Inner diameter</td>
<td>mm 8.41</td>
</tr>
<tr>
<td>Wall thickness</td>
<td>mm 0.61</td>
</tr>
</tbody>
</table>
6.2.1 Operating Conditions and Irradiation History

The test rods were irradiated in flowing steam prior to the transient, then kept in stagnant steam for the transient duration; at the end, re-flooding conditions are introduced to conclude the test. The re-flooding rate is averaged to 5 in/s (~0.127 m/s) in Bison input. Test conditions are summarized in Table 21. The axial power profile used is shown in Figure 44 as well as the pre-transient axial temperature profile in Figure 45. The claddings in general failed during the adiabatic heat-up phase, prior to re-flooding. As we are interested in the failure behavior of the ATF concepts, we will focus our analysis on the time required for failure in comparison to the reference Zircaloy case.

Table 21: Operating conditions for the MT-4 LOCA test

<table>
<thead>
<tr>
<th>Operating condition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power level</td>
<td>kW/m 1.2</td>
</tr>
<tr>
<td>Pre-transient cladding temperature</td>
<td>K 640</td>
</tr>
<tr>
<td>Pre-transient internal gas pressure</td>
<td>MPa 9.3</td>
</tr>
<tr>
<td>Steam pressure</td>
<td>MPa 0.28</td>
</tr>
<tr>
<td>Delay time before reflood</td>
<td>s 57</td>
</tr>
<tr>
<td>Reflood rate</td>
<td>in/s 8 in/s for 6s</td>
</tr>
<tr>
<td></td>
<td>4 in/s for 6s</td>
</tr>
<tr>
<td></td>
<td>1 in/s for 3s</td>
</tr>
<tr>
<td>Reflood temperature</td>
<td>K 311</td>
</tr>
</tbody>
</table>

Figure 44: Axial Power profile for the MT-4 LOCA test
6.2.2 Geometry and Mesh

A 2-D axisymmetric quadratic mesh is used for the simulations. The fuel pellets were modeled as a single smeared fuel column. The fuel and cladding had 12 and 4 radial elements respectively. A sectional view of the mesh is shown in Figure 46. The simulation for the reference zirc-4 case had a total of 1,900 elements.

Figure 45: Pre-transient axial temperature profile for MT-4 LOCA case

\[ f(x) = -24.096x^2 + 152.47x + 437.81 \]

Figure 46: Section of BISON mesh for the LOCA MT-4 simulation (x-axis is scaled 5:1)
6.2.3 Material and Behavioral Models

6.2.3.1. Fuel
The UO$_2$ fuel is modeled as an elastic solid with nonlinear mechanical behavior. Young’s modulus is set to 200 GPa, Poisson’s ratio of 0.345 and a coefficient of thermal expansion is set to $10 \times 10^{-6}$. The following BISON material models were used as well for the fuel [19):

- ThermalFuel: NFIR correlation; burnup and temperature dependent thermal properties.
- Sifgrs: Coupled fission gas release and swelling model, with the burst release effect during transients enabled.
- VswellingUO$_2$: Calculating swelling in fuel due to both solid and gaseous fission products, based on empirical relations from MATPRO.

6.2.3.2. Cladding
The following BISON material models were used for the Zirc-4 cladding [19):

- Constant thermal conductivity of 16 W/m-K is used.
- MechZry: Elastic modulus is set to 75 GPa and a fixed coefficient of thermal expansion of $5 \times 10^{-6}$. Thermal and irradiation creep are turned off. LOCA large deformation creep is modeled and is activated above 900K [19].
- ZrPhase: Models phase transformation of Zr alloy from hexagonal (α-phase) to cubic (β-phase) crystal structure under high-temperature conditions [64]–[66].
- FailureCladding: Failure due to burst of Zircaloy-4 during LOCA accidents [67].

6.3 Results

6.3.1 Zr-based fuels
The results of the simulations are shown in Figures 47-51. The time to rupture, maximum rupture hoop strain, average cladding temperature and the rod pressure at rupture are summarized for the three Zr-based fuels in Table 22. Both coated claddings performed better than the reference Zr-cladding, which failed prior to re-flooding. The Zr-Cr and Zr-Mo/FeCral claddings failed 1.36s and 2.67s after re-flooding respectively. However, such behavior depends on maintaining the structural stability of the coating through such a large deformation. For these simulations, both combined creep and plasticity were included for the coatings. Figure 47 shows the evolution of effective plastic strain for the coating layers.
Table 22: Simulation results for the MT-4 LOCA test

<table>
<thead>
<tr>
<th></th>
<th>Zr</th>
<th>Zr-Cr</th>
<th>Zr-Mo/FeCrAl</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time to Rod Rupture s</td>
<td>53.7946</td>
<td>56.329</td>
<td>59.5867</td>
</tr>
<tr>
<td>Maximum Hoop Strain %</td>
<td>14.22</td>
<td>12.58</td>
<td>12.09</td>
</tr>
<tr>
<td>Rod Pressure at Rupture MPa</td>
<td>7.21</td>
<td>7.54</td>
<td>7.61</td>
</tr>
<tr>
<td>Peak Cladding Temperature K</td>
<td>1073.06</td>
<td>1090.56</td>
<td>1103.14</td>
</tr>
</tbody>
</table>

The claddings in all three cases showed extensive ballooning at the mid-section as shown in Figure 48. The burst location is located at the site with maximum displacement in each case. To finalize, the coated claddings showed better performance for the LOCA conditions. However, experimental verification is required for these conditions as it is not expected that the coatings will survive such extensive plastic deformation. The Zr4-Mo/FeCrAl potential is questionable at this point due to the expected high plastic strains in the molybdenum layers. Failure is calculated to occur for this layer much earlier than the simulation end-point as molybdenum has very low ductility. The process of failure compared to the base Zr4 layer will be thus more complicated to predict since Fe/Zr forms a binary low-melt eutectic at a temperature of 940 °C. Chromium on the other hand is highly ductile, and could possibly
survive such strains. For now, an assumption can be made that the coatings will provide better or at least comparable performance when compared to the reference Zr cladding.

Figure 48: Cladding dimensions at Burst showing extensive ballooning at the mid-section

Figure 49: Sectional view of ballooning at mid-section (x-axis is scaled 50:1).
6.3.1.1. Zr-based fuels: restart case

For modelling purposes, the previous section is basically treated as a fresh fuel except for few prescribed initial conditions. This assumes that the LOCA transient would occur at initiation of a fuel run, as there are no accumulation in plasticity in the coatings or plenum pressure build-up as seen in the steady state case for example. Therefore, to provide for a more realistic scenario, we ran the cladding with the same mesh under a straight power profile of 20 kW/m of linear heat generation to mimic a steady state run up to ~40 MWd/kgU. After that, the simulation case was restarted and subject it to the LOCA transient. The results of the LOCA-restart case is are shown in Table 23 and Figure 50.

Table 23: Simulation results for the MT-4 LOCA test after 40 MWd/kgU burnup

<table>
<thead>
<tr>
<th></th>
<th>Zr</th>
<th>Zr-Cr</th>
<th>Zr-Mo/FeCrAl</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time to Rod Rupture</td>
<td>s</td>
<td>47.5738</td>
<td>45.2281</td>
</tr>
<tr>
<td>Maximum Hoop Strain</td>
<td>%</td>
<td>14.97</td>
<td>13.14</td>
</tr>
<tr>
<td>Rod Pressure at Rupture</td>
<td>MPa</td>
<td>9.00</td>
<td>10.11</td>
</tr>
<tr>
<td>Peak Cladding Temperature</td>
<td>K</td>
<td>1027.72</td>
<td>1037.14</td>
</tr>
</tbody>
</table>

Figure 50: Cladding dimensions at burst for LOCA test after 40 MWd/kgU burnup
In the restart case, the time to failure is still close to the reference Zr-4 case. A slight difference is that the Zr4-Cr cladding shows shorter time to failure compared to the reference case unlike the LOCA simulation for a fresh fuel conducted earlier in section 6.3.1. This might be slightly improved by adjusting the thickness of the Cr coating, but in general it seems the difference is limited to +/- few seconds. The difference in time to failure here is mainly due to a higher starting plenum pressure and accumulated plastic strains for the coatings from the pre-LOCA steady state run. In conclusion, The Zr4-Mo/FeCrAl potential is still questionable due to the very high plastic strains in the molybdenum layer, while the Zr4-Cr cladding is expected to give a comparable performance to the Zr4 reference cladding under LOCA conditions.

### 6.3.2 SiC-based fuels

The results for the SiC-based cladding cases are presented in figures 52-62. For the LOCA case, the enhanced fuel thermal conductivity (1.3x) is used to be consistent with the steady state and power ramp simulations. The Zr4 reference case results is listed in Table 24. As SiC failure is statistical in nature, we plot the expected maximum principal stresses and the expected failure probability based on the respective Weibull material characteristic and
modulus in Figure 52. Agreeing with results from steady-state and power ramp simulations, the SiC-3layers cladding show the highest stresses and failure probabilities, especially at the inner and outer monolith layer, but would still be able to survive a LOCA. The SiC-Cr shows a very low, almost zero, failure probability. The resulting hoop strains shown in Figure 53 puts the SiC/SiC layer SiC/SiC-Cr below the PLS limit (~0.056%). The plastic strain in the Cr coating is kept to 1.3% which matches earlier strains from the steady-state operation. Therefore, the SiC-Cr fuel still looks very promising. In general, the SiC-based fuels are shown to survive LOCA here, in both the heating and re-flooding phase unlike the Zr4-based claddings in section 6.3.1, where it generally failed either just prior to or at the initiation or re-flooding. Therefore, SiC-based fuels might prove more advantageous in more extreme conditions like LOCA. However, the simulations in this section again assume a fresh fuel and so, we repeat the simulations but after running the fuels under steady state simulations up to a burnup of ~40 MWd/kgU in the following section.

Table 24: Simulation results for the MT-4 LOCA test with fuel enhanced thermal conductivity

<table>
<thead>
<tr>
<th></th>
<th>Zr4*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time to Rod Rupture</td>
<td>s</td>
</tr>
<tr>
<td>Maximum Hoop Strain</td>
<td>%</td>
</tr>
<tr>
<td>Rod Pressure at Rupture</td>
<td>MPa</td>
</tr>
<tr>
<td>Peak Cladding Temperature</td>
<td>K</td>
</tr>
</tbody>
</table>

Figure 52: Maximum principal stresses and Failure probability of SiC layers for LOCA
Figure 53: Hoop strains of SiC layers for LOCA-Restart

Figure 54: Von Mises Stress and effective plastic strain of the Cr coating layer in SiC/SiC-Cr
6.3.2.1. SiC-based fuels: restart case

As done earlier in section 6.3.1.1, the SiC-based fuels were run under a straight power profile of 20 kW/m of linear heat generation to mimic a steady state history up to ~40 MWd/kgU, after which the LOCA transient is introduced. This allowed a study of the fuels with higher initial plenum pressures and accumulated swelling and plasticity in the SiC/SiC and Cr coating respectively. The Zr4-reference case is repeated with enhanced fuel thermal conductivity (1.3x) and the results are listed in Table 25. As shown in Figure 55, the resulting stresses for the SiC-3layers are high enough to cause likely failure in the inner monolith (P(f)=~0.9). The SiC/SiC layer in SiC/SiC-Cr failure probability is still negligible. The resulting hoop strain for SiC/SiC-Cr, shown in Figure 56, exceeds the PLS limit in this case (0.056%), but is still much lower than the strain at ultimate tensile strength (0.494%) [42]. While the failure probability of SiC/SiC-Cr is very low, the results warrant further experimental investigation to test its performance under these conditions. As for the Cr coating, the plastic strain reaches ~1.7% as shown in Figure 57, which is in line with steady state operation for both SiC/SiC-Cr and Zr4-Cr cladings. In general, the SiC/SiC-Cr cladding still proves to be promising, unlike the SiC-3layers cladding that has shown a high failure probability across most simulations.

Table 25: Simulation results for the LOCA-Restart test with fuel enhanced thermal conductivity

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Time to Rod Rupture</td>
<td>s</td>
<td>44.0869</td>
</tr>
<tr>
<td>Maximum Hoop Strain</td>
<td>%</td>
<td>13.70</td>
</tr>
<tr>
<td>Rod Pressure at Rupture</td>
<td>MPa</td>
<td>8.95</td>
</tr>
<tr>
<td>Peak Cladding Temperature</td>
<td>K</td>
<td>1033.02</td>
</tr>
</tbody>
</table>
Figure 55: Maximum principal stresses and Failure probability for SiC layers for LOCA-restart

Figure 56: Hoop strain for SiC layers for LOCA-restart
6.3.2.2. SiC-based fuels: Swelling annealing effect

SiC has been reported to anneal out radiation induced defects if heated to temperatures above its irradiation temperature, recovering induced swelling [68], [69] and pre-irradiation material properties such as thermal conductivity [70]. However, to date this annealing effect has not been quantified i.e. how long does it take and at what temperatures. The phenomena itself is observed with Price suggesting that “For annealing times of ~1h, recovery starts at the irradiation temperature and continues almost linearly with increasing temperature until it is complete at ~1300°C (1573 K)” [68]. In this this section, we aim to look at this annealing effect by designing a simple thought experiment. As the LOCA-restart cases start the LOCA after the material has been irradiated to a burnup of ~40 MWd/kgU, the SiC claddings starts with a swelling value of ~1.5% as seen in Figure 60. In the simulation, it was assumed that full annealing is realized if SiC is exposed to ~1200K for 60s. Based on this, an Arrhenius relationship for annealing is assumed. This implementation leads to the swelling annealing profile shown in Figure 60; a slight offset difference in swelling exists at time zero but doesn’t affect initial stresses as shown in Figure 58. Annealing causes the

![Figure 57: Von Mises Stress and effective plastic strain for the Cr coating layer in SiC-Cr for the LOCA-restart case.](image-url)
principal stresses to rise to the point of failure as shown in Figure 58. The stresses are mainly due to the imposed strain gradient in the material as each part anneal differently depending on its temperature, ranging from full annealing to none. The energy release predicted from the annealing process would raise the cladding temperature as seen in Figure 61. The annealed case would also have higher hoop strains (Figure 59) and plastic strain of the Cr coating (Figure 62). In conclusion, this simple analysis of possible annealing effect showed the importance of studying this phenomena as it can prove detrimental to the performance of SiC claddings at extreme conditions such as LOCA. The phenomena needs proper quantification through experimental investigation to enable proper modelling and design of SiC claddings.

Figure 58: Comparison of stresses and failure probability with the inclusion of swelling annealing for SiC-Cr fuel
Figure 59: Comparison of hoop strains with swelling annealing for SiC-Cr fuel

Figure 60: Average swelling for annealed and normal SiC-Cr case for LOCA-Restart
Figure 61: Average cladding temperature for annealed and normal SiC-Cr fuel for LOCA-restart

Figure 62: Comparison of plastic strains of the Cr coating for annealed and normal SiC-Cr fuel for LOCA-restart
7 Conclusion & Future Outlook

7.1 Conclusions

To conclude, this thesis investigated four potential ATFs, two Zr4-based fuels (Zr4-Mo/FeCrAl and Zr4-Cr) and two SiC based fuels (SiC-3layers and SiC/SiC-Cr). The proposed fuel systems were tested under PWR steady-state operation conditions, power ramps and finally LOCA transients. The following is a summary of the findings for each proposed fuel system:

- **Zr4-Mo/FeCrAl**: The performance of this fuel concept is questionable and warrants further investigation. Molybdenum fails at less than ~1% elongation, which is at a comparable scale to the 0.3% plasticity predicted in steady state simulations. The concept needs more work to make the much more ductile FeCrAl layer carry more of the structural load and possible plastic deformations. A sensitivity study of the two layer thicknesses might be of interest for future exploration of this concept. In addition, the diffusion of Fe across Mo needs further attention, especially at accident conditions.

- **Zr4-Cr**: This cladding showed promising performance under steady-state, and power ramp cases. However, the chromium coating plastic strain in the LOCA case is high, reaching ~12%. While chromium is highly ductile, elongating up to 40% before fracture [25], this high plastic strain can be detrimental to its performance and requires more experimental investigation of this condition or modelling of damage and possible fracture, which is not a capability implemented in BISON yet. In general, the Zr4-Cr fuel concept seems to be the more promising choice out of the two Zr4-coated fuels studied.

- **SiC-3layers**: This fuel concept can be easily excluded based on its performance in all three study cases. The cladding showed a high probability of failure for in all cases reaching almost ~1 for some layers. The failure is mainly due to the resulting high stresses at the inner monolith. These results agrees with similar concept studied earlier by Avincola et al. [53] and Stone et al. [42].

- **SiC/SiC-Cr**: The composite SiC coated with fuel showed very promising results in all three study cases, with failure probability reaching a maximum of 0.1 for the LOCA,
while remaining negligible in steady-state and power ramps. The plastic deformation of the chromium coating in steady state and power ramps was the same level as the Zr4-Cr fuel, reaching up to ~2.5% plastic strains. However, the SiC/SiC-Cr shows a clear advantage under LOCA conditions, since no burst is predicted. This kept the Cr layer plastic strain below 2% in comparison to the 12% reached in the Zr4-Cr fuel. This could be explained by the higher stiffness of SiC/SiC in comparison to the base Zr-4, thus causing lower strains in the Cr coating under the same pressures and conditions. In general, the SiC/SiC-Cr proves to be a promising concept and should be further investigated.

In conclusion, the chromium coated fuel systems seem to be the most promising in both Zr4 and SiC based fuel systems. The two fuels should be further investigated experimentally as well as possible modelling of beyond design-basis accidents. The resulting plastic strains in the coatings in general necessitates the addition of possible damage and fracture mechanics models within the BISON/ MOOSE framework to enable the assessment of survival of these kind of concepts and should be included in future work.

7.2 Future work

The potential of chromium coated claddings, SiC/SiC-Cr and Zr4-Cr, as possible ATFs, established in this work opens the door for future work to be done for further verification, validation and optimization to be done before the fabrication of a possible lead test rod (LTR) that can eventually lead to deployment in commercial reactors. The following list will briefly discuss possible future work.

- **Failure prediction:** In this work, only the effective plastic strains are provided as a measure of possible damage in claddings/coatings and to help deduce if failure will occur or not. As plasticity is expected in some cases, such as transient conditions, future work should include the implementation of failure predicting criteria based on the principles of damage and fracture mechanics into the BISON source code. This implementation would prove useful when modeling more extreme conditions such as BDBA and will help better predict the structural stability of the proposed ATF claddings.
Coating thickness optimization: A sensitivity study is required to identify the optimal coating thickness for each ATF; this should include structural, neutronic and economic evaluation to reach an optimal thickness that fits the three criteria.

Pellet-cladding gap thickness: In the SiC/SiC-Cr case, pellet-clad interaction occurred. This interaction can be avoided by increasing the initial gap size to allow more volume for fuel swelling. However, increasing the gap will also increase the fuel temperature due to lower thermal conductivity of the gap. This should be optimized to maintain fuel temperatures within an acceptable range and at the same time avoid pellet-clad interaction in SiC claddings.

Irradiated chromium properties: To date, there is extremely limited publications on irradiation effects on pure chromium. An experimental effort should be carried out to document the effect of irradiation on thermo-mechanical properties of pure chromium, preferably under PWR similar conditions. These properties should integrated into future modelling efforts as well.

Oxidation of claddings: In this work, oxidation of the claddings is not included. The expected oxide layer thickness and thermos-mechanical properties should be included in future simulations.

Friction and wear: The friction between the cladding and spacer grids during normal operation can result in wear; this effect should be studied to understand its effect on the structural integrity of the coatings as these regions will serve as stress concentration regions.

Residual stresses: Depending on the coating technique, residual stresses can form in the base coated material. Such stresses should be calculated and studied as it can help design/choose the coating technique depending on its performance.

Coating delamination: In this work, it is always assumed that the coating is perfectly bonded in all regions. This assumption might not be true in reality and needs to be examined experimentally and corrected in future simulations.
8 References


[14] C. Toffolon-Masclet, C. Desgranges, C. Corvalan-Moya, and J. C. Brachet, “Simulation of the $\beta\rightarrow\alpha(O)$ Phase Transformation due to Oxygen Diffusion during High


