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IMPLEMENTATION AND EVALUATION OF FUEL CREEP USING ADVANCED LIGHT-WATER REACTOR MATERIALS IN FRAPCON 3.5

by

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Abstract

As current reactors approach the end of their operable lifetime, new reactors are needed if nuclear power is to continue being generated in the United States. Some utilities have already began construction on newer, more advanced LWR reactors, which use the same fuel as current reactors and have a similar but updated design. Others are researching next generation (GEN-IV) reactors which have new designs that utilize alternative fuel, coolants and other reactor materials. Many of these alternative fuels are capable of achieving higher burnups and are designed to be more accident tolerant than the currently used UO₂ fuel. However, before these new materials can be used, extensive research must be done in order to obtain a detailed understanding of how the new fuels and other materials will interact.

New fuels, such as uranium nitride (UN) and uranium carbide (UC) have several advantages over UO₂, such as increased burnup capabilities and higher thermal conductivities. However, there are issues with each that prevent UC and UN from being used as direct replacements for UO₂. Both UC and UN swell at a significantly higher rate than UO₂ and neither fuel reacts favorably when exposed to water. Due to this, UC and UN are being considered more for GEN-IV reactors that use alternative coolant rather than for current LWRs. In an effort to increase accident tolerance, silicon carbide (SiC) is being considered for use as an alternative cladding. The high strength, high melting point and low oxidation of SiC make it an attractive cladding choice, especially in an accident

scenario. However, as a ceramic, SiC is not ductile and will not creep outwards upon pelletclad mechanical interaction (PCMI) which can cause a large build up in interfacial pressure.

In order to understand the interaction between the high swelling fuels and unyielding SiC cladding, data on the properties and behaviors of these materials must be gathered and incorporated into FRAPCON. FRAPCON is a fuel performance code developed by PNNL and used by the Nuclear Regulatory Commission (NRC) as a licensing code for US reactors. FRAPCON will give insight into how these new fuel-cladding combinations will affect cladding hoop stress and help determine if the new materials are feasible for use in a reactor.

To accurately simulate the interaction between the new materials, a soft pellet model that allows for stresses on the pellet to affect pellet deformation will have to be implemented. Currently, FRAPCON uses a rigid pellet model that does not allow for feedback of the cladding onto the pellet. Since SiC does not creep at the temperatures being considered and is not ductile, any PCMI create a much higher interfacial pressure than is possible with Zircaloy. Because of this, it is necessary to implement a model that allows for pellet creep to alleviate some of these cladding stresses. These results will then be compared to FEMAXI-6, a Japanese fuel performance code that already calculates pellet stress and allows for cladding feedback onto the pellet. This research is intended to be a continuation and verification of previous work done by USC on the analysis of accident tolerant fuels with alternative claddings and is intended to prove that a soft pellet model is necessary to accurately model any fuel with SiC cladding.

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LIST OF ABBREVIATIONS

BWR	Boiling Water Reactor
LWR	Light Water Reactor
PWR	Pressurized Water Reactor
SiC	Silicon Carbide
UC	Uranium Carbide
UO ₂	Uranium Dioxide
UN	

CHAPTER 1

INTRODUCTION

Nuclear utilities have been looking towards fuels and materials that are considered accident tolerant for use in new LWR designs as well as in the new GEN-IV reactor designs. Since the Fukushima accident, efforts to better understand these new fuels and claddings have greatly increased. The fuels and materials would be able to prevent and survive an accident scenario much better that the current UO₂ pellet with Zircaloy cladding combination. These fuels tend to have higher thermal conductivities as well as higher uranium densities. This allows for the reactor to achieve higher burnups while maintaining low temperatures. New claddings that have reduced oxidation, lower hydrogen production and higher melting points are also being studied.

Uranium carbide (UC) and uranium nitride (UN) are two of the above mentioned fuels that are being considered for use in current light water reactors (LWRs) as well as for GEN-IV designs such as sodium or gas cooled reactors. Each of these fuels has advantages over UO₂ but also several major disadvantages which would cause them to not be easily adaptable to current LWRs without major design changes. For this reason, UN and UC are not major considerations for use in current reactors, but would instead be used primarily in GEN-IV reactors. Gen-IV reactors are new reactor designs that aim to replace current reactors as many of the reactors now in use are nearing the end of life. These reactors seek to achieve higher fuel burnups while being much safer in the event of an accident due to a higher thermal conductivity resulting in lower temperatures and less stored energy. Gen-IV reactors are radically different than currently used reactors, with some utilizing the fast neutron spectrum instead of the thermal spectrum and most using different coolants and operating at higher temperatures.

The main issues with the accident tolerant fuels being considered is that they all have a higher swelling rate than UO_2 and some aren't compatible with current reactor designs. For example, UN has a higher uranium density and higher thermal conductivity than UO_2 but reacts poorly with water, making it unsuitable as an accident tolerant fuel in current generation reactors. UC also has a higher uranium density and thermal conductivity, but has a much high swelling rate and poor compatibility with water which limits its application in current reactors.

The high swelling rates of these new fuels coupled with the rigidity of the SiC cladding can cause massive interfacial pressure when contact is made; something that is not an issue when considering UO₂ and Zircaloy. In order to accurately represent what is happening after the fuel pellet comes in contact with the cladding, a soft pellet model had to be implemented into the code. This model allows for feedback onto the pellet from the cladding which can cause the pellet to deform and lessen the stress on the cladding. Unlike the current Zircaloy cladding, SiC is a ceramic and therefore extremely brittle. Instead of deforming outwards under stress like the Zircaloy, the SiC cladding will crack once pressures get too high. If there is no model allowing for pellet deformation, the stress will build up too quickly due to the high swelling rate of UC. However, if the pellet is allowed to creep inward due to the high interfacial pressure between the pellet and cladding, then the hoop stress on the cladding may be reduced enough to prevent cladding failure.

Therefore, in order to accurately capture what is occurring, creep of the pellet must be allowed to achieve understanding of how the fuel and cladding interact.

Since FRAPCON does not natively calculate the stress on the pellet or pellet creep, it is not enough to just include a creep equation in the code. The method of implementation must be validated in order to prove that the soft pellet model is affecting the results of the code in the correct manner. In order to do this, a soft pellet model was created for UO₂ in FRAPCON and the results were compared to an identical case run in FEMAXI. In order to prove that FRAPCON is predicting pellet creep correctly, the results from both cases should be nearly identical. With the method of implementation for UO₂ validated, the soft pellet model can then be used for other fuel such as UC and UN. Implementing a soft pellet model for each of these fuels gives a better understanding of how high swelling fuels will interact with advanced claddings. This knowledge can then be used to determine what conditions are necessary to make SiC cladding a feasible choice for high swelling advanced fuels.

CHAPTER 2

ADVANCED LWR MATERIALS

In the nuclear power industry, there has been a growing desire for safer, higher burnup fuels as well as interest in new reactor designs that could incorporate these advanced fuels. Two of the most promising fuels in contention for use in advanced LWRs and GEN-IV reactors are uranium nitride and uranium carbide (S.J. Zinkle 2013). While each fuel is unique, they share certain characteristics, such as high uranium density and high thermal conductivity, that make them suitable candidates for some of the high temperature, high burnup GEN-IV reactor designs that are being proposed.

	UO2	UN	UC
Melting point (°C)	2865	2762±40	2350
Density/U Density (g/cc)	10.96 / 9.6	14.3 / 13.5	13.63 / 12.97
Thermal Conductivity @500 °C (W/m*K)	4.0	18	20.1
Irradiation Induced Swelling (Relative)	Low	Medium	Medium
Stability (Water)	Medium	Low	Low
Ease of Manufacture	Easy	Difficult	Medium

 Table 2.1: Comparison of Fuel Properties

2.1 URANIUM NITRIDE PROPERTIES

On the surface, UN may seem to be an excellent choice for use in GEN-IV reactors and also a possibility in current LWR designs. It has a very good thermal conductivity and uranium density and does not swell as rapidly as some of the other advanced fuels. However, due to unfavorable reactions when it comes in contact with water, it is unsuited for use in any water cooled reactor without serious safety considerations (Arai 2012) (G.A. Rama Roa 1991). In addition, there is little experience in working with it and it can be quite difficult to manufacture correctly, especially when compared with the extremely fine-tuned UO₂ manufacturing process.

2.1.1 Thermal Properties

As previously mentioned, one of the most attractive features of UN is its high thermal conductivity. At 500°C, it has a thermal conductivity of 18.0 W/m-K, which is much higher than the 4.0 W/m-K of UO₂ at the same temperature (Frost 1994) (Khromov 1980). In addition to a higher base value, the thermal conductivity of UN also increases with temperature.



Figure 2.1: Thermal Conductivity Comparison

The equation implemented in FRAPCON for thermal expansion is a function of temperature and is affected by the porosity of the fuel, especially at higher temperatures. The thermal expansion for UN is entirely dependent on temperature and is valid up to 2273 K, a far higher temperature than will be reached in a reactor environment (Matzke 1986).

Thermal Conductivity	
$k = 1.37 \times T^{.41} \left(\frac{1-p}{1+p}\right)$	k =Thermal Conductivity Coefficient (W/m-K) T =Temperature (K) p =Fuel Porosity (as a decimal)
Thermal Expansion Coefficient	
$\alpha = 7.096 \times 10^{-6} + 1.409 \times 10^{-9}T$	α = Thermal Expansion Coefficient T = Temperature (K)

Due to the high thermal conductivity of the fuel, it is not predicted that UN will relocate upon reactor startup, at least at the power levels used in this study. Therefore, relocation for UN has been disabled.

2.1.2 Irradiation Properties

The swelling model implemented for UN was chosen based on results from several different studies which predicted a wide variety of different swelling rates. The model implemented in FRAPCON is burnup dependent for temperatures under 1200 °C (Bo Feng 2012). Past 1200 °C, the formula changes and becomes much more temperature dependent. However, due to the high thermal conductivity of UN, these temperatures will not be reached in typical reactor settings (Ross 1990).

Swelling

T < 1200 °C	
$\frac{\Delta V}{V} = 1\% \text{ per atomic \% Burnup}$ $T > 1200 \text{ °C}$	T_{av} = Fuel Average Temperature (K) Bu = atomic percent burnup ρ = percent of theoretical density
$\frac{\Delta V}{V} = 4.7 \times 10^{-11} T_{av}^{3.12} B u^{0.83} \rho^{0.5}$	
Creep $\varepsilon_{cr}^{irr} = 1.81 \times 10^{-26} (1 + 1250P^2) f\sigma$	ε_{cr}^{irr} = Creep due to irradiation (s ⁻¹) P = fraction of porosity in the pellet f = Fission rate (fissions/cm ³ s)

The creep equation that was implemented for UN is a function of stress, porosity and fission rate. It was implemented into FRAPCON in same way that the creep for UO_2 was implemented. While there is also a thermal creep term, the thermal creep is overwhelmed by irradiation creep as long as fuel temperatures are below 1200 K (J. T. S.L. Hayes 1990). As with UO_2 creep, the creep rate for UN was implemented so that it modifies the swelling rate of the fuel. However, the code separates and distinguishes between the two phenomena and outputs the results accordingly.

2.1.3 Viability of UN as a Fuel

The main advantage that UN has over UO₂ is the higher uranium density and higher thermal conductivity. With the higher uranium density, reactors would be able to operate longer without exceeding burnup limits set by the NRC, resulting in less reactor downtime. The high thermal conductivity that increases with temperature makes UN an excellent candidate for GEN-IV reactors which use alternative coolants, such as high temperature gas cooled reactors. Despite these advantages, there are limitations in working with UN. It is a relatively new fuel and there is very little experience with it when compared to UO_2 , especially in terms of mass fabrication (Josef Bugl 1964). However, once more experienced is gained with UN, manufacturing costs will inevitably be driven down as the process is fine-tuned and longer operating cycles could offset the increased cost of enrichment. While UN is not suitable for use in LWRs due to the reactivity with water, it is an excellent candidate for use in GEN-IV reactors.

2.2 URANIUM CARBIDE OVERVIEW

For several reasons, uranium carbide is being considered as a replacement fuel for UO_2 as reactor owners seek to operate their reactors for longer cycles and get more power out of the fuels. However, due to the lack of experience with UC, this concept is at best a long way from becoming a realistic prospect and at worst an unfeasible possibility. The benefits of using UC lie in its high uranium density and high thermal conductivity. Due to both of these attributes, the fuel will be able to produce more power while remaining at a lower temperature. Keeping the fuel centerline temperature lower is important in the case of an accident scenario. In a loss of coolant accident (LOCA), having less thermal energy in the fuel at the time of accident helps to keep the fuel from melting down. However, despite these advantages, the fuel does have an extremely high swelling rate which is not desired in a reactor because of the large pressures it puts on the cladding. Also, since UO_2 has been used for many years and is well understood and easily manufactured, there would have to be substantial differences in using UC fuel for it to be considered.

2.2.1 Thermal Properties

The primary thermal properties of interest for UC are thermal conductivity and thermal expansion. As previously mentioned, the thermal conductivity of UC is one of its most attractive features. At 500 °C, UC has a thermal conductivity of 20.1 W/m-K significantly higher than UO_2 and slightly higher than UN (A. K. Sengupta 2012). This value also increases with temperatures, similarly to UN. The thermal expansion model is entirely dependent on temperature.

Thermal Conductivity $k = 21.7 - 3.04 \times 10^{-3}T + 3.61 \times 10^{-6}T^2 \left(\frac{1-p}{1+p}\right) \qquad k = \text{conductivity (W/m °C)}$ T = temperature (°C)

Thermal Expansion	
-------------------	--

	$\alpha = \text{Coefficient} (1/{^{\circ}\text{C}})$
$\alpha(T) = 1.007 \times 10^{-5} + 1.17 \times 10^{-9}T$	$T = temperature (^{\circ}C)$

Relocation for UC is not predicted to occur at most power levels. Due to the high thermal conductivity of UC, the thermal gradient across the fuel does not cause enough thermal stress for the fuel to crack when operating at normal power levels. A subroutine implemented in the code by a previous USC student Luke Hallman will calculate the stress caused by the thermal gradient and if a high enough stress occurs, the fuel will relocate (Jr. 2013). Using an identical case as for the other research cases, it took increasing the power levels to about 35 kW/m to cause the fuel to relocate. When the fuel relocates, the relocation amount is based on the gap between the pellet and cladding at beginning of life.

2.2.2 Irradiation Properties

The swelling model implemented in FRAPCON for UC was based on work done by W. Dienst. Studies were done at temperatures at or below ½ of the melting point of the fuel; about 1200° C for both restrained and unrestrained swelling. In order to best incorporate the fuel into FRAPCON in the way that gives the most accurate results, the unrestrained swelling model needs to be used. Changes in swelling due to restraints on the fuel can then be modeled as creep. The model for swelling in FRAPCON for UO_2 uses an unrestrained swelling model and keeping with this method will allow for the best comparisons and greater accuracy. The formula used for swelling is a function of burnup which is converted to %FIMA and then multiplied by 1.5% to obtain the solid swelling rate of UC.

Swelling $\frac{\Delta V}{V} = 1.5$ volume percent per 10 GWD/MTU

Based on studies done by Dienst, if the uranium carbide pellet has high enough porosity, then it will densify immediately at the beginning of life. However, this densification will only cause the pellet to reach about 90% TD. Since the cases being run for the purpose of this research use an as manufactured pellet porosity of 95% TD, densification is not predicted to occur. However, if the as manufactured %TD was lowered to 85%, then densification of the pellet would occur according to this formula:

Densification	
	P = Porosity Reduction
$\Delta P = \Delta P_{\text{rescal}} \left[1 - \exp\left(-\frac{B}{B}\right) \right]$	$P_{total} = -3.4 \text{ vol\%}$
$\Delta I = \Delta I_{total} I = CAP \left(B_{densif} \right)^{I}$	$\mathbf{B} = \mathbf{Burnup}$
	B = 0.6 at% U+Pu

The creep formula implemented for UC is a function of pressure and fission density and, like UO_2 modifies the swelling term instead of being a separate phenomenon. However, in order to implement this formula in FRAPCON, the fission density needed to be converted into burnup. This creep model was developed based on work done by Dienst. The process of implementing the creep formula will be discussed in detail later in this paper but, in short, it is implemented in such a way that it modifies the swelling rate of the fuel.

Creep	
	F = Fission rate (fissions/m3-s)
$\varepsilon_{cr}^{irr} (h^{-1}) = 3.0 \times 10^{-27} F \sigma$	σ = Interfacial pressure (MPa)

2.3 SILICON CARBIDE OVERVIEW

Silicon carbide is being considered for use as a more accident tolerant cladding. As a ceramic, it has several advantages over current Zircaloy claddings such as an extremely high melting point and a low neutron absorption cross-section. In addition, a lower oxidation results in a lower hydrogen production. However, there are drawbacks to be considered. Due to the brittle nature of ceramics, large stresses on the cladding will cause instant failure if the yield strength is reached. This heavily contrasts the behavior of Zircaloy, which deforms easily under stress.

SiC Properties	
Theoretical Density (g/cm ³)	3.21
Melting Temperature (K)	3000
Thermal Conductivity (W/m-K)	350
Thermal Conductivity (irradiated) (W/m-K)	3.6
Thermal Expansion Coefficient (10 ⁻⁶ /K)	2.2
Elastic Modulus (GPa)	384
Yield Strength (MPa)	261-551
Poisson's Ratio	0.21

The thermal conductivity of SiC before it is irradiated is very high. However, after only a short time in the reactor, radiation causes it to drastically decrease to about 3.6 W/m-K (Lance L. Snead 2007). As a ceramic, it boasts an extremely high melting point of about 3000 K. The elastic and shear modulus for SiC were added into FRAPCON and are functions of neutron fluence and temperature (Li 2013). Results from research suggest that the irradiation creep rate of SiC is extremely low below 1400 °C and would negligibly affect the results (M. Ben-Belgacem 2014). Therefore, when SiC was implemented in FRAPCON, creep was disabled. Research on the yield strength of SiC has produced a variety of results based on who manufactured the material. To be conservative, the lower value will be used for this research.

CHAPTER 3

IMPLEMENTATION OF SOFT PELLET MODEL IN FRAPCON

3.1 BACKGROUND

Uranium dioxide (UO_2) is the standard fuel for use in light water reactors. The nuclear industry has a good understanding of its mechanical, thermal and irradiation properties and behaviors as well as many years of experience manufacturing it for use in reactors. However, as industry begins to research new GEN-IV reactor designs, interest is shifting to different fuels as UO_2 is limited by its low thermal conductivity, especially at high temperatures.

3.1.1 Methodology

As previously discussed, in order to accurately model the interactions between high swelling fuels and SiC, the fuel pellet needs to be allowed to deform based on the high stress that it will be under. However, as this is new ground for FRAPCON, it makes sense to first implement a soft pellet model for UO₂, a fuel that is extremely well modeled and understood. Due to the wide usage of UO₂ as a fuel, there are other countries with other fuel performance codes that FRAPCON can be compared against. One of these codes is FEMAXI, a code developed by the Japanese to regulate their reactors. FEMAXI is similar to FRAPCON in that both are fuel performance codes that are centered on UO₂ modeling. However, one major difference is that FEMAXI allows for pellet deformation based on stresses on the fuel. This feature can be used to validate the approach used to implement the soft pellet model in FRAPCON for UO₂. With the method of implementation verified, the UO_2 soft pellet model can then be adapted for use with both UN and UC as well as any other future fuel types.

3.1.2 FRAPCON Overview

FRAPCON is a nuclear fuel performance code developed by PNNL and used by the NRC to license reactors in the United States. It is a steady state code intended to be used to calculate the performance of a LWR fuel rod from beginning to end of life. The official version of FRAPCON models the fuel as a rigid pellet that is unable to be deformed, even when under stress from the cladding and is only capable of modeling UO₂ pellets with a zirconium alloy cladding. Work done by USC has altered the code so that it is able to be used to model fuels such as UC, UN and U₃Si₂ as well as other new materials such as SiC as a cladding and helium as a coolant. Many of the models in FRAPCON have been altered slightly to fit test reactor data.

3.1.3 FEMAXI Overview

FEMAXI-6 is used by the Japanese Atomic Energy Agency (JAEA) to license their reactors. Many of the same phenomena that are represented in FRAPCON are also modeled in FEMAXI and the two codes should provide similar results when running the same case. One major difference is that FEMAXI provides a detailed mechanical analysis of stresses on the pellet which includes inward creep of the pellet, something that FRAPCON does not calculate. Also, while FRAPCON has chosen one model to use for each of the different fuel phenomena, FEMAXI has many different models implemented for most of the phenomena that occur within the reactor and the user is able to choose between these. 3.2 CROSS-CODE COMPARISON OF UO2 SURFACE DISPLACEMENT PHENOMENA

Since this comparison is being done to verify the implementation of creep how it affects the fuel, it is important to be able to directly compare the results from each code. Therefore, each code needs to be using the same design parameters in order to get the cases as similar as possible. In order to begin analyzing the differences of how all the phenomena are represented within the two codes, it is necessary to understand a fundamental difference between the two codes. While both codes are able to accurately represent what is happening within the reactor, they make use of known data differently to achieve this goal. As previously mentioned, FRAPCON has altered many of its models so that the predicted results more closely match test reactor data. FEMAXI, however, does not alter its models to fit data. Instead, each model is represented as it was in the study from which the model was taken. Results from identical cases run with each code which better illustrate the differences are plotted below. Case parameters are as follows:

- Linear average power: 200 W/cm
- Coolant pressure: 15.5 MPa
- Coolant inlet temperature: 580 K
- Coolant inlet mass flux: 3800 kg/m²-s
- Rod fill gas: helium
- Fill gas initial pressure: 2.0 Mpa
- Initial fuel density: 95%

3.21 Swelling

The model used in FRAPCON for swelling is a modified version of the MATPRO UO₂ swelling model. This model is entirely burnup dependent and predicts that swelling occurs at a constant rate until 80 GWD/MTU, at which point the swelling rate is increased (W.G. Luscher 2014). FRAPCON has modified the MATPRO model so that swelling does

not begin until 6 GWD/MTU and when it does begin it occurs at a slightly lower rate than is predicted by MATPRO.

Burnup	
0 – 6 GWD/MTU	Swelling = 0
6 – 80 GWD/MTU	<i>Swelling</i> = $A \times (2.315 \times 10^{-23} + 2.315 \times 10^{-24})$
> 80 GWD/MTU	Swelling = $A \times (3.211 \times 10^{-23} + 3.211 \times 10^{-24})$
	$A = density \times 2974 \times 10^{10} \times (burnup)$

The model chosen for swelling in FEMAXI is the unaltered MATPRO-09 formula. This model predicts a mostly burnup dependent swelling rate but the rate changes slightly at certain temperature intervals. However these changes do not appear until the fuel centerline temperature is about 1400 °C and this temperature is not often reached during regular reactor operation.

Temperature at Pellet Center (°C)	Swelling ratio (% per 10^{20} /cm ³)
$T \le 1,400$	0.28
$1,400 \le T \le 1,800$	0.28[1 + 0.00575(T - 1,400)]
$1,800 \le T \le 2,200$	0.28[3.3 - 0.004(T - 1,800)]
2,200 < T	0.476



Figure 3.1: FRAPCON/FEMAXI Swelling Comparison

As shown in Figure 1 above, FEMAXI predicts swelling to occur immediately at the beginning of life. Swelling continues to occur at a constant rate throughout the cycle. FRAPCON, however, delays the start of swelling until about 6 GWD/MTU as well as predicts swelling to occur at a slightly lower rate. At end of life, the differences in swelling models for this case has accounted for about 10 microns of radial displacement difference between the two codes.

3.22 Thermal Expansion

FRAPCON uses the MATRPO version of thermal expansion but has altered the coefficients slightly to account for new data from studies done by Martin (1988) and Momin (1991). This model is entirely temperature dependent for the first 40 GWD/MTU of burnup. However, after 40 GWD/MTU and if the temperature is above 1370 °C, the thermal expansion of the fuel increases. These conditions are not often met in normal reactor operation. FEMAXI also uses a MATPRO model it is a different version of

MATPRO than is used by FRAPCON. This model is entirely based on temperature. Despite the differences in MATPRO versions, the two codes predict almost the exact same values for thermal expansion with the only slightly differences that are attributed to temperature differences.



Figure 3.2: FRAPCON/FEMAXI Thermal Expansion Comparison

3.23 Densification

As a reactor starts up, the high temperatures of the reactor environment cause some of the voids within the pellet to disappear. This results in a rapid 1% decrease in fuel pellet volume. This phenomena was first discovered in 1972 when it was noticed some PWR rods had flattened or collapsed sections. Upon discovery, fuel manufacturers began programs to better understand how densification could be limited. Through the efforts of these manufactures, it was discovered that a resintering anneal at 1700 °C causes a density change that limits the amount of densification that can occur in the reactor (Meyer 1976).



Figure 3.3: FRAPCON/FEMAXI Densification

Due to these limits, densification is a fairly simple phenomena to model and therefore both codes predict it to affect the fuel in a very similar way. The model used in FRAPCON predicts slightly less than 1% densification. In FEMAXI, the densification can be specified so that the user inputted amount of densification occurs over the desired amount of time. In the cases used in this research, densification is set so that 1% volumetric change occurs within the first 5 GWD/MTU.

3.24 Relocation

One of the most noticeable difference when comparing FRAPCON and FEMAXI surface displacement results is the relocation value. Relocation is a displacement phenomenon that is unique to the reactor environment and because of this it can be difficult to tell exactly how relocation occurs. In general, relocation occurs due to the extreme thermal gradient caused by reactor startup. As the pellet rapidly heats up as the reactor starts, the thermal stress across the pellet causes it to crack radially. Once the pellet cracks,

the pieces may relocate outwards towards the cladding. As the cladding creeps inward and the fuel swells outward, there is some recovery of the relocation displacement as the fuel fragments are forced back together. The way this is predicted to affect fuel performance can vary and both FRAPCON and FEMAXI represent relocation and recovery in different ways.

In FRAPCON, relocation occurs over a period of 6 GWD/MTU, starting at the beginning of life of the reactor. At 6 GWD/MTU, the full relocation value is reached. FEMAXI does not use the same relocation model that FRAPCON currently employs but instead predicts that the fuel cracks and that the fragments relocate at the beginning of life. Both codes predict about the same amount of initial relocation.

At first, it may seem as though there is not much difference between the relocation models of both codes. This is because the real difference is in how this relocation is recovered. Relocation recovery occurs as the cladding creeps down enough to come in contact with the pellet and exert pressure on it. When discussing relocation and relocation recovery, there are three stages that must be understood.

No Contact Soft Contact Hard Contact



As shown in the above picture, when the fuel first relocates, there is no contact between the pellet and the cladding since cladding creep down has not yet began. During this phase, the fuel fragments move towards the cladding as the cladding creeps inward. Eventually, due to the creep of the cladding and other surface displacement phenomena causing the fuel pellet to expand, soft contact occurs. The soft contact phase must be looked at from a thermal and mechanical standpoint.

Thermally, the gap between the pellet and cladding is effectively closed. As far as heat transfer from the pellet to the cladding is concerned, there is not a gap between the pellet and the cladding. However, despite the contact between the pellet and the cladding, the fuel pellet is not yet solid enough to mechanically influence the cladding. This stage is what is referred to as soft contact and marks where relocation recovery begins. Although the pellet fragments have spread out to the point where they are in contact with the cladding, there is still a lot of space between the pellet pieces. As the cladding creeps down even more, it forces the pellet pieces together until the pellet is roughly solid again from a mechanical stand point. It is at this point that the relocation is said to have been recovered and it can now resist the inward creep of the cladding. This is referred to as hard contact. It is important to note that all of the relocation is not recovered. Since only enough must be recovered to cause the pellet fragments to be forced together, there are still gaps between the fragments, but not large enough gaps to affect the pellet stiffness.

In FRAPCON, relocation is represented through the use of a mechanical and thermal radius. The thermal radius is used to calculate the heat transfer and other thermal properties of the fuel at that time. The pellet's thermal radius is what is used to determine when soft contact occurs.

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Figure 3.5: Pellet Thermal and Mechanical Radius

At soft contact, the thermal radius begins to decrease at the same rate as the cladding's inward creep as shown in the graph above. This continues to occur over the next 6 GWD/MTU until hard contact. It is important to note that the thermal radius will never be equal to the cladding inner radius, even when they are in contact. Since neither the cladding nor the pellet are perfectly smooth, there will never be perfect heat conduction between the pellet and the cladding. This results in the gap between the pellet and cladding radius.

The mechanical radius is used to calculate when the pellet has recovered the allotted amount of the relocation value. When calculating the mechanical radius, the relocation value is multiplied by the percentage of relocation that can be recovered; in most cases, 50%. This altered relocation value, along with the other fuel displacement

phenomena, is used to calculate the mechanical radius. The mechanical radius is used to determine what the radius of the pellet and cladding are when relocation has been recovered and once the mechanical radius is equal to the cladding radius, the fuel is said to be in hard contact with the cladding and the pellet begins to push the cladding outwards as it swells (K.J. Geelhool 2014).

Instead of using a thermal and mechanical diameter, FEMAXI represents relocation and recovery by altering the Young's Modulus of the fuel once it relocates. As soon as the fuel relocates, which is at BOL, the Young's Modulus of the fuel is set to an extremely low value, making it unable to resist the inward creep of the cladding. As the fuel makes soft contact, the Young's Modulus begins to increase until it is solid enough to resist the cladding's inward creep. This is represented by the following formulas:

$$E_{i} = \begin{cases} E_{c} , & 0 \leq \varepsilon_{i} - \varepsilon_{i}^{0} \\ -\frac{\varepsilon_{i} - \varepsilon_{i}^{0}}{\varepsilon_{i}^{rel}} (E - E_{c}) + E_{c} , & -\varepsilon_{i}^{rel} < \varepsilon_{i} - \varepsilon_{i}^{0} < 0 \\ E , & \varepsilon_{i} - \varepsilon_{i}^{0} \leq -\varepsilon_{i}^{rel} \end{cases}$$
(3.2.34)

Here,

 ε_i : strain in *i* direction

 ε_i^0 : initial strain in *i* direction

 ε_i^{rel} : initial relocation strain in *i* direction (input data)

 E_c : effective Young's modulus of pellet with cracks in a tensile state.

Figure 3.6: FEMAXI Relocation Recovery

The phase of increasing Young's modulus is the relocation recovery. Once enough of the relocation has been recovered, the fuel is considered hard enough to push out against the cladding. It's worth noting that since the increase of Young's Modulus is a gradual affect, there is a smoother transition between soft and hard contact, unlike the abrupt change as it is on FRAPCON. In FEMAXI, soft contact occurs from when the fuel first contacts the cladding and persists until the fuel is hard enough to cause the cladding to push outwards. Once it is rigid enough to do this, it is considered hard contact. When recovering the relocation, cladding creep inwards is not the only factor when strain is calculated. The total strain of the pellet is taken into account. For example, if a rigid pellet model is used and the pellet is not allowed to creep, the pellet recovers more relocation than it normally would.



Figure 3.7: FEMAXI Young's Modulus Recovery

In FEMAXI, the amount that the pellet relocates is calculated by examining the difference between the cladding inner radius and the pellet outer radius at hot stand-by multiplied by a radial relocation parameter. This parameter is 0.5 by default but is able to be changed by the user. As previously mentioned, FEMAXI alters the Young's Modulus of the fuel to make it weak enough to be pressed inward by the cladding. As it is pressed inward, it regains its hardness. Until the allotted amount of relocation is recovered, the

pellet's Young's Modulus is a function of the inward strain of the pellet (Motoe Suzuki 2005). Once the inward strain of the pellet is equal to the amount of strain caused by relocation, the pellet's Young's Modulus is considered fully recovered. (eq. 3.2.34 in Femaxi Manual)



Figure 3.8: FRAPCON/FEMAXI Relocation Comparison

The graph above displays the differences in the two models quite clearly. FRAPCON predicts relocation to initially occur at a rapid rate and then taper off until it plateaus at about 32 microns of total radial displacement. The relocation stays constant until the pellet and cladding come into contact at about 13 GWD/MTU. Once contact is made, the allotted amount of relocation is recovered over about 6 GWD/MTU. At this point, the pellet is considered to be in hard contact with the cladding and immediately begins pushing out the cladding at the same rate as the fuel is swelling.
FEMAXI represents relocation recovery in a much different way which results in a large discrepancy in the two codes' predicted relocation values. As previously discussed, FEMAXI represents relocation recovery as more of the degradation and recovery of pellet strength instead of modeling a separate thermal and mechanical radius. As shown, relocation occurs instantly as soon as the reactor starts up and reaches a maximum value of about 35 microns of radial displacement. At about 16 GWD/MTU, the fuel comes into contact with the cladding. However, unlike FRAPCON, the fuel's strength isn't completely disregarded until the relocation is recovered. Instead, the Young's modulus of the fuel is reduced so that it is not strong enough to force the cladding outwards. FEMAXI predicts that the fuel takes about twice as long to fully recover the relocation and during that time the pellet isn't compressed nearly as much as the cladding creeps inwards. Instead, the pellet and cladding diameter are held roughly constant until, as it is interpreted by FEMAXI, the pellet begins to regain some of its strength.



Figure 3.9: FRAPCON/FEMAXI Total Surface Displacement Comparison

The difference of how each code interprets relocation recovery is most noticeable directly after relocation is recovered. In FEMAXI, since the pellet is just weakened, there is much less inward displacement as the pellet relocation recovers which results in a large discrepancy between the results at about 20 GWD/MTU.

3.2.5 Thermal Conductivity

For the thermal conductivity model, the origin of the data that each code uses comes from the same source. However, FRAPCON alters the thermal conductivity equation slightly while FEMAXI uses it in its original form. This results in FRAPCON using a slightly higher thermal conductivity model, with differences especially noticeable at lower temperatures and burnups.

Frapcon uses a modified version of the model developed by NFI (Ohira and Itagaki, 1997). They altered the model at first in a way that raised low burnup thermal conductivity at low temperatures and lowered thermal conductivity at very high temperatures. This involved changing the temperature dependent portion of the burnup function in the phonon term and changing the electronic term. The formula was later altered again to account for the porosity of the fuel.

FEMAXI has an option to use the original, unaltered Ohira and Itagaki model so that is what is used for these cases. The equation in FEMAXI does not take into account the electronic term of the equation. When plotted at various temperatures and burnups, alongside the FRAPCON thermal conductivity model, the FEMAXI model predicted a slightly lower thermal conductivity with larger discrepancies at low temperatures and low burnups.

3.25 Creep

Other than densification, creep is the only phenomena that actually causes the pellet to reduce in size. As the pellet swells outward and the cladding creeps inward, there is a lot of interfacial pressure buildup. In addition to the creep caused by the interfacial pressure between the pellet and the cladding, the pressure from the gap gas begins to affect the pellet from the beginning of life. These pressures on the pellet, along with the high temperatures of the reactor environment and the fission process that is occurring within the pellet cause pellet creep. Temperature, stress and fission density are all variables that affect the amount of pellet creep that occurs. It is important to note here that although creep always occurs, it is not represented as a separate phenomenon in FRAPCON and is accounted for empirically elsewhere in the code through altering other displacement phenomena as it is not believed to be a significant source of displacement when coupled with Zircaloy. For the purpose of comparison, however, a creep module has been added that calculates pellet creep based on fission density and interfacial pressure despite it possibly being accounted for elsewhere in the code.

In order for the pellet to be able to creep at all, there first must be space for it to creep into. Previously it was discussed that 50% of the relocation value must be recovered before the pellet can begin to affect the cladding. This remaining 50% relocation value is still available as space that can be crept into and is the first space that will be occupied. Other than the relocation space, the pellet can also theoretically creep into any remaining porosity. Usually, UO_2 is manufactured at 95% of its theoretical density. After densification, which is a 1% volumetric reduction, is accounted for there is still 4% remaining porosity. Once the remaining relocation is filled, the pellet can then creep into

some of this remaining porosity. Obviously it is not reasonable to assume that the pellet is able to creep in enough to reach 100% theoretical density, so the amount the pellet can creep in must be limited. Unlike FRAPCON, FEMAXI has allows for creep by default as a separate phenomenon that is more deeply ingrained in the code. The FEMAXI creep model comes from MATPRO Version 09 and is the most commonly accepted creep formula for UO₂. The FEMAXI model allows the gap gas pressure in the plenum to affect the fuel until hard contact is made. At this point the interfacial pressure drives the fuel creep until a limit based on relocation and fuel porosity is reached. The model for UO₂ creep implemented in FRAPCON will be discussed later in this paper.

3.3 Development of UO_2 Soft pellet Model in FRAPCON

To implement a soft pellet model in FRAPCON for UO_2 , several other displacement phenomena had to be altered. As previously discussed, several of the models used in FRAPCON have been slightly altered so that the code results would match test data. These changes have been reverted to match the original models so that results using the soft pellet model closely match what is predicted by the official version of FRAPCON as well as FEMAXI.

3.31 Swelling

FRAPCON has been altered so that when using the soft pellet model, the swelling regimen changes slightly. It is no longer delayed 6 GWD/MTU and the rate has been increased slightly so that it now matches the MATPRO model for swelling. Since the swelling models for UN and UC and not altered to fit any data, this is only significant for UO₂.

3.32 Relocation Recovery

As previously discussed, the model for relocation recovery is not as concrete as some of the other FRAPCON phenomena. The code currently predicts that after soft contact is made, 50% of the relocation value will be recovered. This 50% value is used so that code will better fit test data. With the addition of creep, the soft pellet model was under-predicting the total surface displacement of the fuel by a fairly significant amount. To counter this, the amount of relocation that could be recovered was reduced from 50% to 15%, a value that is much more in line with the relocation recovery predicted by FEAMXI. This new value will also be used for UC and UN in the event that they do relocate.

3.33 Creep

The model developed for UO₂ creep includes both a low and high stress regime and is a function of temperature, stress, fission rate and grain size. Creep was implemented in such a way that it modifies the swelling rate of the fuel instead of being a separate phenomenon. The UO₂ creep rate equation that was implemented into FRAPCON was developed by Solomon et al (1971) and is the same formula that is currently being used in FEMAXI. For the low stress regime, the creep rate is directly proportional to the stress and the pellet. In addition, there is a high stress regime where the creep rate is proportional to $\sigma^{4.5}$. The formula implemented is as follows:

$$\varepsilon = A(F)\sigma^{4.5} \exp\left(-\frac{Q}{RT}\right) + A_1(F) = \sigma G^{-2} \exp\left(\frac{Q_1}{RT}\right) + c\sigma F$$

$$A(F) = \frac{1.38 \times 10^{-4} + 4.6 \times 10^{-17}}{-90.5 + \delta}$$

$$A_1(F) = \frac{9.73 \times 10^6 + 3.24 \times 10^{-17}}{-87.7 + \delta}$$
Q = 552.3 kJ/mol
Q_1 = 376.6 kJ/mol
c = 7.10 \times 10^{-23}
\sigma = Stress (psi)
G = grain size (µm)
T = temperature (K)
R = Universal Gas Constant
F = Fission Rate (f/cm³ s)
\delta = \% theoretical density

During the initial comparison of the soft pellet model results to FEMAXI, it was noticed that FRAPCON was predicting a much higher amount of creep despite both codes using the same model and coming into hard contact at about the same point. Other displacement phenomena, such as thermal expansion and swelling were extremely similar in both codes and didn't seem to be the cause of the higher creep displacement.



Figure 3.10: Initial FRAPCON/FEMAXI Creep Results

As previously mentioned, the pellet in FRAPCON is treated as a solid right cylinder that cannot be deformed. Therefore, there is no need to know what kind of stresses are acting on the pellet since it is not affected by them. Because of this, when calculating the creep, the interfacial pressure is what is used by FRAPCON. FEMAXI, however, allows for feedback onto the pellet and therefore calculates the stress on the pellet as well as the PCMI pressure. Therefore, when FEMAXI calculates creep, it uses the pellet stress value.

Comparing results from FRAPCON and FEMAXI gives insight into how the soft pellet model affects the pressure and stress on the pellet. For this test, FRAPCON and FEMAXI were altered so that the exact same displacement results would be obtained. Relocation was disabled as it was causing issues in displacement similarities. Once this was done, a case was run using a soft and rigid pellet model for both FEMAXI and FRAPCON and the interfacial pressures and pellet stress differences were examined.



Figure 3.11: FRAPCON Interfacial Pressures

In FRAPCON, using a soft pellet model results in about a 4 MPa drop in the interfacial pressure at 30 GWD/MTU which is about a 15% reduction. This interfacial pressure value, about 22 MPa, is what is used for the creep calculations in FRAPCON. In FEMAXI, the soft pellet model affects pellet stress in a slightly different way.



Figure 3.12: FEMAXI Pressures and Stresses

FEMAXI also calculates a PCMI pressure but additionally calculates the radial stress on the pellet. The value predicted for interfacial pressure in FEMAXI for a rigid pellet is about 14 MPa, which is significantly less than the 28 MPa predicted by FRAPCON. When the soft pellet model is turned on, the interfacial pressure is reduced by about the same percentage as in FRAPCON, about 15% at 30 GWD/MTU. The more important comparison though is what happens to the stress on the pellet when a soft pellet model is enabled. For a rigid pellet model, the stress on the pellet ranges from 20 to 30 MPa after contact has been made. However, when a soft pellet model is used, the pellet stress is reduced to about 11 MPa, which is a far more substantial reduction than the interfacial pressure reduction. This 11 MPa value is what is used when calculating the creep rate of the pellet in FEMAXI and is about half of the value used in FRAPCON. The difference between these two values would explain the difference in creep rates between FRAPCON and FEMAXI.





From these results, it was decided that the interfacial pressure value in FRAPCON was too high to use in the creep calculations. Therefore, the value in the creep equations will be multiplied by 0.6 in order to make the creep calculation accurately match what is predicted by FEMAXI. The multiplier was chosen based on the stresses used in FEMAXI to calculate pellet creep. This multiplier was then tested by running cases with both codes at different power levels.



Figure 3.15: Creep Modifier Power Level Tests

Investigating further into the assessment data for both codes reveals that FRAPCON-3.5 is known to significantly over-predict cladding hoop strain due to the rigid pellet model. This lends more credibility to using a modifier for the pellet creep calculation. 3.34 Verification

The soft pellet model has been compared to both FEMAXI-VI and FRAPCON-3.5 and was based on results from the FEMAXI-VI model. FRAPCON and FEMAXI are assessed using test reactor data from a large variety of sources. These sources overlap in some cases, but for the most part FRAPCON and FEMAXI area validated against different sets of test reactor data. Results from the FRAPCON soft pellet model match up well with both the FRAPCON 3.5 rigid pellet model and the FEMAXI-VI model.

3.34 Creep Limitation

Since creep is not a standard part of the FRAPCON code, there is nothing to keep the pellet from creeping into space that isn't actually there. Therefore, the pellet creep must be limited based on the amount of volume that is available. The sources of space for the pellet to creep into come from the initial porosity of the fuel as well as the remaining relocation that is not recovered upon soft contact. A flag was put into the input deck that allows the user to set a maximum % theoretical density. Based on this number as well as the amount that the pellet relocates, the available volume for creep is calculated. Once this is known, the code calculates the volumetric displacement caused by creep based on the pellet's radius at the time. This radius takes into account the displacement caused by thermal expansion, densification, swelling and relocation. If the volumetric displacement caused by creep is greater than the volume available for creep, then the creep rate is set to zero. For the purpose of this research, the creep limitation so that the fuel is able to creep into 100% of the allotted space. This value is able to be changed so that the space available for creep can be limited based on the density of the fuel. For most UO_2 – Zircaloy cases, this limit will not be reached. However, for a case where PCMI occurs early and SiC is the cladding, it is more likely a limit will be reached. Due to relocation not occurring for UN and UC, these fuels have a much higher chance at reaching 100% TD if PCMI is allowed to occur since there is less space for them to creep into. The graphs below show results from when the creep limitation is set to 95.5% of the fuel's theoretical density.



Figure 3.16: Creep Limitation - UO2 - Zircaloy - FRAPCON

Figure 3.13 shows the effect creep limitation has on the pellet surface displacement. As the pellet creep occupies all of the volume allotted for it, the pellet creep rate is set to zero and the rate of radial displacement of the fuel increases.



Figure 3.17: Creep Limitation Calculation

Figure 3.14 shows how the creep occupies the volume available from relocation and porosity. At the low %TD limits set for these graphs, the relocation provides most of the space for the pellet to creep into. Implementing a creep limitation calculation prevents the pellet from becoming unrealistically dense.

CHAPTER 4

EFFECT OF SOFT PELLET MODEL IN FRAPCON

Before FRAPCON and Femaxi are compared to each other to validate the creep model, it must first be understood how creep effects the results within each code. In the soft pellet model for FRAPCON, a model was implemented that allows the pellet to creep inward based on interfacial pressure. In addition to this, the swelling model was altered so that it swells at a higher rate and begins swelling at the beginning of life.

$4.1 \ UO_2 \ \text{with} \ Zircaloy$

Before results from FRAPCON and FEMAXI can be compared, it must be understood how using a soft pellet model affects the results predicted by each code.



Figure 4.1: Effect of Soft Pellet Model on UO₂ with Zircaloy Cladding - Radial Displacements

Figure 4.1 shows the effect that the soft pellet model has on the radial displacement of a UO_2 when it is used with Zircaloy cladding. The most notable difference is the addition of creep as well as the difference in relocation recovery and swelling. Altering the relocation recovery results in about an 11 microns difference between the relocation values and the soft pellet swelling model causes about 9 microns higher swelling displacement. These differences are countered by the added creep of the pellet. Although the pellet begins to creep slightly at beginning of life due to gap gas pressure, creep is not a substantial cause of surface displacement until hard contact is made.

The change in relocation recovery causes a large discrepancy between the soft and rigid pellet models at 20 GWD/MTU, however, the total displacement at beginning and end of life is very similar to what is predicted by FRAPCON 3.5.



Figure 4.2: Effect of Soft Pellet Model on Cladding Hoop Stress - UO₂ Pellet with Zircaloy Cladding

When studying the effects of the soft pellet model, one of the main interests is how allowing for pellet creep can alleviate stress on the cladding. Due to the ductile nature of Zircaloy, interfacial pressures never reach the point where having a pellet creep model is absolutely necessary. However, with interest in new, unyielding claddings such as SiC, understanding how much the soft pellet model alleviates is very important.



Figure 4.3: Effect of Soft Pellet Model on Cladding Hoop Stress - UO₂ Pellet with Zircaloy Cladding

Even though the soft pellet model predicts an early point of hard contact, the reduction of cladding hoop stress is fairly significant. Due to pressure from the coolant, the cladding is in compression until hard contact is made. After contact, the cladding hoop

stress rapid increases as it is forced outward by the pellet swelling. Even without pellet creep, the hoop stress when using a rigid pellet model begins to level off due to the relaxation of the cladding as it creeps outward. Due to the addition of creep in the soft pellet model, it takes less interfacial pressure to offset the stress caused by pellet swelling.

Overall, the biggest difference that results from using a soft pellet model is in cladding stress. Due to the altered relocation recovery, hard contact is predicted to occur about 6 GWD/MTU earlier than when a rigid pellet model is used. However, even though this causes the cladding to be under tension for a longer amount of time, the amount of stress is significantly less. This reduced hoop stress is an initial confirmation that the soft pellet model is functioning as intended.

4.2 COMPARISON OF FRAPCON SOFT PELLET MODEL TO FEMAXI

A favorable comparison with FEMAXI fuel performance code is imperative to verifying the implementation of a soft pellet model for UO₂ in FRAPCON. As previously mentioned, creep in FEMAXI is a standard part of its fuel surface displacement models. However, there is an option to turn off pellet plasticity and creep which will simulate the rigid pellet model used by FRAPCON. Since in FEMAXI creep is treated as a separate phenomenon and is more deeply ingrained in the code, altering the creep also slightly affects the relocation recovery.





In FEMAXI, the addition of creep and a slight change in the pellet's relocation term are the only changes when a soft pellet model is used instead of a rigid pellet model. These differences make up the difference between the total displacements for the soft and rigid models. It is interesting to note that after the pellet comes into contact with the cladding, more of the relocation value is recovered when using a rigid pellet model. In FEMAXI, relocation recovery is calculated based on strain on the surface pellet. Once the total surface strain is equal to the amount of strain that was caused by relocation, the pellet is considered solid again. When creep is turned off, it takes longer for this strain value to be reached.



Figure 4.3: FRAPCON/FEMAXI Soft Pellet Comparison

After the previously mentioned changes were made to FRAPCON to implement the soft pellet model, FRAPCON predicts very similar results that are very similar to what is predicted by FEMAXI with the main difference being within the first 6 GWD/MTU. The rate of creep, which is the main interest in this verification is almost exactly the same in both codes. Due to differences in relocation recovery, hard contact is made a few GWD/MTU earlier in FRAPCON which results in a slightly larger total displacement due to creep.

When the soft pellet model is used in FRAPCON for UO_2 with Zircaloy cladding, the results very closely resemble what is predicted by FEMAXI, with only minor differences due to the relocation recovery models. The fuel pellets creep at almost exactly the same rate once hard contact has been made and both codes predict very similar total surface displacements. In FEMAXI, there is an elastic displacement term that is calculated but it is small enough that is does not significantly affect the results. Judging from these results, the soft pellet model in FRAPCON was implemented correctly and is accurately representing the effects of allowing fuel creep.

4.3 UO_2 with Silicon Carbide

For the purposes of understanding PCMI, the main difference between Zircaloy and silicon carbide is that SiC does not creep. Without the inward creep of the cladding, the gap must be closed entirely by pellet swelling, thermal expansion and relocation which results in a significantly longer period of no contact between the pellet and cladding. However, since the cladding does not creep outward either, there is a massive build-up of interfacial pressure once contact is made.



Figure 4.6: Effect of Soft Pellet Model on Radial Displacement - UO₂ - SiC

While the radial displacement of the fuel is not heavily affected by the introduction of a soft pellet model, the interaction between the pellet and the cladding is extremely different when using SiC cladding. As a ceramic, SiC cladding is not ductile like Zircaloy cladding and thusly will not deform elastically under pressure as Zircaloy does. However, without the use of a soft pellet model, the cladding has no choice but to deform as the rigid pellet swells outward. If the pellet is allowed to deform, cladding hoop stress is massively relieved as the pellet creeps inwards.

In Figure 4.6, the slight pellet creep inward due to gap gas pressure is enough to cause soft contact to occur at about the same time, despite differences in the swelling models. After hard contact, the influence of the soft pellet model is most noticeable. As mentioned previously, the SiC cladding has no choice but to deform as the rigid UO₂ pellet swells outwards. However, this causes a massive hoop stress on the cladding, even with the cladding yielding to the pellet.



Figure 4.5: Effect of Soft Pellet Model on Cladding Hoop Stress - UO₂ - SiC



Figure 4.7: Effect of Soft Pellet Model on Cladding Hoop Stress - UO_2 - SiC - FRAPCON

When using a soft pellet model for UO₂ with SiC, there is an interesting interaction which causes the peak on cladding hoop stress shown in Figure 4.7. This peak is due to a change in the thermal expansion regimen that is only noticeable when using SiC cladding due to the high fuel temperatures that it causes. In FRAPCON for UO₂, there is an increase in thermal expansion rate at 40 GWD/MTU which stops at 50 GWD/MTU that only occurs at temperatures above 1370 °C. When the fuel comes into contact with the cladding, the increased thermal expansion rate causes a larger increase in cladding hoop stress than it would if the thermal expansion rate was steady. At 50 GWD/MTU, once the rate stops increasing, there is a sharp dip in the hoop stress of the cladding which continues to decrease as pellet creep alleviates stress on the cladding.



Figure 4.8: Effect of Soft Pellet Model on Cladding Hoop Stress - SiC and Zircaloy Comparison

At end of life, there is about a 565 MPa difference in the hoop stress of the cladding when the soft pellet model is used. Compared to using Ziracloy cladding, where the soft pellet model only decreases the hoop stress of the cladding by about 50 MPa, this is a massive decrease in hoop stress. If creep is not predicted to occur, then any case where the pellet comes into contact with the SiC cladding will cause the cladding to rupture shortly after contact. While it may not be imperative to use a soft pellet model when modeling with Zircaloy as a cladding, the interfacial pressure when using SiC is so high that the only way to accurately model any fuel as a rigid pellet with SiC cladding is to never allow PCMI to occur. However, judging from the hoop stresses obtained during the soft pellet case, it would be possible to design a $UO_2 - SiC$ combination in a way that would prevent cladding fracture.



Figure 4.9: Effect of Cladding Type on Centerline Temperature

One downside to the SiC cladding is that the lack of cladding inward creep delays soft contact which causes about a 100 degree increase in fuel centerline temperature at end of life due to the thermal gap being open longer. Thus, creating a configuration where the pellet never comes into contact with the cladding would be detrimental to the heat conduction from the pellet to the coolant. This further exemplifies the importance of using a soft pellet model to accurately model fuel with a SiC pellet and shows how big of an impact creep can have. By allowing for fuel creep, the rod can be modeled in such a way that the thermal gap can be closed while keeping the cladding from fracturing. Therefore, in order to accurately model any fuel with SiC cladding, fuel creep must be considered, otherwise either the pressure on the cladding or the centerline temperature of the fuel will be too high.

4.4 UC WITH ZIRCALOY

Interest in using UC fuel with SiC cladding is one of the main reasons that FRAPCON is being altered to allow for pellet creep. As shown in the previous section, when UO_2 is used with SiC, there is only a short amount of time where the pellet is in contact with the cladding. However, due to the high swelling rate of UC, there will be a much longer period of PCMI and the interfacial pressures will be much higher.

As shown with a UO₂ pellet, running FRAPCON using a soft pellet model can cause the code to predict very different results than the same case run with a rigid pellet model. These differences are significant enough that not allowing the pellet to creep could cause the cladding to fracture upon PCMI. When a UC pellet is considered, these differences are magnified due to the swelling rate being over twice that of UO₂. This means that the pellet will come in contact with the cladding sooner and provide even more of a pressure between the pellet and the cladding.

Cases for UC with both Zircaloy and SiC need to be run in order to obtain results which can be compared to UO_2 results. This will help ensure that the soft pellet model was implemented correctly and affecting the results as predicted.



Figure 4.10: Effect of Soft Pellet Model on UC Radial Displacement - Zircaloy Cladding

With Zircaloy cladding, the interfacial pressure isn't high enough to cause large amounts of creep, but it is still enough to cause a drop in fuel surface displacement. The Zircaloy cladding will creep outward quickly enough to accommodate the high swelling of UC. Swelling and thermal expansion have been omitted from this graph as they are not changed by the soft pellet model.



Figure 4.11: Effect of Soft Pellet Model - UC Pellet – Zircaloy

The difference in cladding hoop stress between the soft and rigid pellet model is as to be expected based on the results from the radial surface displacement. The stresses increase at about the same rate and have a similar slope. However, the soft pellet model causes the cladding hoop stress to be about 20 MPa less than when the rigid model is used.

As with UO_2 , the effect of the soft pellet model is most evident when using SiC cladding. The rigidity of the cladding causes large amounts of feedback onto the pellet. This creates a massive amount of interfacial pressure between the pellet and cladding unless some of that pressure is relieved through fuel creep.

4.5 UC WITH SILICON CARBIDE

When uranium carbide is paired with SiC cladding, using a soft pellet model causes drastically different results when compared with the results from using a rigid pellet model. Since the SiC cladding does not creep outwards, there is a very large amount of interfacial pressure between the pellet and cladding upon contact. This causes the pellet to creep inwards which in turn alleviates some of the stress on the cladding and in theory prevents the cladding from fracturing.



Figure 4.12: Effect of Soft Pellet Model - UC Pellet - SiC Cladding



Figure 4.13: Effect of Soft Pellet Model on Cladding Radius - UC Pellet - FRAPCON

Figure 4.13 shows how the soft pellet model affects cladding radius after contact is made. For both the soft and rigid pellet model, the pellet swells until it comes into contact with the cladding at about 28 GWD/MTU. For UC, the mechanical radius will be used instead of the thermal radius since there is not relocation occurring. When there is no relocation, the thermal and mechanical radius are the same other than the thermal radius never contacts the cladding due to there being a thermal gap. When a soft pellet model is used, the rigidity of the cladding causes the pellet to creep inward and there is very little change in the inner radius of the cladding. However, with the rigid pellet model, the swelling of the pellet. Since UC and a non-ductile ceramic, it would not be able to realistically creep outwards as is shown in the results from the rigid pellet model.



Figure 4.14: Effect of Soft Pellet Model on Cladding Hoop Stress - UC Pellet - SiC Cladding

When the cladding stress is examined, it is obvious that for UC fuel and SiC cladding to be a successful combination, creep has to play a significant role in reducing the hoop stress on the cladding. Without a soft pellet model being used, the hoop stress in the cladding is almost 8000 MPa, far higher than the cladding is capable of withstanding. If the pellet is allowed to creep, the code predicts a cladding hoop stress of about 1000 MPa. While this stress is still too high for the SiC cladding to be able to withstand, it is a much more reasonable amount of stress when compared to the hard pellet model. The graph above also assumes that the pellet is able to creep is about 50 microns, which is a substantial amount of displacement.

From the results of the graph above, it is obvious that a UC pellet with SiC cladding could not be used when manufactured to the same specifications as UO_2 and Zircaloy cladding. For UC to be used with SiC, the fuel must be designed so that it never contacts the cladding or the cladding must be thick enough to withstand the high hoop stresses.

4.7 UN WITH ZIRCALOY

UN is another advanced fuel with many desirable qualities but also a few drawbacks, including a high swelling rate more similar to that of UC than UO_2 . As with UC, it is important to understand how it will interact with current and future reactor materials, such as Zircaloy and SiC.





Similar to UC, using a soft pellet model for UN with Zircaloy cladding does not have a major effect on the total surface displacement of the fuel as the outward creep of the cladding alleviates a lot of the stress on the pellet.



Figure 4.16: Effect of Soft Pellet Model on Radius - UN - Zircaloy - FRAPCON



Figure 4.17: Effect of Soft Pellet Model on Pellet Hoop Stress - UN - Zircaloy - FRAPCON

Due to the higher swelling rate, the UN pellet puts a higher amount of stress on the Zircaloy cladding than UO_2 and since the creep rate is less, the amount of stress reduction

caused by pellet creep is less than that for UO_2 . Even with UN causing 40 more MPa of hoop stress, implementing a soft pellet model only reduces stress by about 30 MPa, compared to a 50 MPa reduction for UO_2 . However, as UN reacts poorly with water, it would not make for a suitable fuel in current LWRs, and is instead more viable in Gen-IV reactors. Therefore, it is of more interest to understand how UN will interact with SiC.

4.8 UN WITH SILICON CARBIDE

The same issues that exist for UC with SiC cladding are also present of UN with SiC cladding. The high swelling rate and lower creep rate cause massive hoop stress on the cladding.



Figure 4.18: Effect of Soft Pellet Model on Radial Displacement - UN - SiC - FRAPCON

The lack of creep in the SiC cladding causes pellet creep to occur at a much later burnup but also causes the pellet to creep at a much fast rate due to the high interfacial pressures. These two things results in the total creep of the pellet to be about the same as it is with Zircaloy cladding.



Figure 4.19: Effect of Soft Pellet Model on Radius - UN - SiC - FRAPCON



Figure 4.20: Effect of Soft Pellet Model on Cladding Hoop Stress - UN - SiC - FRAPCON

Despite nearly the exact same amount of creep occurring for UN with Zircaloy and SiC claddings, the soft pellet model has a much bigger impact when UN is coupled with SiC. The lack of creep in SiC causes an extremely large hoop stress in the cladding. If the pellet is not allowed to creep inwards, there is nothing to relieve the hoop stress and it will continually increase as the fuel swells outwards. However, if the pellet is allowed to creep, it reduces the amount of hoop stress on the cladding by almost 1000 MPa.



Figure 4.21: SiC - Zircaloy UN Centerline Temperature Comparison

Even with this significant reduction in cladding hoop stress, the stress on the cladding is still too high when using the UO_2 – Zircaloy specifications. If the fuel is not allowed to contact the cladding at all, there are significantly increased temperatures as shown above. As with UC, significant alterations in fuel design would have to be made for SiC to be a viable cladding.

CHAPTER 5

COMPARISON OF ADVANCED FUELS TO UO_2

The soft pellet model will be used to compare UO_2 and UC since the effect of creep is what is of interest in this study. A case with the same parameters as was previously used for the UO_2 comparisons will be used for these comparisons despite the fact that if UC were to be used in a reactor it would likely have different as manufactured specifications than those currently used for UO_2 .



Figure 4.22: UO₂ – UC - UN Swelling Comparison

The graph above illustrates how much more the UC fuel swells under the same conditions as the UO_2 pellet. At the end of life, the UC pellet has swelling over twice the amount of the UO_2 pellet, causing a final displacement of about 119 microns. This high
swelling rate is the main reason that adjustments would have to be made to current reactor fuel rod designs if they were to accommodate UC pellets. The UN pellet still swells at a significantly high rate than UO_2 but would be far more manageable, especially considering that UN will densify unlike UC. When considering only the swelling rate, UN would be much more easily adapted than UC into current fuel rod designs.



Figure 4.23: UC - UO₂ – UN Thermal Expansion Comparison

Thermal expansion for UC is dependent only on temperature and keeps the same model throughout, unlike UO_2 which uses different models for thermal expansion based on burnup. The higher thermal conductivity of the UC keeps the pellet at a lower temperature than UO_2 , causing the thermal expansion value to be much lower. For the same linear average power, the centerline temperature of UC is 400 K to 500 K lower, depending on how long it has been in the reactor. Again, UN is in between UO_2 and UC. Neither UN nor UC relocates so both come into soft contact a few GWD/MTU later than UO_2 .



Figure 4.24: UO₂ - UC Centerline Temperature Comparison

Due to the high thermal conductivity of UC, the thermal stress across the fuel are not high enough to cause the fuel to relocate. However, due to the high swelling rate, UC makes hard contact about 5 GWD/MTU before the UO₂ pellet and from there continues to swell outward at a much greater rate. The total surface displacement of UC is over twice that of UO₂.



Figure 4.25: Soft Pellet Hoop Stress Comparison UC - UO₂

The large difference in total fuel displacement is evident when examining how much more stress the Zircaloy cladding is under when the UC pellet is used. The stress caused by the UC pellet is about three times as much as that caused by UO_2 and also occurs over a longer period of time. UN comes into hard contact at about the same time as UO_2 but builds up more stress due to a higher swelling rate. In addition, the UC and UN pellets do not creep as fast as the UO_2 pellet which results in the cladding hoop stress for UC and UN to continue to increase after contact.

CHAPTER 6

CONCLUSIONS

Understanding and accurately representing how materials interact within the reactor is the first step to being able to use these new materials for future reactor designs. Without a thorough understanding of what happens when these new materials interact, it isn't possible to even begin to design a fuel rod that uses a new cladding and a new fuel. From these results, significant changes will have to be made to the existing UO_2 – Zircaloy design specifications. Even with pellet creep, the stress on the cladding from UC and UN is too much for the SiC to handle.

 UO_2 would be able to be combined with SiC cladding without changing any design specifications. However, using SiC instead of Zircaloy would cause the pellet centerline temperatures to be much higher due to hard contact being delayed. It is possible that the gap size could actually be decreased if the pellet is able to continually creep.

For both UN and UC there are two options for use with SiC cladding. If pellet creep is assumed, then the cladding can be thickened to the point where it would be able to withstand the stress from the high swelling rates of both fuels. In doing this, the pellet would come into contact with the cladding more quickly, however, the thicker cladding would hurt the neutron economy of the reactor as well as negatively affect heat transfer. The other option is to increase the gap size to a point where the pellet never comes into contact with the cladding. The large gap would greatly affect the transfer of heat from the pellet to the cladding but in general this would be the more conservative method. However, a large factor of safety would have to be allowed. As previously shown, the hoop stress of SiC increases so rapidly upon contact that any contact at all would cause fracture.

Based on these result, significant design changes would have to be made before UC, UN or SiC could be used safely and effectively in a LWR reactor. It is much more possible that UN and UC with SiC as a cladding will be used in a GEN-IV reactor that does not use water as a coolant. Regardless of reactor type, to accurately model either of these fuels with SiC a soft pellet model must be used unless to accurately represent PCMI between any reactor fuel and SiC cladding.

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