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Modeling of Metallic Fuel for Liquid-Metal Fast Reactors

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ABSTRACT

Computational models to analyze in-reactor behavior of U-Zr and U-Pu-Zr metallic alloy fuel pins have been developed and implemented in a new code, the Fuel Engineering And Structural analysis Tool (FEAST). FEAST consists of several modules working in coupled form with an explicit numerical algorithm. These modules are (1) Fission Gas Release and Swelling, (2) Fuel Constituent Redistribution, (3) Temperature Distribution, (4) Fuel-Clad Chemical Interaction and (5) Fuel-Clad Mechanical Analysis.

The main purpose of FEAST is to model metal fuel performance by adopting non-empirical approaches to increase the ability to extrapolate the existing database with a reasonable accuracy. As a consequence, mechanistic models for the fission gas release and swelling module, the fuel constituent redistribution and the Fuel Clad Chemical Interaction, were adopted. The mechanical analysis and temperature distribution modules adopt 1D approaches.

The code was benchmarked against the available EBR-II experimental database. The results show that FEAST is able to predict the important phenomena such as axial fuel swelling, cladding strain and fission gas release satisfactorily. Moreover, a code to code benchmark has been performed against ALFUS by using PHENIX reactor irradiation data. Again, the agreement is reasonably good for fuel swelling, while some discrepancies are observed in the cladding strain predictions.
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FEAST: A New Irradiation Behavior Code for Metal Fuels

1. Introduction

Liquid-metal-cooled fast reactors, particularly sodium-cooled reactors, have regained worldwide interest in recent years thanks to international nuclear programs such as Generation-IV and GNEP. Several fast reactor concepts use metal fuel as their primary fuel option. Metal fuel typically consists of a binary alloy of uranium and zirconium or a ternary alloy of uranium, plutonium and zirconium. Addition of about 10% by weight zirconium to a uranium-plutonium alloy raises the solidus temperature of the fuel and prevents fuel-cladding interdiffusion at temperatures typical of steady operating conditions [1]. The fuel/clad gap is filled with liquid sodium, which acts as a thermal bond. The attractive characteristics of metal fuel include:

- High thermal conductivity which, combined with a highly conducting gap, maintains fuel temperatures low and reduces stored energy, an important feature during unprotected transients, such as the unprotected loss of primary flow and loss of heat sink.
- High heavy metal density and low moderating power, which provide for a very hard spectrum and excellent neutron economy.
- Low Fuel Clad Mechanical Interaction (FCMI), which enables achievement of high burnup.
- Good compatibility with the coolant.
- Ease of manufacturing and reprocessing by pyrochemical methods.

However, various phenomena limit the in-core performance of metal fuel assemblies, including clad thermal and irradiation creep, fuel restructuring and Fuel/Clad Chemical Interaction (FCCI). It is obvious that any credible attempt at assessing the performance of metal fuel must include a model that is able to predict the temperature, stress and strain time-dependent distributions within the clad and fuel for given operating and abnormal conditions, including the effects of fuel restructuring, FCCI, thermal expansion, thermal creep, irradiation creep, fuel swelling and fission gas release. Benchmarking of these models against the experimental data is perhaps the most crucial step. However, the metal fuel irradiation database is limited and mostly based on irradiations in the EBR-II during the integral fast reactor program, which was protected as Applied Technology.

1.1. Description of a Typical Metal Fuel Pin

A typical metal fuel pin is shown in Figure-1.1. A solid cylindrical metal fuel slug is submerged into liquid sodium and is encapsulated within the cladding. The reference cladding material for the past twenty years has been HT9, a low swelling ferritic-martensitic stainless steel. Note that

\[\text{Some researchers however feel that the relatively low melting point of metal fuel is a serious drawback compared to oxide fuel [2].}\]
a certain free volume is provided in the upper part of the fuel pin to relief the pressure due to fission gas release from the fuel.

![Diagram of metallic fuel element](image)

**Figure-1.1: Description of the metallic Fuel**

### 1.2. Project Objectives and Review of Current Metal Fuel Codes

The objective of this work is to develop a robust and reliable code, which we will call Fuel Engineering And Structural analysis Tool (FEAST), to model the irradiation behavior of metal fuels in sodium-cooled fast reactors. Given the fuel pin geometry, composition and irradiation history, FEAST can analyze the fuel slug and cladding thermo-mechanical behavior at both steady state and transient conditions. In this report we will focus only on the steady behavior. The ultimate goal is to use FEAST in the licensing process of metal-fuelled fast reactors for the GNEP and Generation-IV programs.

A literature review has been completed to identify and assess the major metallic fuel codes in use or being developed to date. A comparison of the features of the various codes is given in Table-1.1. Note that in all cases the overall code structure consists of several modules describing the important phenomena.

<table>
<thead>
<tr>
<th>Fuel</th>
<th>U-Pu-Zr</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gap</td>
<td>Liquid Sodium</td>
</tr>
<tr>
<td>Clad</td>
<td>HT9</td>
</tr>
<tr>
<td>Coolant</td>
<td>Liquid Sodium</td>
</tr>
</tbody>
</table>

The LIFE code was originally developed for oxide fuel and was later modified to analyze mixed-carbide and mixed nitride fuel. LIFE-METAL [3] is the metal-fuel version of the carbide/nitride version of LIFE. It implements a detailed thermo-mechanical analysis of the fuel-cladding system in the radial direction. Axial variations in operating conditions are accounted for by assigning specific powers and fast fluxes at up to nine axial nodes. The axial nodes are thermally coupled through the calculated coolant temperatures, however, axial heat conduction is ignored and there are no provisions for mechanical coupling between axial nodes. LIFE-METAL calculates the fission gas release fraction and fuel swelling strains by empirical correlations of burnup, temperature and porosity. The fuel constituent redistribution is also based on an empirical model. The code cannot model anisotropic fuel deformation, which is observed in experiments.
Table-1.1:  Steady-State Metallic Fuel Codes

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Developer</td>
<td>ANL (US)</td>
<td>CRIEPI</td>
<td>CRIEPI</td>
<td>KAERI</td>
<td>MIT (US)</td>
</tr>
<tr>
<td>General Capabilities</td>
<td>Steady-state and Transient Behavior</td>
<td>Steady-state Behavior</td>
<td>Steady-state Behavior</td>
<td>Steady-state Behavior</td>
<td>Steady-state and Transient Behavior</td>
</tr>
<tr>
<td>Fission Gas Release and Fuel Swelling</td>
<td>Empirical Correlation</td>
<td>Empirical Correlation</td>
<td>Mechanistic Model, based on $\text{UO}_2$ Fuel</td>
<td>Mechanistic Model, Based on $\text{UO}_2$ Fuel</td>
<td>Mechanistic Model, Based on Metallic Fuel</td>
</tr>
<tr>
<td>Constituent Redistribution</td>
<td>Empirical Correlation</td>
<td>Chemical Equilibrium Model</td>
<td>Thermo-transport theory</td>
<td>Thermo-transport theory</td>
<td>Thermo-transport theory</td>
</tr>
<tr>
<td>Temperature Distribution</td>
<td>1D Model</td>
<td>1D Model</td>
<td>1D Model</td>
<td>1D Model</td>
<td>1D Model</td>
</tr>
<tr>
<td>Mechanical Analysis</td>
<td>1D Model</td>
<td>1D Model</td>
<td>2D Model</td>
<td>1D Model</td>
<td>1D Model</td>
</tr>
<tr>
<td>FCCI</td>
<td>Empirical Correlation</td>
<td>Not Included</td>
<td>Empirical Correlation</td>
<td>Not Included</td>
<td>Empirical Correlation (mechanistic model under development)</td>
</tr>
</tbody>
</table>

The SESAME [4] code was developed to predict only the steady-state performance of both U-Fissium and U-Pu-Zr alloy metallic fuels. A single fuel element is divided into several axial nodes, each containing several equiaxial radial meshes in which the important performance variables such as stress, strain, temperature and material properties are assumed to be spatially uniform. Temperature and mechanical analysis modules adopt a 1D finite element method. The fission gas release and swelling module adopts the same empirical model developed for LIFE-METAL. The fuel constituent redistribution model is based on the chemical equilibrium assumption. Anisotropic fuel slug deformation is accounted for by an empirical approach.

The ALFUS code [5] has been developed for stress-strain analysis of U-Pu-Zr ternary metallic fuel pins. The mechanical analysis model is based on axisymmetric 2D r-z finite element method, which is similar to FEMAXI-III, the light water reactor fuel performance code [7]. The fuel constituent redistribution model is based on thermal-transport theory, but is not coupled to the mechanical analysis module, so an implicit assumption is made that the mechanical properties are insensitive to local fuel composition. The code uses a mechanistic model, originally developed for $\text{UO}_2$ fuel, for calculation of the fission gas release and fuel swelling [8]. Empirical models are included for compressibility of the interconnected gas pores and anisotropic deformation of the fuel slug.

The MACSIS code [6] analyzes the irradiation behavior of U-10Zr fuel for steady state conditions. It calculates the temperature distribution, dimensional changes, axial growth, fission gas release and radial redistribution of the fuel alloying elements. Axial heat conduction and mechanical coupling of axial nodes are not considered. The fuel constituent redistribution model is based on thermo-transport theory. The fission gas release and swelling module is based on Booth’s diffusion theory which was originally developed for ceramic fuels.

It was decided to develop a new metal fuel code, FEAST, for the following reasons:
- The older codes (LIFE [3] and SESAME [4]) are highly empirical and cannot be extrapolated beyond the narrow database for which they were developed
- There is a need for a robust code for analysis of fuel behavior during transients
- Regulators will need an independent tool to verify the performance of metal fuel for the next-generation of fast reactors
- The newer codes being developed in Asia (ALFUS [5] and MACSIS [6]) may not become available to researchers/vendors/regulators in the US

The FEAST code is developed for analysis of the steady-state and transient irradiation behavior of U-10Zr and U-Pu-10Zr metal fuels. It is being developed to be highly flexible, so that constitutive models for other alloys of interest (e.g., TRU-Zr alloys) can be easily added to the code. FEAST’s mechanical model is similar to the respective LIFE code algorithm. Variation of material properties (fuel creep, thermal expansion, Young’s modulus) with local fuel composition is taken into account. The fuel and cladding regions can be divided into up to 8 radial nodes each; however, six radial nodes in the fuel region and at least two radial nodes within the cladding region are recommended. Axial nodes are also user specified. A maximum of twenty nodes can be assigned in the axial direction. Axial heat conduction is neglected. The fission gas release and swelling module implements the GRSIS algorithm [9] which was originally developed for metal fuel. The fuel constituent redistribution model is based on thermo-transport theory. Empirical models developed for the compressibility of open pores and anisotropic deformation of the fuel slug in ALFUS [5] are implemented into the FEAST code. Finally, an Arrhenius-type empirical relation was developed to model cladding wastage. A more mechanistic approach is being developed for FCCI and will be included in the next version of FEAST.

This report provides a detailed description of the FEAST code structure (Section-1) and constitutive models (Section-2 through 6). Validation of the code using the available irradiation data is shown in Section-7. Conclusions and Future Work are discussed in Section-8 and 9, respectively.

1.3. Thermo-mechanical Behavior of the Metal Fuel

Table-1.2 reports the sequence of key physical phenomena during the irradiation of a typical metal fuel pin, as deduced from the operating experience in the EBR-II reactor at ANL-West in Idaho.
Table-1.2: Description of the burnup history (72 % smear density U-19Pu-10Zr Fuel)

<table>
<thead>
<tr>
<th>Burnup (at %)</th>
<th>Relevant phenomena</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>Irradiation begins</td>
</tr>
</tbody>
</table>
| 0.5-1.0       | (1) Due to swelling and cracking, the fuel reaches the clad and becomes axially restrained at the ‘hot’ axial location.  
(2) Resulting axial friction force is enough to stop the axial growth of the fuel by compressing the existing open gas pores. Furthermore, swelling rate reduces due to axial frictional force.  
(3) The radial contact stress between fuel and clad is low due to extrusion of the inner zone fuel into the cracks.  
(4) Fission gas release into the plenum begins. |
| 1.0-2.0       | (1) Cracks are closed and fuel becomes both axially and radially restrained at the hot axial location.  
(2) Radial contact stress between fuel and clad rises to a level somewhat higher than plenum pressure. Open gas pores start to be compressed to accommodate for solid/liquid fission product swelling.  
(3) Fission gas release fraction rises rapidly to 50 %. |
| 2.0-13.0      | Contact stress holds at a level somewhat higher than the plenum pressure as the open pores are further compressed to accommodate accumulation of solid products. |
| 13-20         | Fuel does not have enough open pores to accommodate solid fission product accumulation. The resulting fuel-clad contact pressure rises significantly. When open pores are less than 5 %, the contact pressure rises rapidly and breach may result. |

1.4. FEAST Code Structure

The FEAST code is composed of several modules in coupled form to simulate metal fuel thermo-mechanical behavior, as described in Table-1.1. The code is written in FORTRAN-90 language.

The code implements an explicit numerical algorithm. The flow sheet of the calculations is given in Figure-1.2. Note that the very high rate of creep strain of the fuel slug requires short time steps, of the order of 10-20 seconds, therefore a typical irradiation simulation requires use of about $10^6$ time steps, resulting in an execution time of the order of minutes, when run on a single CPU personal computer.

The input file for the code allows specification of the operating conditions and initial fuel pin and coolant flow path geometry.

The code performs the following steps for each axial node at each time step:

1- Radial power distribution within the fuel slug is calculated based on the actinide concentration within each radial node.
2- Contact pressure between the fuel and clad is calculated as a function of displacement of fuel and cladding.

3- The code calculates the fuel constituent redistribution, which is a relatively slow process, every 10000 seconds to reduce the computational time. Given the phase diagram and thermo-chemical activity of each phase, the code calculates the zirconium current and solves the diffusion equation by an explicit algorithm. Note that, both explicit and semi-implicit algorithms exist for this module. The semi-implicit algorithm could only be computationally efficient if one million second or higher time steps area selected. However, the rapid variation of the temperature distribution does not allow such high time steps; thus, an explicit algorithm is recommended for this module.

4- Temperature distribution of the fuel pin is calculated as a function of radial power, zirconium, porosity distribution and sodium infiltration. Furthermore, the coolant axial temperature distribution is calculated with the Single Mass Velocity Model [10]. Consistently with the fuel constituent redistribution module, the calculation is performed every 10000 seconds. The Jacobi matrix solver algorithm is used [11].

5- Having calculated the radial temperature distribution, the fuel stress/strain analysis is performed. Using the creep strains and axial strains calculated at the previous step, the average radial displacement can be calculated for each radial ring by using the Jacobi matrix solver algorithm. After that, the axial force balance is used to calculate either the axial strain if the gap between the fuel and the clad is open; or, the friction force, if the gap between the fuel and the clad is closed. Finally, the creep and plasticity strains and open pore compressibility strain are calculated which will be used in the next time step.

6- Given the hydrostatic stress, temperature and fission rate of each radial ring, the fission gas release and swelling behavior of the fuel is calculated. Swelling due to diffusion of gas atoms into gas bubbles, coalescence of gas bubbles due to growth and bubble diffusion and open porosity formation have been accounted for. Moreover, an empirical relation is adopted for solid fission product swelling. No matrix solver is necessary in this module.

7- Cladding wastage is calculated using an Arrhenius type empirical relation.

8- Given the contact pressure between fuel and cladding and coolant pressure outside the cladding, the radial displacement for each radial ring in the cladding are solved using the Jacobi matrix solver. After that, the axial force balance is used to calculate the axial strain. Finally, cladding creep strains are updated again and used in the next time step.

9- The plenum pressure calculation is performed by assuming that the perfect gas law applies. The sum of the open porosity within the fuel slug and the plenum region at the top of the fuel slug is the volume occupied by gas.
Figure-1.2: Flow Sheet of FEAST
2. Fission Gas Release and Swelling Module

2.1. Introduction

The main contributors to fission gas release in metal fuel are xenon and krypton because of their virtually complete insolubility in the fuel matrix. Therefore, if kinetically favorable, xenon and krypton will be rejected from the fuel matrix. These gases are either directly released into the plenum, or they accumulate in small bubbles within the fuel. Because the density of the gas in such bubbles is considerably lower than that of the solid fuel, gas atoms residing in bubbles occupy more volume than either the fissile atoms they replaced or fission-product atoms that segregate as solid phases. The precipitation of fission gases thus leads to swelling of the fuel to a larger degree than volume expansion that would occur if the xenon and krypton had remained dispersed on an atomic scale in the fuel matrix. Swelling adversely affects fuel performance because it promotes fuel-cladding mechanical interaction, which may shorten the cladding lifetime.

Fission gases are considered to be released from the fuel when they reach any space that is connected to the free volume within the fuel pin. Gas connection zones include the fuel/cladding gap and the porosity within the fuel which communicates directly with the gap (open porosity). The following is assumed regarding the gas in the closed bubbles and that in the free volumes (plenum above the fuel slug and open porosity within the fuel slug):

1- Once the gas is released into the free volumes, its probability of reentering the closed bubbles is zero.
2- The gas pressure in open porosity is equal to that in the plenum. Because of the insolubility of xenon and krypton in solids, there is no direct influence of plenum pressure on the rate of gas escape from the fuel.
3- While the fission gas within the closed bubbles tends to cause swelling, the fission gas in the free volume promotes shrinkage by pressurizing the solid and thereby encouraging collapse of the internal porosity.

2.2. Fission Gas Release and Swelling Behavior of Metal Fuel

When the U-Pu-10Zr metallic fuel is irradiated at around 600°C or higher, fission gas bubbles nucleate and grow at a rate much higher than the ceramic $UO_2$ fuel due to a lower gas-solid stress level and higher gas diffusivity characteristics. Figure-2.1 shows the fractional fission gas release as a function of burnup for the ANL U-Pu-10Zr irradiation database [9]. Fission gases at the fuel rod of peak power start to be released through open channels formed by interconnection of the bubbles at a burnup of about 0.5%. Then, the fractional fission gas release increases to 70% when the burnup reaches 4-5 at % burnup and levels off at about 80% at 10 at % burnup.
Figure-2.1: Fission gas release of ANL fuel irradiation tests [9]

Many models have been developed for fission gas release and swelling behavior of the U-Pu-10Zr metallic fuel for liquid metal fast reactors. The model in the LIFE-METAL [3] code is empirical, and calculates the fission gas release by a simple correlation using burnup, porosity and temperature. It does not explicitly consider fission gas bubbles. The ALFUS [5] model considers the bubble formation and growth based upon a model originally developed for $UO_2$ fuel. Therefore, it is assumed that fission gases are generated inside the fuel grains and then diffuse to the grain boundaries to nucleate a new bubble or be absorbed by an existing bubble at the grain boundaries. However, in metal fuel the fission gas bubbles could nucleate at the phase boundaries inside grains as well as at the grain boundaries. The phase boundaries are distributed quite randomly inside the grains in U-Pu-10Zr metallic fuel. Therefore, the effect of grain size on fission gas behavior in metallic fuel may not be as important as in $UO_2$ fuel.

2.3. Modeling of the Fission Gas Behavior

The FEAST user can select either a mechanistic fission gas release model or an empirical one.

Mechanistic Model

The GRSIS model [9] is adopted to model the fission gas behavior of the metallic fuel in the FEAST code. A schematic diagram of the fission gas bubble nucleation and growth in the metallic fuel according to the GRSIS approach is shown in Fig.2.2. Fission gas atoms are generated by fission, and then form (nucleate) new bubbles or diffuse into existing bubbles. The bubbles are assumed to nucleate uniformly from the gas atoms in the metallic fuel matrix, since they nucleate at both the grain boundaries and the phase boundaries which are randomly distributed inside grain. The closed bubbles can grow by the diffusion of newly created fission gas atoms, and are classified into two groups depending on their sizes. Small bubbles and large bubbles are defined as having 0.5 and 10 micron radius, respectively. The third group of bubbles is the open bubbles (or open pores), which are connected to each other and open to the external free space. They are assumed to be same of the type as the closed bubbles. When a closed
bubble-i becomes an open bubble, it is assumed to be transformed into bubble-3i. When the fuel matrix swelling due to the closed bubbles reaches a threshold value, it is assumed that a certain fraction of the bubbles become interconnected and release their gas into the free volume (i.e., they become open bubbles).

Figure-2.2: Fission gas and bubble movement model

According to the bubble classification given in Figure-2.2, the behavior of the fission gas atoms and bubbles can be described as follows.

Bubbles in group 1 are nucleated from the fuel matrix. They can collide with each other by both diffusion and growth, to become bubbles in group 2, with the probability of this process depending on the difference of the bubble sizes between groups 1 and 2. When bubbles in group 1 or 2 collide with bubbles in group 3, they become part of group 3. Bubbles in group 3 (open bubbles) are designated as bubbles-31 and 32, depending on the bubble group from which it came. Open bubbles are assumed not to move (diffuse) since gases in the open bubbles are released into the free volume.
Empirical Model

The upper part of the fission gas release data band given in Figure-2.1 represents the typical peak fuel pin fission gas release behavior of EBR-II reactor. The data has been fitted to an exponential function as given in Eq.2.1 and shown in Figure-2.3.

\[
f = \begin{cases} 
0 & \text{Bu < 0.8} \\
0.8 \times \exp \left( -\frac{Bu}{1.8} \right) & \text{Bu \geq 0.8} 
\end{cases}
\]  

(2.1)

\(f\): Fission gas release fraction  
\(\text{Bu}\): Average fuel rod burnup (at %)

This type of a relation is recommended for use only in rough comparative analyses. Because the metal fuel fission gas release behavior shows strong dependency on axial power profile, operating temperature and linear heat rate, such a simplified relation should not be used for studies, in which accuracy is required.

Finally note that the empirical treatment has been developed only for fission gas release, whereas the swelling behavior of the fuel is simulated with the GRSIS model, even when the FG release empirical correlation is selected.

Figure-2.3: Empirical correlation for fission gas release

2.4. Governing Equations for GRSIS Model

The governing equations for the gas atoms and bubble groups are:

\[
\frac{dC_g}{dt} = YF - (J_{g1} + J_{g2} + J_{g3}) - J_{b,nucl},
\]

(2.2)
\[
\frac{dC_{gb1}}{dt} = J_{b,nucl} + J_{g1} - (ab_{12} + ab_{13}) - (gab_{12} + gab_{21} + gab_{13}) - f_{12}(ab_{11} + gab_{11}) \tag{2.3}
\]
- instantaneous release by bubble interconnection at threshold closed bubble swelling

\[
\frac{dC_{gb2}}{dt} = J_{g2} + ab_{12} + gab_{12} + gab_{21} + f_{12}(ab_{11} + gab_{11}) - ab_{23} - gab_{23} \tag{2.4}
\]
- instantaneous release by bubble interconnection at threshold closed bubble swelling.

\[
\frac{dC_{gb3}}{dt} = J_{g3} + ab_{13} + ab_{23} + gab_{13} + gab_{23} \tag{2.5}
\]
+ instantaneous release by bubble interconnection at threshold closed bubble swelling.

\(C_g\): Gas atom concentration in the fuel matrix (atoms/m^3)

\(C_{gb1}\): Concentration of gas atoms present as bubble-1 in the matrix (atoms/m^3)

\(C_{gb2}\): Concentration of gas atoms present as bubble-2 in the matrix (atoms/m^3)

\(C_{gb3}\): Concentration of gas atoms present as bubble-3 in the matrix (atoms/m^3)

\(Y\): Fission yield of gas atoms is assumed to be 0.25 atoms/fission [12]

\(F\): Fission density (fission/s/m^3)

\(J_{g1}\): Gas diffusion rate to bubble-i (atoms/s/m^3),

\(J_{b,nucl}\): Bubble-1 nucleation rate (atoms/s/m^3),

\(ab_{ij}\): Transfer rate of bubble-i into bubble-j by bubble diffusion (atom/s/m^3),

\(gab_{ij}\): Transfer rate of bubble-i into bubble-j by radial growth of bubble-i (atom/s/m^3),

\(f_{i,i+1}\): Transition probability of bubble-i into bubble-(i+1) by collision with bubble

The relation between bubble density, \(N_{bi}\), and the total gas atom density of bubble-i, \(C_{gbi}\) is

\[
C_{gbi} = \rho_{gi} N_{bi} \tag{2.6}
\]

\(\rho_{gi}\): Density of gas atom in a bubble-i (atoms/bub-i)

\(N_{bi}\): the bubble-i concentration (bub-i/m^3).

\[
\rho_{gi} = \left( B + \left[ \frac{2\gamma}{kT} \frac{1}{R_i} + \frac{\sigma}{kT} \right]^{-1} \right) \times V_{bi} \tag{2.7}
\]

\(B\): Van der Waals Parameter (85 \times 10^{-30} \text{ m}^3/\text{atom})

\(\gamma\): Surface Tension = 0.8 N/m from refs. [8] and [13]

\(R_i\): Radius of Bubble-i

\(\sigma\): Hydrostatic Stress

\(k\): Boltzman Constant

\(V_{bi}\): Volume of the Bubble-i (m^3/bubble-i)
The hydrostatic stress is given as follows:

\[ \sigma_h = -\frac{\sigma_r + \sigma_\theta + \sigma_z}{3} \]  

(2.8)

The collision rate of a closed bubble-i with the open pores by diffusion and growth are given by, respectively:

\[ ab_{i3} = ab_{i31} + ab_{i32} \]  

(2.9)

\[ gab_{i3} = gab_{i31} + gab_{i32} \]  

(2.10)

Then, the balance equations of open pores are as follows:

\[ \frac{dC_{gb_{31}}}{dt} = \rho_{g1} \frac{d}{dt} N_{b_{31}} = ab_{i31} + ab_{i32} + gab_{i31} + gab_{i32} \]  

(2.11)

\[ \frac{dC_{gb_{32}}}{dt} = \rho_{g2} \frac{d}{dt} N_{b_{32}} = ab_{i32} + ab_{232} + gab_{231} + gab_{232} \]  

(2.12)

The specific parameters of the gas atoms and bubbles in the above equations can be obtained as follows.

### 2.5. Bubble-1 Nucleation Rate

Bubble-1 nucleation rate, \( J_{b_{1\text{nucl}}} \) is obtained from the bubble nucleation constant and the gas atom concentration in the fuel matrix, such that

\[ J_{b_{1\text{nucl}}} = k_{b_{1\text{nucl}}} C_g \rho_{g1} \]  

(2.13)

\( k_{b_{1\text{nucl}}} \) : Bubble-i nucleation constant (bub-1/s atom)

### 2.6. Gas Diffusion

Diffusion of gas atoms into the bubbles can be calculated from the analytical solution in the case that gas atoms diffuse into a spherical sink. The atomic flux into bubble-i by diffusion, \( J_{gi} \), can be calculated as a function of the gas diffusion constant and the concentrations of gas and bubbles as follows:

\[ J_{gi} = k_{gi} C_g N_{bi} \]  

(2.14)

\[ k_{gi} = E_{ghi} (4\pi r_{bi}) D_g \]  

(2.15)

\( k_{gi} \) : Gas diffusion constant to bubble-i (m³/s),

\( E_{ghi} \) : Empirical bias factor for gas diffusion to the bubble-i,
$r_{bi}$: Radius of bubble-i (m)
$D_g$: Diffusion coefficient of gas atom (m²/s)

$$D_g = D_{go} \exp\left(-\frac{Q_g}{RT}\right)$$  \hspace{1cm} (2.16)

$D_{go}$: Diffusion Constant (m²/s)
$Q_g$: The activation energy for a mole of jumps = 52000 cal/g-mol from Ref. [14]
$R$: Gas Constant (1.98 cal/g-mol/K)

In Ref. [9] it is noted that there exist large discrepancies in reported gas diffusion coefficients, by up to a factor of 100. In this study, the diffusion factor, $D_{go}$, is being used as one of the fitting parameters to match the calculated and measured fission gas release and swelling behavior of the metallic fuel. The selected values are given in Table-2.2. Comparing the metal fuel diffusion coefficient with the oxide fuel in Table-2.1, the metal fuel has many orders of magnitude higher diffusion coefficient within the temperature range of interest.

Table-2.1: Comparison of metal and oxide fuel diffusion coefficients

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>Metal Fuel (FEAST)</th>
<th>$UO_2$ Fuel [12]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>9.9E-15</td>
<td>3.0E-24</td>
</tr>
<tr>
<td>900</td>
<td>5.4E-16</td>
<td>1.9E-26</td>
</tr>
<tr>
<td>800</td>
<td>1.4E-17</td>
<td>3.3E-29</td>
</tr>
<tr>
<td>700</td>
<td>1.3E-19</td>
<td>9.3E-33</td>
</tr>
</tbody>
</table>

2.7. Coalescence by Bubble Diffusion

The bubble diffusion coefficient can be calculated as a function of surface diffusion coefficient ($D_s$) and bubble characteristics.

$$D_{si} = \frac{3a_o^4}{2\pi r_{bi}^4} D_s$$  \hspace{1cm} (2.17)

$D_{si}$: Diffusion coefficient of bubble-i (m²/s)
$a_o^2$: Area occupied by a gas atom at the bubble surface (m²).

Surface diffusion coefficient, $D_s$ can be obtained by [9]

$$D_s = 1000D_g$$  \hspace{1cm} (2.18)

Bubbles can collide by diffusional movement so that the collision constant of bubble-i and bubble-j by bubble diffusion, is $k_{ij}$ (m³/s)
\[ k_{ij} = E_{bh} 4\pi (r_{bi} + r_{bj})(D_{bi} + D_{bj}) \quad (2.19) \]

\( E_{bh} \): Empirical bias factor for bubble diffusion to other bubbles
\( k_{ij} \): Collision or integration constant of bubble-i into bubble-j (m³/s).

Then, the transfer rate of bubble-i into bubble-j by bubble diffusion is

\[ ab_{ij} = k_{ij} N_{bi} N_{bj} \rho_{gi} \quad (2.20) \]

Jump or transition rate of bubble-i into bubble-i+1 after the collision with bubble-i can be obtained by

\[ ab_{ii} = k_{ii} N_{bi}^2 2 \rho_{gi} \quad (2.21) \]

\( ab_{ij} \): Jump or transition rate of bubble-i into bubble-i+1 (atoms/m³/s).

If two bubbles from the same group coalesce, they will be transformed into the higher size bubble with a certain probability given by

\[ f_{i,i+1} = \frac{2 \rho_{gi}}{\rho_{gi+1}} \quad (2.22) \]

### 2.8. Coalescence by Bubble Growth

When the number density of bubble-i is \( N_{bi} \), the average distance between bubble-i’s can be calculated by assuming faced-centered cubic (FCC) lattice. As a result, the average distance between bubbles can be obtained by

\[ l_j = 1.122 N_{bj}^{-1/3} \quad \text{(m)} \quad (2.23) \]

When there is a bubble-i in the space where bubble-j’s are evenly distributed at the number density, \( N_{bj} \) with their distance, \( l_j \), the average distance between the centers of bubble-i and bubble-j becomes 0.5\( l_j \) which we calculated by means of a simple Monte Carlo simulation of randomly distributed bubbles in 3D space. Note that Ref. [9] recommended using 0.25\( l_j \) for the average distance between the centers of bubble-i’s, which was based on a (likely incorrect) 2D calculation.

The probability per unit time of a closed bubble-i colliding with a closed bubble-j due to radial growth of bubble-i, \( P_{ij} \) is
\[ P_{ij} = \frac{\text{radial growth of bubble-i}}{\text{distance between the surfaces of bubble-i and j}} = \frac{\Delta r_{bi}}{0.5l_j - (r_{bi} + r_{bj})} \quad (1/\text{sec}) \tag{2.24} \]

\( \Delta r_{bi} \): Change rate of radius of bubble-i

\( r_{bi} \): Radius of bubble-i

\( r_{bj} \): Radius of bubble-j

On the other hand, this expression has been modified for the collision probability per unit time of a closed bubble-i with an open bubble-j as follows:

\[ P_{ij} = \frac{\Delta r_{bi}}{d_l l_j} \tag{2.25} \]

Thus, it is assumed that the probability is proportional to the radial growth of bubble-i and inversely proportional to the average distance between two open bubble-j’s. \( d_l \) is one of the fitting parameters to match the predicted and measured fission gas release and swelling behavior of the fuel. Its value is given in Table-2.2.

The radial growth of bubble-i by gas diffusion can be calculated from the following equations. The volume increase (\( \Delta V_{bi} \)) and radial growth (\( \Delta r_{bi} \)) of bubble-i by gas diffusion are:

\[ \Delta V_{bi} = \frac{J_{gbi} V_{bi}}{C_{gbi}} \tag{2.26} \]

\[ \Delta r_{bi} = \frac{\Delta V_{bi}}{4\pi r_{bi}^2} = \frac{J_{gbi} r_{bi}}{3C_{gbi}} \tag{2.27} \]

Then, the collision (or integration) rate of bubble-i with bubble-j by radial growth of bubble-i, \( g_{ab_{ij}} \) (atoms/m³/s) can be calculated as

\[ g_{ab_{ij}} = P_{ij} C_{gbk} \quad k = \min(i, j) \tag{2.28} \]

Thus, a certain fraction of smaller bubbles will become larger bubbles.

In parallel with coalescence by bubble diffusion process, when two bubbles from the same group coalesce by growth, they will be transformed into the higher size bubble with a certain probability given by

\[ f_{i,i+1} = \frac{2\rho_{gi}^i}{\rho_{gr,i+1}} \tag{2.29} \]

**2.9. Open Bubble Surface Area and Volume Correction**

When a bubble-i is incorporated into the open bubble group, it is designated as open bubble-3i. After absorption of bubble-i by an open bubble, the gases in bubble-i are assumed to be released
into the free space which has a lower pressure than bubble-i and therefore its surface area and volume may decrease. Therefore, when a bubble-i becomes an open bubble, its volume and surface area may be reduced to certain fractions of the initial values such as \( f_v \) and \( f_s \), respectively. In Ref. [9], \( f_v \) is assumed to be equal to one and \( f_s \) has been used as a fitting function to shape the high burnup behavior of the fission gas release curve. Consistently with Ref. [9], the FEAST code assumes \( f_v = 1 \). The value of \( f_s \), yielding the most accurate fit of the experimental fission gas release curve is given in Table-2.2.

### 2.10. Swelling

The swelling volume of the closed bubbles, \( S_c \) is

\[
S_c = V_1 + V_2
\]

\[
V_i = \frac{4}{3} \pi r_{bi}^3 N_{bi}
\]

When swelling due to the closed bubbles reaches the threshold value \( S_{th} \) for bubble interconnection and opening to the external free space, a certain fraction of the closed bubbles become instantaneously open. Therefore, when \( S_c \geq S_{th} \) the volume and surface area of the closed and open bubbles change as follows, respectively:

\[
V_i \rightarrow (1 - f_{th}) V_i \quad i = 1, 2
\]

\[
V_3 = f_{th} f_v (V_1 + V_2)
\]

\[
A_i \rightarrow (1 - f_{th}) A_i \quad i = 1, 2
\]

\[
A_3 = f_{th} f_s (A_1 + A_2)
\]

\( f_{th} \): Fraction of closed bubbles that interconnect to the open bubbles when the threshold swelling is exceeded

\( f_v \): Fractional surface area of a closed bubble after interconnecting to the open bubbles,

\( f_s \): Fractional volume of a closed bubble after interconnected to the open bubbles.

The swelling volume by the open and closed bubbles is

\[
S_g = V_1 + V_2 + V_3
\]

To obtain the total fuel swelling, one needs to account for the swelling due to solid fission products. It is recommended in Ref. [5] that swelling rate due to solid fission products be assumed to be 1.5 \% per unit burnup (at \%).

Thus, the total swelling becomes as follows
Then the fission gas release can be calculated as follows:

\[ FGR = 0, \quad S_g < S_{th} \]

\[ = f_{th}(C_{gb1} + C_{gb2}), \quad S_g = S_{th} \]

\[ = C_{gb3}, \quad S_g > S_{th} \]  

(2.38)

2.12. Critical review of the simplifying assumptions made by the GRSIS model

As stated previously, the fission gas release and fuel swelling model in FEAST is based on the GRSIS model. The parameters in GRSIS (i.e., bubble size, bubble nucleation constant, threshold swelling, fraction of bubbles interconnecting at the threshold swelling, volume and surface area correction factors for open bubbles) were used by its developers as fitting parameters, to match the generic fission gas release behavior of the metal fuel given in Figure-2.1. The following simplifying assumptions were made in the original development of GRSIS:

1- The fuel is at 550 °C

_Metal fuel usually operates within (400-750°C) temperature range. However, mechanical properties and phases change significantly within this temperature range; so this assumption may lead to major inaccuracies._

2- Anisotropic fuel slug deformation is neglected.

_Metal fuel shows strongly anisotropic fuel slug deformation due to grain boundary tearing (in U-Zr fuel) and radial cracks (in U-Pu-10Zr fuel). Thus, an isotropic swelling behavior may seriously overestimate the time at which the fuel/cladding contact occurs._

3- After the contact stress reaches the fuel yield stress, further swelling of the fuel is compensated for by the fuel plastic strains.

_Fuel plastic behavior depends on the equivalent stress. Due to the very high creep rate of metal fuel, the equivalent stress stays at a level lower than the yield stress, even when the contact stress exceeds the yield stress of the fuel, so plastic behavior is not encountered. Note that this conclusion is consistent with the prediction of the ALFUS code [5]._

4- As the fuel is assumed to freely expand in the axial direction, fuel clad mechanical interaction is neglected even after all open pores are filled with solid fission products at high burnup.

_The experimental data [1] do not support this assumption._
The threshold swelling is assumed to be 20%. According to Ref. [5] 85 % smear density fuel only swells by 17 % and at the end of life, and 60 % of the fission gases are released to the plenum. This behavior can not be explained by GRSIS.

Based on these observations, some of the original GRSIS parameters were changed when the model was implemented in FEAST. Table-2.2 shows the important parameters for the fission gas release and swelling modules in FEAST and GRSIS.

Table-2.2: Reference Data for FEAST and GRSIS

<table>
<thead>
<tr>
<th>Variable</th>
<th>FEAST</th>
<th>GRSIS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radius of Bubble-1 (μm)</td>
<td>0.5 [15]</td>
<td>0.5</td>
</tr>
<tr>
<td>Radius of Bubble-2 (μm)</td>
<td>10 [15]</td>
<td>12.5</td>
</tr>
<tr>
<td>Surface Tension (N/m)</td>
<td>0.8 [8], [13]</td>
<td>1.0</td>
</tr>
<tr>
<td>Gas Diffusion Factor, $D_{go}$ (m²/s) (fitting factor)*</td>
<td>2.3×10⁻³</td>
<td>9.5×10⁻⁸</td>
</tr>
<tr>
<td>Activation Energy of the gas diffusion, $Q_g$ (cal/g-mol)</td>
<td>52000 [14]</td>
<td>32000</td>
</tr>
<tr>
<td>Surface Diffusion Factor, $D_{so}$ (m²/s)**</td>
<td>2.3</td>
<td>9.5×10⁻⁵</td>
</tr>
<tr>
<td>Activation Energy of the gas diffusion, $Q_s$ (cal/g-mol)**</td>
<td>52000</td>
<td>32000</td>
</tr>
<tr>
<td>Area occupied by surface molecule, $a_o^2$ (m²)</td>
<td>9×10⁻²⁰ [9]</td>
<td>9×10⁻²⁰</td>
</tr>
<tr>
<td>Bubble-1 Nucleation constant $k_{nuc}$ (bub-1/s atom)</td>
<td>1×10⁻²⁰ [9]</td>
<td>1×10⁻²⁰</td>
</tr>
<tr>
<td>Bias factor of gas diffusion to closed bubble, $E_{gh1}$, $E_{gh2}$</td>
<td>1.0 [9]</td>
<td>1.0</td>
</tr>
<tr>
<td>Bias factor of gas diffusion to open bubble, $E_{gh3}$</td>
<td>1.0 [9]</td>
<td>1.0</td>
</tr>
<tr>
<td>Bias factor of bubble diffusion to closed bubble, $E_{bh1}$, $E_{bh2}$</td>
<td>1.0 [9]</td>
<td>1.0</td>
</tr>
<tr>
<td>Bias factor of bubble diffusion to open bubble, $E_{bh3}$</td>
<td>1.0 [9]</td>
<td>1.0</td>
</tr>
<tr>
<td>Threshold Closed Bubble Swelling ($S_{sh}$)</td>
<td>0.1 [5]</td>
<td>0.2</td>
</tr>
<tr>
<td>Fraction of interconnected bubbles at threshold swelling, $f_{sh}$</td>
<td>0.01 [5]</td>
<td>0.3</td>
</tr>
<tr>
<td>Correction factor for bubble volume after becoming open bubble, $f_c$</td>
<td>1.0 [9]</td>
<td>1.0</td>
</tr>
<tr>
<td>Correction factor for bubble volume after becoming open bubble, $f_s$</td>
<td>0.3</td>
<td>0.6</td>
</tr>
<tr>
<td>Open bubble formation coefficient, $d_i$ (fitting factor)*</td>
<td>0.232</td>
<td>N/A</td>
</tr>
</tbody>
</table>

* $D_{go}$, $f_s$ and $d_i$ are the fitting parameters to match the fission gas release and swelling behavior of the metal fuel.
** Surface diffusion coefficient is assumed to be 1000 times the gas diffusion coefficient [9].

Table-2.3 shows a comparison of fitted diffusion coefficient and reference diffusion coefficient. The reference gas diffusion coefficient given in the GRSIS description was evaluated at high temperatures (>950 K) in which the single gamma phase is dominant within the fuel. FEAST and GRSIS diffusion coefficients seem to match well within the range of the GRSIS diffusion.
3. Modeling of Constituent Redistribution in U-Zr and U-Pu-Zr Fuel

3.1. Introduction

Fuel constituent migration, which has been observed in irradiated metallic fuel, affects the fuel slug material properties such as solidus and liquidus temperatures, thermal conductivity, mechanical properties such as modulus of elasticity, fuel cladding eutectic reaction rate, and radial power density profile, particularly in enriched uranium alloy fuels. Thus, modeling of constituent redistribution is essential when developing a metallic fuel performance code.

Upon constituent redistribution the microstructure of irradiated metal fuel exhibits three distinct concentric zones, a zirconium-enriched central zone, a zirconium-depleted and uranium-enriched intermediate zone, and a zirconium-enriched zone on the outer periphery. The migration of zirconium atoms is driven by the chemical activity gradients that develop with the radial temperature distribution creates multiple crystalline phases of the fuel alloy.

3.2. Major Assumptions

The model given by Kim in [16] is implemented into the FEAST code. It is based on thermo-transport theory. The following assumptions are adopted from [16] and [17].

1- Local equilibrium assumption. Phase changes (determined by a change in local concentration and/or temperature) are assumed to occur very rapidly compared with the migration of alloy constituents.
2- Pu does not migrate, thus the U and Zr concentration profiles are opposite.
3- The equilibrium phases of the ternary U-Zr-Pu system are described by using a quasi-binary U-Zr phase diagram (with constant Plutonium content), which is produced from ternary phase diagrams, assuming uniformity of Plutonium in each phase of the multiphase zones.
4- The minimum allowed Zirconium concentration in the Zirconium depleted middle region is 5 at % due to the solubility limit. When the concentration of a radial node drops below 5 at % further diffusion from this node to the adjacent nodes is not allowed. This limit corresponds to depletion of the matrix $\gamma$ phase in the middle region.
The cross-terms, relating the flux of one species to the chemical potential gradient of another species, in the constitutive equations are negligible.

The presence of plutonium in the alloy at levels greater than 8 wt% enhances uranium and zirconium migration by an order of magnitude.

Only radial migration of zirconium is considered. Axial temperature gradients are relatively small and axial zirconium redistribution has not been observed experimentally.

The radial power distribution in the fuel slug is assumed to be directly proportional to the actinide concentration distribution.

The plutonium uniformity assumption is partly justified on the basis of the following observations from Ref. [17]:

1- Plutonium shows relatively large miscibility in various phases of the system in the in-reactor temperature range.
2- Irradiation data of the ternary system show that redistribution of plutonium is minimal.
3- Theoretical calculations show that the equilibrium tie lines in the vicinity of the ternary fuel compositions of interest run approximately parallel to the constant plutonium line in the isothermal sections of the U-Pu-Zr ternary phase diagram for the in-reactor temperature range.

3.3. Fundamental Data

The phase diagrams, diffusion coefficients and effective heats of transport of zirconium and uranium in the ternary alloy are the fundamental data required in this model.

3.3.1. Phase Diagrams

The thermochemical driving force for constituent migration is determined by the various phases present in the fuel at the operating temperatures, an accurate estimate of the phase diagram is essential to the development of the fuel restructuring model. Assuming a fixed Pu concentration of 19 wt %, a simplified pseudo-binary phase diagram was developed for U-Pu-Zr alloys [16], which is based on the available ternary phase diagrams for the temperatures of interest. The U-Zr phase diagram is given in Ref. [18].

Figure-3.1 shows a generic pseudo-binary phase diagram for U-Pu-Zr alloys. The solubility lines 1 through 6 are linearly interpolated between U-Zr and U-19Pu-Zr fuels, and are given as functions of temperature in Table-3.1. This approach is adopted to examine the fuel for varying plutonium contents (0-26 wt %). Note that, similar approaches are recommended in Ref. [16] and [17].
Figure-3.1: Pseudo Binary Phase Diagram for U-Pu-Zr Fuel for fixed Pu content [16]

Table-3.1: Solubility Lines

<table>
<thead>
<tr>
<th>Solubility Line</th>
<th>U-Zr [18]</th>
<th>U-19Pu-Zr [16]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$x_{Zr} = 0.01$</td>
<td>$x_{Zr} = 0.001 + (T-773.15)/2968.8$</td>
</tr>
<tr>
<td>2</td>
<td>$x_{Zr} = \frac{T-813.15}{935.15-813.15} \times (0.588-0.676) + 0.676$</td>
<td>$x_{Zr} = 0.539 - \frac{T-773.15}{9500.0}$</td>
</tr>
<tr>
<td>3</td>
<td>$T= 935.15$</td>
<td>$T= 868.15$</td>
</tr>
<tr>
<td>4</td>
<td>$x_{Zr} = 0.01$</td>
<td>$x_{Zr} = 0.032 - \frac{T-868.15}{6111.1}$</td>
</tr>
<tr>
<td>5</td>
<td>$x_{Zr} = \frac{T-935.15}{965.15-935.15} \times (0.444-0.588) + 0.588$</td>
<td>$x_{Zr} = 0.529 - \frac{T-868.15}{440.5}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$x_{Zr} = 0.445 - \frac{T-905.15}{200}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$T &lt; 905$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$T \geq 905$</td>
</tr>
<tr>
<td>6</td>
<td>$T= 965.15$</td>
<td>$T= 923.15$</td>
</tr>
</tbody>
</table>

$x_{Zr}$: Zirconium molar fraction  
$T$: Temperature (K)

### 3.3.2. Enthalpy of Solution

The enthalpy of solution of Zirconium in $\alpha$ and $\beta$ phases is negligible [18]. On the other hand, the enthalpy of solution of the $\gamma$ and $\delta$ matrix phases are given in [16] as follows:

$$\Delta H_s = G^E_{Zr} - T \frac{\partial G^E_{Zr}}{\partial T}$$

(3.1)
\[ G^{E}_{Zr} = x^2_U (43764.5) - 22.0T - 44174.7x_{Zr} + 38635.1x^2_{Zr} + x^2_{Pu} (6574.7) + x_U x_{Pu} (15884.0) \]

\[ \Delta \overline{H}_s : \text{Enthalpy of solution (J/mol)} \]

\[ G^{F}_{Zr} : \text{Free energy of Zirconium (J/mol)} \]

\[ x_U : \text{Uranium mole fraction} \]

\[ x_{Zr} : \text{Zirconium mole fraction} \]

\[ x_{Pu} : \text{Plutonium mole fraction} \]

\[ T : \text{Temperature (K)} \]

### 3.3.3. Effective Heat of Transport

The heats of transport for each phase field were obtained by a best fit in Ref. [16] and Ref. [13] to reproduce the measured redistribution profile of U-Pu-Zr and U-Zr fuels, respectively. The results are given in Table-3.2.

Table-3.2: Effective heat of transport

<table>
<thead>
<tr>
<th>Phase</th>
<th>U-&gt;8Pu-Zr</th>
<th>U-Zr</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \alpha ) (kJ/mol)</td>
<td>200</td>
<td>0.0</td>
</tr>
<tr>
<td>( \delta ) (kJ/mol)</td>
<td>160</td>
<td>0.0</td>
</tr>
<tr>
<td>( \beta ) (kJ/mol)</td>
<td>450</td>
<td>0.0</td>
</tr>
<tr>
<td>( \gamma ) (kJ/mol)</td>
<td>-200</td>
<td>-150</td>
</tr>
</tbody>
</table>

Note that the effective heat of transport values are linearly interpolated between their values for the U-Zr and U-8Pu-Zr alloys. For plutonium concentrations above 8 wt %, it is assumed that the effective heat of transport values stay constant.

The negative heat of transport in the \( \gamma \) phase generates the driving force for zirconium to migrate towards the center (hotter) region of the fuel slug, even after zirconium accumulation in the center region creates an opposing concentration gradient. The positive heats of transport for the \( \alpha \), \( \beta \) and \( \delta \) phases let zirconium migrate toward the fuel surface.

### 3.3.4. Effective Interdiffusion Coefficients

The interdiffusion coefficient of Zirconium for U-Pu-Zr is not available. Therefore it was estimated to best fit the experimental data in Ref. [16].

The influence of plutonium addition and irradiation on the zirconium migration kinetics is handled by some enhancement factors. The existence of plutonium in a ternary fuel has been assumed to increase the interdiffusion coefficient [16], and the diffusion coefficients for each phase have been found by matching the experimental data for the T-179 fuel rod [16]. The results are given in Table-3.3 for the U-Zr alloy [18] and Table-3.4 for the U-Pu-Zr alloy with Plutonium weight fraction greater than 0.08. The gamma phase diffusion coefficient given in Ref. [18] depends on the zirconium molar fraction. Note that the quadratic dependency of the
diffusion coefficient on the zirconium mole fraction is preserved for both U-Zr and U-Pu-Zr fuels.

Table-3.3: Diffusion Coefficients for U-Zr alloy phases

<table>
<thead>
<tr>
<th>Phases</th>
<th>$D_o$ (m²/s)</th>
<th>$Q$ (kJ/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>$2 \times 10^{-7}$</td>
<td>170</td>
</tr>
<tr>
<td>$\delta$</td>
<td>$2 \times 10^{-7}$</td>
<td>150</td>
</tr>
<tr>
<td>$\beta$</td>
<td>$5.7 \times 10^{-5}$</td>
<td>180</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>$10^{(-5.1-8.05x_{Zr}+9.13x_{Zr}^2)}$</td>
<td>$128-107x_{Zr}+174x_{Zr}^2$</td>
</tr>
</tbody>
</table>

Table-3.4: Diffusion Coefficients for U-Pu-Zr alloy phases (Pu is > 8 wt %)

<table>
<thead>
<tr>
<th>Phases</th>
<th>$D_o$ (m²/s)</th>
<th>$Q$ (kJ/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>$2 \times 10^{-6}$</td>
<td>170</td>
</tr>
<tr>
<td>$\delta$</td>
<td>$2 \times 10^{-6}$</td>
<td>150</td>
</tr>
<tr>
<td>$\beta$</td>
<td>$4.0 \times 10^{-4}$</td>
<td>180</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>$10^{(-5.1-8.05x_{Zr}+9.13x_{Zr}^2)}$</td>
<td>$128-107x_{Zr}+174x_{Zr}^2$</td>
</tr>
</tbody>
</table>

The Zr diffusion coefficient for the dual phase $\beta + \gamma$ is calculated by the diffusion coefficient of the $\beta$ and $\gamma$ phases from Table-3.4 multiplied by a factor of 10 depending on whether the $\beta$ or $\gamma$ phases exceed 50 %, respectively.

3.4. Model Development

The one dimensional continuity equation for zirconium can be expressed in cylindrical coordinates as follows:

$$\frac{\partial C_{Zr}}{\partial t} = -\frac{1}{r} \frac{\partial (rJ_{Zr})}{\partial r} + s$$  \hspace{1cm} (3.2)

$C_{Zr}$: Zirconium concentration

$J_{Zr}$: Interdiffusion flux

$s$: Zirconium production rate by fission. The Zirconium yield is 0.2 for the fission of Plutonium.

Within a single $\gamma$ phase field the zirconium interdiffusion flux is given by

$$J_{Zr} = -D_{Zr}^{\text{eff}} \left( \frac{\partial C_{Zr}}{\partial r} + \frac{Q_{Zr}C_{Zr}}{RT^2} \frac{\partial T}{\partial r} \right)$$  \hspace{1cm} (3.3)

$D_{Zr}^{\text{eff}}$: Effective interdiffusion coefficient of zirconium in $\gamma$ phase

$Q_{Zr}$: Heat of transport of zirconium in $\gamma$ phase
When the concentration gradient becomes equal to the chemical potential gradient, the diffusion in the $\gamma$ phase inherently stops.

Within a dual phase field such as $\alpha + \delta$ and $\beta + \gamma$, the driving force for diffusion is affected by the solubility of zirconium in the precipitation phases.

$$J_{Zr} = -V_1 D_{Zr,1}^eff C_{Zr,1} \frac{\Delta H_{s,1} + Q_{Zr,1}}{RT^2} \frac{\partial T}{\partial r} - V_1 D_{Zr,2}^eff C_{Zr,2} \frac{\Delta H_{s,2} + Q_{Zr,2}}{RT^2} \frac{\partial T}{\partial r}$$  \hspace{1cm} (3.4)

$V_i$: Volume fraction of a phase-$i$

Note that subscript “1” represents the first phase and subscript “2” represents the second phase.

Discretization of the radial continuity equation results in

$$C_{Zr}^i = C_{Zr}^{i-1} + 2\Delta t \frac{J_{+}^{i-1} \times rc^{i-1} - J_{+}^{i} \times rc^{i} + J_{-}^{i} \times rc^{i} - J_{-}^{i-1} \times rc^{i+1}}{(r^i)^2 - (r^{i-1})^2} + s\Delta t$$  \hspace{1cm} (3.5)

$rc^i$: Weight center of the radial node-$i$,
$r^i$: Outer boundary of node-$i$.

$J_{+}^i$: Positive zirconium current emerging from node-$i$ towards outer part of the fuel. Its sign is positive.

$J_{-}^i$: Negative zirconium current emerging from node-$i$ towards inner part of the fuel. Its sign is negative.

### 3.5. Boundary Conditions

The boundary conditions are that the negative current at the origin of the fuel slug as well as the positive current at the surface of the fuel slug are zero. That is:

at $r=0.0$ \hspace{0.5cm} $J_{-}^i = 0.0$  \hspace{1cm} (3.6)

at $r=R$ \hspace{0.5cm} $J_{+}^i = 0.0$  \hspace{1cm} \text{(Zirconium cannot migrate out of the fuel)}  \hspace{1cm} (3.7)

### 3.6. Model Verification

This section reports comparisons between the model predictions and experimental measured data for pin T179. Predictions of the redistribution profiles in the fuel for the 4S reactor [16] are also
compared to Kim’s Model predictions. Finally, a benchmark has been accomplished against data for the X447 U-Zr fuel assembly irradiated in EBR-II.

### 3.6.1. T179 Benchmark

Figure-3.2 gives the fuel pin data and the fuel temperature distribution of T-179 estimated based on both experimental data and calculation from fuel microstructure observations [16]. The experimental data for the zirconium radial distribution at 230 mm from the bottom of the fuel slug are given in Figure-3.3. The calculation for both Kim’s model and the FEAST code has been performed for the given temperature profile in Figure-3.2. The FEAST results in Figure-3.3 which is performed at constant temperature given in Figure-3.2, consistently with Kim Model calculation, are matching the experimental data reasonably well.

![Figure-3.2: T-179 fuel data and temperature profile at a location 230 mm above the bottom of the fuel.](image1)

<table>
<thead>
<tr>
<th>Fuel Alloy Composition (wt %)</th>
<th>U-19Pu-10Zr</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel Slug length (mm)</td>
<td>343</td>
</tr>
<tr>
<td>Fuel Slug Radius (mm)</td>
<td>2.16</td>
</tr>
<tr>
<td>Fuel Slug Density (g/cm³)</td>
<td>15.8</td>
</tr>
<tr>
<td>Fuel Smear Density (%)</td>
<td>72.3</td>
</tr>
<tr>
<td>Fuel-cladding gap material</td>
<td>Liquid Na</td>
</tr>
<tr>
<td>Sodium level above fuel (mm)</td>
<td>6.35</td>
</tr>
<tr>
<td>Cladding thickness (mm)</td>
<td>0.381</td>
</tr>
<tr>
<td>Linear heat rate (kW/m)</td>
<td>42</td>
</tr>
<tr>
<td>Subassembly coolant temperature (°C)</td>
<td>Inlet: 371, Outlet: 486</td>
</tr>
<tr>
<td>Irradiation Burnup (at %)</td>
<td>1.9</td>
</tr>
</tbody>
</table>

![Figure-3.3: Radial zirconium distribution within the T179 fuel pin at an axial location 230 mm from the bottom of the fuel.](image2)
3.6.2. 4S Benchmark

Kim’s model and its FEAST implementation were applied to predict the 4S reactor fuel constituent redistribution. The calculation was performed for the fuel specifications given in Table-3.5. Fuel surface, centerline and phase transformation temperatures are given. Three different cases have been analyzed. The temperature distribution is given in Figure-3.4, and was assumed to be constant with burnup.

Table-3.5: 4S Design Fuel Data [16]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel Type (wt %)</td>
<td>U-20Pu-10Zr</td>
</tr>
<tr>
<td>Fuel Length (m)</td>
<td>2.5</td>
</tr>
<tr>
<td>Fuel density (g/cm³)</td>
<td>15.8</td>
</tr>
<tr>
<td>Slug Radius (mm)</td>
<td>4.83</td>
</tr>
<tr>
<td>Clad Inner Diameter (mm)</td>
<td>10.8</td>
</tr>
<tr>
<td>Peak Linear Heat Rate (kW/m)</td>
<td>21.4</td>
</tr>
</tbody>
</table>

Figure-3.4: Fuel Temperature distribution

Case-1

In Case-1 the fuel surface temperature is 535 °C and the burnup is 3.7 at %. Figure-3.5 shows that the predictions of the Kim model and the FEAST code match reasonably well.
Case-2

In Case-2 the fuel surface temperature is 555 °C and the burnup is 7.5 at %.
Figure-3.6 shows that in this case the FEAST code predicts a lower Zirconium concentration in the inner region of the fuel and higher in the outer region. However, the agreement is again reasonable.

Case-3

In case-3 the fuel surface temperature is 605 °C and the burnup is 3.2 at %. The predictions are reasonably close as shown in Figure-3.7, but FEAST now predicts a higher Zr concentration near the center.
3.6.3. X447 Benchmark

The X447 assembly operated at higher peak cladding temperatures than typical EBR-II conditions. As a result, a significant part of the fuel element was subjected to constituent migration. The input data for X447 are shown in Table 3.6.

Table 3.6: X447 Fuel Specifications

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel Type (wt %)</td>
<td>U-10Zr</td>
</tr>
<tr>
<td>Fuel Length (m)</td>
<td>0.343</td>
</tr>
<tr>
<td>Fuel smear density (%)</td>
<td>75</td>
</tr>
<tr>
<td>Slug Radius (mm)</td>
<td>2.2</td>
</tr>
<tr>
<td>Clad Inner Radius (mm)</td>
<td>2.54</td>
</tr>
<tr>
<td>Clad Outer Radius (mm)</td>
<td>2.92</td>
</tr>
<tr>
<td>Peak Linear Heat Rate (kW/m)</td>
<td>33.0</td>
</tr>
<tr>
<td>Peak Clad Inner Temperature (°C)</td>
<td>660</td>
</tr>
</tbody>
</table>

The irradiation history for the DP-11 fuel pin is shown in Figure-3.8. The end of cycle experimental data and the FEAST predictions are compared in Figure-3.9. The predicted distribution matches the trend of the experimental data.
4. Temperature Distribution Model

4.1. Introduction

The temperature distribution module adopts a 1D approach; thus, heat conduction in the axial and azimuthal directions is neglected. The key factors affecting the temperature distribution of metal fuel are known to be porosity, bond sodium infiltration into the porosity and thermal conductivity dependence on fuel constituent redistribution. These parameters are incorporated into the fuel temperature calculation in FEAST. The position-dependent porosity of the fuel is evaluated by means of the fission gas release and swelling module which was described in Section-2. The fuel constituent redistribution module was described in Section-3.
4.2. Coolant Temperature Distribution

Normally a detailed subchannel analysis would be required to calculate coolant temperature distribution within a fuel assembly. Due mainly to differences in the hydraulic diameter of the subchannels, the sodium coolant may have a non-negligible flow distribution across the fuel assembly in EBR-II. However, in FEAST a simpler single-channel approach is adopted. To estimate the coolant axial temperature distribution associated with the fuel pin of interest, the code uses a user-specified linear heat rate profile, and coolant inlet and exit temperatures to find the effective mass flow rate in the subchannel from an energy balance. Then the coolant temperature at each axial node can be calculated.

The Single Mass Velocity Model [10] is applied. Thus, the flow is assumed to be incompressible and thermally expandable.

\[
\frac{d\dot{m}_{\text{eff}}}{dz} = 0 \quad (4.1)
\]

\[
\dot{m}_{\text{eff}} = \frac{Q_{\text{tot}}}{(h_{\text{out}} - h_{\text{in}})} \quad (4.2)
\]

\[
T_c^j = \frac{Q^j}{\dot{m}_{\text{eff}} c_p^j} + T_c^{j-1} \quad \text{where } j = 0, \text{axn} \quad (4.3)
\]

\( \dot{m}_{\text{eff}} \): Effective subchannel mass flow rate
\( Q_{\text{tot}} \): The total power produced in the fuel rod
\( h_{\text{in}} \): Coolant inlet enthalpy
\( h_{\text{out}} \): Coolant outlet enthalpy
\( T_c^j \): Node-\( j \) coolant inlet temperature
\( T_c^{j-1} \): Node-\( j \) coolant exit temperature
\( Q^j \): Power produced in the fuel section associated with node-\( j \)
\( c_p^j \): Specific heat of the coolant evaluated at \( T_m^j \)
\( \text{axn} \): Total number of axial nodes

The average coolant temperature at node-\( j \) is computed as:

\[
T_m^j = \frac{T_c^{j-1} + T_c^j}{2} \quad (4.4)
\]

\( T_m^j \): Mean coolant temperature at axial node-\( j \)
Coolant Heat Transfer Coefficient

The Schad-Modified Correlation has been selected to calculate the coolant heat transfer coefficient [20]. It is known to be one of the most accurate correlations within its range. The Nusselt number is given as a function of pitch to diameter ratio and Peclet number as follows:

$$Nu = \left[ -16.15 + 24.96 \left( \frac{P}{D} \right) - 8.55 \left( \frac{P}{D} \right)^2 \right] Pe^{0.3} \quad (4.5)$$

$$1.1 \leq \frac{P}{D} \leq 1.5$$

$$150 \leq Pe \leq 1000$$

The resulting coolant heat transfer coefficient becomes:

$$h = \frac{Nuk_{Na}}{D_h} \quad (4.6)$$

$$Nu$$: Nusselt Number

$$\frac{P}{D}$$: Pitch to diameter ratio

$$Pe$$: Peclet Number = Re × Pr = \(\frac{\rho V c_p D_e}{k}\)

$$k_{Na}$$: Sodium Conductivity

$$D_h$$: Heated Diameter

h: Coolant heat transfer coefficient

$$\rho$$: Coolant density

$$V$$: Coolant velocity

$$c_p$$: Specific heat

$$D_e$$: Equivalent diameter

k: Thermal conductivity

4.3. Fuel Pin Radial Temperature Calculation

The radial temperature profile is calculated for each axial node. First the clad outer temperature is found from Newton’s law of cooling:

$$T_{co}^{j} = \frac{Q^{j}}{h^{j} 2\pi R_{co}^{j} L^{j}} + T_{m}^{j} \quad (4.7)$$

$$T_{co}^{j}$$: Clad outer temperature at axial node-j

$$R_{co}^{j}$$: Clad outer radius at axial node-j

$$L^{j}$$: The axial length of node-j.
Energy Balance Method

Figure-4.1 shows the generic radial nodes for the fuel, gap and cladding regions. The numerical relation for node-i is formulated by assuming that all the heat goes into node-i [21]

\[
\begin{array}{l}
\text{Figure-4.1: Radial Discretization of the fuel pin.}
\end{array}
\]

\[
\dot{E}_{in} + \dot{E}_{g} = 0.0 \quad (4.8)
\]

\[\dot{E}_{in} : \text{Heat flow into node-i from node-(i-1) and (i+1)}\]

\[\dot{E}_{g} : \text{Energy generated within node-i} \]

\[
\frac{T_{i-1} - T_{i}}{\ln \frac{r_{i}}{r_{i-1}}} + \frac{T_{i+1} - T_{i}}{\ln \frac{r_{i+1}}{r_{i}}} + q_{i}''A_{i} = 0.0 \quad (4.9)
\]

\[T_{i} : \text{Temperature of node-i}, \]

\[T_{i-1} : \text{Temperature of node-(i-1)}\]

\[k_{i-1,i} : \text{Thermal conductivity between node-(i-1) and node-i evaluated at the average temperature} \]

\[q_{i}'' : \text{Heat generation rate. It is assumed to be zero for the gap and clad and coolant regions.}\]

Thus, all the fission heat is assumed to deposit in the fuel

\[A_{i} : \text{Cross-sectional area of the radial node-i.}\]

Fuel Thermal Conductivity

The fuel thermal conductivity depends on the fuel temperature, composition, porosity and fraction of the sodium infiltrated into the fuel, and is given in Ref. [22].

Note that the Zirconium weight percent for each radial node is given by the fuel constituent redistribution module; whereas Plutonium is assumed to be immobile (see discussion in Section 3).

Sodium infiltration is described quantitatively in Ref. [22] and semi-quantitatively in Ref. [16]. Based on these descriptions, it is assumed that sodium infiltrates 40 % of the open (interconnected) porosity.
\[ k_0 = a + bT + cT^2 \]
\[ a = 17.5 \left( \frac{(1-2.23W_{Zr})}{(1+1.61W_{Zr})} - 2.62W_{Pu} \right) \]
\[ b = 1.54 \times 10^{-2} \left( 1 + 0.061W_{Zr} + 0.9W_{Pu} \right) \]
\[ c = 9.38 \times 10^{-6} (1 - 2.7W_{Pu}) \]
\[ P_c = 1 - \frac{3P_{Na} \times 1 - k_{Na}/k_o}{1 - P} \]
\[ 1.163 + 1.837k_{Na}/k_o \]
\[ k_f = P_c \times (1 - P)^{1.5} \times k_o \]

\( k_0 \): As-fabricated thermal conductivity,
\( W_{Zr} \): Zirconium weight percent in the fuel,
\( W_{Pu} \): Plutonium weight percent in the fuel,
\( P_c \): Porosity correction factor for sodium infiltration,
\( P_{Na} \): Fraction of the fuel which is filled with sodium,
\( k_{Na} \): Sodium thermal conductivity,
\( P \): Fuel porosity fraction,
\( k_f \): Fuel thermal conductivity,

**Thermal Conductivity of liquid sodium**

Thermal conductivity of liquid sodium is given in [23] as follows:

\[ k_{Na} = 93-0.0581T + 1.173 \times 10^{-5}T^2 \text{ (W/m/K)} \text{ (T in Celsius)} \]  
\[ (4.11) \]

Equation-4.11 is valid within the temperature region of interest for sodium fast reactors.

**Clad Conductivity**

Thermal Conductivity of HT9 is given in [24] as follows:

\[ k_c = \begin{cases} 17.622 + 2.42 \times 10^{-2}T - 1.696 \times 10^{-5}T^2 & T < 1030 \\ 12.027 + 1.218 \times 10^{-2}T & T \geq 1030 \end{cases} \text{ (T in Kelvin)} \]  
\[ (4.12) \]
4.4. Sensitivity Study and Benchmarking

The sensitivity of the temperature distribution to the important effects is shown in Figure-4.2 under the assumptions listed in Table-4.1. Note that the fuel centerline temperature is predicted within less than 10°C of the value reported in Ref. [16].

Table-4.1: Fuel Specifications

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel</td>
<td>U-20Pu-10Zr</td>
</tr>
<tr>
<td>Radius (mm)</td>
<td>4.83</td>
</tr>
<tr>
<td>Linear Heat Rate (kW/m)</td>
<td>19.7</td>
</tr>
<tr>
<td>Porosity</td>
<td>~0.3</td>
</tr>
<tr>
<td>Sodium Fraction within the pores</td>
<td>0.08</td>
</tr>
<tr>
<td>Fuel Surface Temperature (°C)</td>
<td>535</td>
</tr>
<tr>
<td>Estimated Fuel Centerline Temperature with FEAST code (°C)</td>
<td>663</td>
</tr>
<tr>
<td>Estimated Fuel Centerline Temperature Reported in Ref. [16] (°C)</td>
<td>671</td>
</tr>
</tbody>
</table>

Figure-4.2: Sensitivity of the fuel temperature distribution to important irradiation effects

To assess the sensitivity of the temperature distribution to the number of radial nodes, a calculation was performed for the as fabricated fuel given in Table-4.2, and the results are shown in Figure-4.3 including the closed form solution of the heat equation. It seems that adequate accuracy would be preserved with as low as five radial nodes.
### Table-4.2: Fuel Specifications

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel</td>
<td>U-19Pu-10Zr</td>
</tr>
<tr>
<td>Radius (mm)</td>
<td>2.86</td>
</tr>
<tr>
<td>Linear Heat Rate (kW/m)</td>
<td>50.0</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.0</td>
</tr>
<tr>
<td>Sodium Infiltration</td>
<td>0.0</td>
</tr>
<tr>
<td>Fuel Surface Temperature (°C)</td>
<td>600</td>
</tr>
</tbody>
</table>

#### Figure-4.3: Node sensitivity to temperature distribution calculation

5. **Fuel Clad Chemical Interaction Module**

The chemical reaction between the fuel slug and the cladding material is one of the most important issues limiting the in-pile performance of metal fuels. As a result of fuel cladding contact during steady state irradiation, the cladding constituents may diffuse into the fuel and form a low-melting point alloy (eutectic). As the burnup increases, some fission products (particularly lanthanides) diffuse into the cladding to form low-melting phases with iron. Furthermore, lanthanide diffusion creates a brittle band, which hardness measurements have shown to be very hard and containing numerous cracks [25].

In addition to the lanthanide layer, the effect of decarburization and grain coarsening of the cladding also contributes to cladding wastage. This layer, which is soft, uncracked and small with respect to the lanthanide layer, is thought to be carbon depleted and was found in areas outside the lanthanide regions. [25]

The presence of zirconium in the fuel decreases Fuel/Cladding Chemical interaction significantly. Fabrication of metal fuel is performed in a nitrogen environment. As a result, a thin ZrN layer forms at the surface of the fuel. This layer hinders diffusion of fuel constituents.
into the cladding and vice versa. On the other hand, the layer loses its strength above 600 °C and it totally disappears at 700 °C. Reported cladding wastage values at normal operating conditions (500-600 °C peak cladding temperatures) are less than 5 % for HT9, while operation at 630 °C to 660 °C may result in more than 20 % thinning of the clad [25].

Figure-5.1 shows the cladding wastage as a function of axial location for the X447 fuel assembly. This assembly was irradiated at 630 to 660 °C peak cladding temperatures at EOL and BOL, respectively; hence, significant fuel cladding chemical interaction is expected. Note that cladding wastage is lower at lower temperatures (lower axial regions). DP70 and DP75 designate the breached fuel pins in Figure-5.1. The data in Figure-5.1 (except for the very high wastage data of the breached fuel pins) can be well reproduced using an Arrhenius-type correlation for the cladding wastage rate as follows:

\[
i_w = 1.8 \times 10^{-3} \exp \left( - \frac{12800}{T} \right) \text{ (mm/s)}; \quad (5.1)
\]

T: Clad inner temperature (K)

This correlation is used to describe FCCI in FEAST for the steady state analysis.

Figure-5.1: Rare earth (lanthanides) penetration in metal fuel (X447 assembly) [25]

6. Mechanical Analysis Module for Fuel and Cladding

6.1. Introduction

The first barrier against the release of radioactive fission products into the environment is the cladding of the nuclear fuel rod. The assessment of the cladding stresses and associated deformations is therefore essential in fuel performance calculations. The stress-strain analysis module of FEAST adopts the LIFE algorithm [12] with a 1D finite difference solution.
6.2. General Assumptions

1- The fuel and clad are assumed to be axially symmetric.
2- The planes perpendicular to the axial z-direction in each material remain plane during deformation. This is the plane strain assumption.
3- Axial friction between the fuel slug and cladding is considered.
4- The time dependence is inherent in the analysis due to the swelling and creep, which are time-dependent phenomena. However, inertia effects are neglected, so the system is treated as undergoing a succession of (mechanical) equilibrium states.
5- The outer radius of the fuel and inner radius of the cladding are loaded by the plenum pressure if the fuel-cladding gap is open and by the fuel-cladding interfacial pressure if the gap is closed.
6- The outer radius of the cladding is subject to the coolant pressure. The axial variation of the coolant pressure is neglected.

As a result of assumptions 1 and 2, only the normal stresses along the three principal directions in the cylindrical coordinate system are non-zero; these are denoted by the symbols $\sigma_r$, $\sigma_\theta$ and $\sigma_z$ and are positive if tensile, and negative if compressive, according to the usual sign convention. There are no shear stresses.

6.3. Governing Relations

6.3.1. Equilibrium Condition

The equilibrium conditions are simplified by the elimination of the shear stresses and axial tangential derivatives, which leads to the single equation:

$$
\frac{d\sigma_r}{dr} + \frac{\sigma_r - \sigma_\theta}{r} = 0
$$

(6.1)

6.3.2. Kinematics

Letting $\varepsilon_r$, $\varepsilon_\theta$ and $\varepsilon_z$ be the total strains in the three principal directions, the strain displacement relations become:

$$
\varepsilon_r = \frac{du}{dr}
$$

(6.2)

$$
\varepsilon_\theta = \frac{u}{r}
$$

(6.3)

$$
\varepsilon_z = \text{Constant with } r \text{ (as per assumption 2 above)}
$$

(6.4)

“u” is the radial displacement. The total strain in each direction is the sum of the thermal strains, elastic strains, creep/plastic and swelling strains due to accumulation of fission gas bubbles, open porosity and nongaseous fission products.
6.3.3. Constitutive Relations

The constitutive relations used in fuel modeling analysis are the generalized Hooke’s law:

\[
\varepsilon_r = \frac{1}{E} \left[ \sigma_r - \nu (\sigma_\theta + \sigma_z) \right] + \alpha T + \varepsilon^s + \varepsilon^c
\]  
(6.5)

\[
\varepsilon_\theta = \frac{1}{E} \left[ \sigma_\theta - \nu (\sigma_r + \sigma_z) \right] + \alpha T + \varepsilon^s + \varepsilon^c
\]  
(6.6)

\[
\varepsilon_z = \frac{1}{E} \left[ \sigma_z - \nu (\sigma_r + \sigma_\theta) \right] + \alpha T + \varepsilon^s + \varepsilon^c
\]  
(6.7)

Equations 6.5 to 6.7 apply to both the fuel and the cladding provided the linear thermal-expansion coefficient \(\alpha\), Young’s Modulus \(E\), and Poisson’s ratio \(\nu\) are chosen accordingly and appropriate material-specific functions are used for the swelling (\(\varepsilon^s\)) and creep/plastic (\(\varepsilon^c\)) strains in each part of the fuel element. The thermal expansion coefficient, Young’s modulus and Poisson’s ratio of the HT-9 cladding material and U-Pu-10Zr fuel alloy are given in Appendix-A.

6.4. Solution Method

The presence of time-dependent permanent (irreversible) strains and the sizeable variation of the mechanical properties of the fuel with position (mainly due to the radial temperature distribution) require a numerical solution of the relevant equations. Moreover, the creep and swelling phenomena introduce time as an explicit variable.

The total strains \(\varepsilon_r\) and \(\varepsilon_\theta\) are eliminated by combining Eq-6.5 to 6.7 with Eq-6.2 and 6.3 and the stresses are expressed in terms of the radial displacement.

\[
\sigma_r = \frac{E}{1+\nu} \left[ \frac{du}{dr} + \frac{\nu}{1-2\nu} \left( \frac{du}{dr} + \frac{u}{r} + \varepsilon_z - 3\alpha(T-T_o) - 3\varepsilon^s \right) - \left( \alpha(T-T_o) + \varepsilon^s + \varepsilon^c \right) \right]
\]  
(6.8)

\[
\sigma_\theta = \frac{E}{1+\nu} \left[ \frac{u}{r} + \frac{\nu}{1-2\nu} \left( \frac{du}{dr} + \frac{u}{r} + \varepsilon_z - 3\alpha(T-T_o) - 3\varepsilon^s \right) - \left( \alpha(T-T_o) + \varepsilon^s + \varepsilon^c \right) \right]
\]  
(6.9)

\[
\sigma_z = \frac{E}{1+\nu} \left[ \varepsilon_z + \frac{\nu}{1-2\nu} \left( \frac{du}{dr} + \frac{u}{r} + \varepsilon_z - 3\alpha(T-T_o) - 3\varepsilon^s \right) - \left( \alpha(T-T_o) + \varepsilon^s + \varepsilon^c \right) \right]
\]  
(6.10)

Eq-6.8 and 6.9 are substituted into the equilibrium condition, Eq-6.1, and the following differential equation for the radial displacement is obtained [12]:

\[
\frac{d}{dr} \left[ \frac{1}{r} \frac{d(ru)}{dr} \right] = \left( \frac{1-2\nu}{1-\nu} \right) \left( \frac{d\varepsilon_z^c}{dr} + \frac{\varepsilon_z^c + \varepsilon_z^c}{r} \right) + \left( \frac{1+\nu}{1-\nu} \right) \frac{d}{dr} \left( \alpha(T-T_o) + \varepsilon^s \right)
\]  
(6.11)
The step leading to Eq-6.11 requires that the elastic constants $E$ and $\nu$ be assumed independent of $r$ (and hence temperature). This approximation is valid only when the radial interval over which the resulting equation applies is small.

Eq. (6.11) is applied to each ring in the fuel element. Each ring is characterized by subscripts $i$ and $j$, representing the radial and axial positions in the pin, respectively. Eq. (6.11) is integrated from the inner boundary of the $i$-th radial zone ($r_{ai}$) to radial position “r” within the ring.

$$u(r) = \frac{C_{hi}}{r} + C_{zi}r + \left(1 + \frac{1}{1 - \nu}\right)\int_{r_{ai}}^{r} \frac{r'}{r^2} (\alpha T + \varepsilon^\prime) dr'$$

$$+ \frac{1}{2} \left(1 - 2\nu\right) \left[\int_{r_{ai}}^{r} (\varepsilon_r^\prime + \varepsilon_\theta^\prime) r' dr' + \int_{r_{ai}}^{r} (\varepsilon_r^\prime - \varepsilon_\theta^\prime) \frac{dr'}{r'}\right]$$

(6.12)

where $C_{hi}$ and $C_{zi}$ are constants of integration for the $i$-th zone which remain to be determined. At this point, it is assumed that the thermal, swelling and permanent strains are constant within each ring which reduces Eq. (6.12) to

$$u(r) = \frac{C_{hi}}{r} + C_{zi}r + \left(1 + \frac{1}{1 - \nu}\right)\left[\alpha_i (T - T_o) + (\varepsilon^\prime)_i\right] \frac{r^2 - r_{ai}^2}{2r} +$$

$$\frac{1}{2} \left(1 - 2\nu\right) \left[\left(\varepsilon_r^\prime\right)_i + \left(\varepsilon_\theta^\prime\right)_i\right] \frac{r^2 - r_{ai}^2}{2r} + \left[\left(\varepsilon_r^\prime\right)_i - \left(\varepsilon_\theta^\prime\right)_i\right] r \ln\frac{r}{r_{ai}}$$

(6.13)

Eq-6.13 is applied to each ring in the fuel element depicted in Figure-6.1. Each ring is characterized by the subscripts “i” and “j” representing the radial and axial positions in the pin, respectively. Note that $M_f$ and $M_c$ are the number of radial nodes within the fuel and clad regions, respectively.

Since the radial boundary conditions needed to determine the integration constants apply to the radial stress component as well as to the displacement, Eq-6.13 is substituted into Eq-6.8 which leads to an equation for $\sigma_r(r)$ as a function of $C_{hi}$, $C_{zi}$, the strain components $(\alpha(T - T_o))$, $(\varepsilon^\prime)_i$, $(\varepsilon_r^\prime)_i$, and $(\varepsilon_\theta^\prime)_i$, the zone boundaries $r_{ai}$ and the axial strain $\varepsilon_z$. 

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The number of axial zones and radial zones are chosen to find an acceptable balance between computing time and accuracy. The original LIFE code divided the fuel into three radial zones and represented the entire cladding cross-section into one radial zone. In the FEAST code it is recommended that the fuel be divided into six radial nodes and the cladding in four radial nodes. Note that increasing the radial nodes in the cladding region does not result in any further gain in accuracy as shown in Figure-6.2. A finer mesh pattern of the fuel region may increase the accuracy somewhat; however, it seriously increases the computational time and may result in a code more susceptible to numerical instabilities, as the solution method used in this algorithm is explicit.
6.5. Boundary conditions

1- \( r = 0 \Rightarrow u = 0 \) \hspace{1cm} (6.14)

2- To ensure continuity of stress and displacement at the radial zone boundaries (\( a_i \): inner boundary of node-\( i \); \( b_i \): outer boundary of node-\( i \)) within the fuel, we have

\[
\begin{align*}
\sigma_r(r_{b_{i-1}}) &= \sigma_r(r_{a_i}) \\
u(r_{b_{i-1}}) &= u(r_{a_i}) \\
(1 < i \leq M_f)
\end{align*}
\] \hspace{1cm} (6.15)

3- The condition at the fuel-cladding interface depends on whether the gap is open or closed. For an open gap:

\[
\sigma_r(R_f) = -P_p \] \hspace{1cm} (6.16)

If the gap is closed the condition becomes,

\[
\sigma_r(R_f) = -P_{fc} \] \hspace{1cm} (6.17)

where \( P_p \) and \( P_{fc} \) are plenum pressure and fuel-cladding interfacial pressure, respectively.

4- The continuity conditions within the cladding are expressed as

\[
\begin{align*}
\sigma_r(r_{i-1,b}) &= \sigma_r(r_{ia}) \\
u(r_{i-1,b}) &= u(r_{ia}) \\
(1 < i \leq M_c)
\end{align*}
\] \hspace{1cm} (6.18)

5- At the outer surface of the cladding

\[
\sigma_r(R_f + t_c) = -P_c \] \hspace{1cm} (6.19)

where \( P_c \) is the coolant pressure and \( t_c \) is the cladding thickness.

**Unknowns**

Since the boundary conditions were used to determine the integration constants \( C_{li} \) and \( C_{2i} \) in each radial zone, the displacement distribution \( u(r) \) is now a function of:

1. The strain components \( \alpha(T-T_o) \), \( \epsilon^\alpha \), \( \epsilon^c \), and \( \epsilon^\theta \) in each ring,
2. The axial strain \( \epsilon_z \), which may take on different values in the fuel and in the cladding,
3. The plenum pressure \( P_p \) and if the fuel-cladding gap is closed, the interfacial pressure \( P_{fc} \).

At this point the interfacial pressure between fuel and cladding, and the axial strains of fuel and cladding are unknown.
6.6. Calculation of the Interfacial Pressure

If the fuel-cladding gap is closed, the incremental change of the fuel outer surface radial displacement within a unit time step should be equal to the change of cladding inner surface radial displacement in the same time step. Thus, the fuel and clad have to move together. The following relation is applied to find the interfacial pressure:

\[ \delta u_{rf} = \delta u_{re} \]  

(6.20)

If the fuel-cladding gap is open, the clad is pressurized solely by the plenum pressure. According to the perfect gas equation, the plenum pressure is given as follows:

\[ P_p = \frac{nRT_{av}}{V_{pl} + \sum_{j=1}^{\text{ann}} V_{\text{void}}(j)} \]  

(6.21)

\[ T_{av} = \frac{V_{pl} + \sum_{j=1}^{\text{ann}} V_{\text{void}}(j)}{T_{pl} + \sum_{j=1}^{\text{ann}} T_{\text{void}}(j)} \]  

(6.22)

- \( P_p \): Plenum Pressure
- \( n \): # of moles of gas
- \( R \): Gas Constant
- \( T_{av} \): Average Temperature
- \( V_{pl} \): Plenum Volume
- \( V_{\text{void}}(j) \): Radially averaged open porosity in axial node-\( j \). It does not include sodium infiltrated porosity.
- \( T_{\text{void}}(j) \): Radially averaged temperature of the open porosity in axial node-\( j \).

6.7. Axial Force Balance

Axial forces acting on the fuel slug between an axial zone “\( j \)” and the upper surface of the fuel consist of an average axial stress, the plenum pressure, weight \( (W) \) and the sum of the friction forces acting vertically on the outer surface of the fuel \( (F) \). These forces are positive if they restrict axial growth of the fuel and are zero if the fuel cladding gap is open.

Fuel:

\[ -2\pi \int_0^{R_f} \sigma_z(r) rdr = \pi R_f^2 P_p + \sum_{k=j}^N F_k + \sum_{k=j}^N W_k \]  

(6.23)
Clad:

\[-2\pi \int_0^{R_{c2TP}} \sigma_z(r) r dr = \pi (R_{c1} + t_c)^2 P_p - \pi R_{c1}^2 P_p \sum_{k=j}^{N} F_k - \sum_{k=j}^{N} W_{ck} \quad (6.24)\]

Note that the axial strain of metal fuel remains constant after the fuel and the clad make contact. Thus, Eq-6.23 is used to calculate the fuel axial strain before the fuel touches the clad. After the fuel touches the clad, the axial strain remains constant, and the only remaining unknown becomes the frictional force exerted on the clad, and it is again calculated with Eq-6.23. Eq-6.24 is used to calculate the cladding axial strain during the irradiation history.

### 6.8. Creep and Plasticity

The permanent strains labeled \( \varepsilon_i^p \) \( (i = r, \theta, \text{ or } z) \) in the equations are the sum of the creep and plastic strains.

\[ \varepsilon_i^c = \varepsilon_i^{creep} + \varepsilon_i^{plastic} \quad (6.25) \]

Creep and plastic deformations occur at constant volume \( [12] \); so the radial, azimuthal and axial components of \( \varepsilon_c \) are related by the following equation:

\[ \varepsilon_r^c + \varepsilon_\theta^c + \varepsilon_z^c = 0 \quad (6.26) \]

Formulation of the permanent strains is based on the von Mises assumption that creep and plastic deformations occur only when the stress state deviates from pure hydrostatic tension or compression. This assumption leads to the stress-strain relations known as the Prandtl-Reuss flow laws or the Soderberg equations:

\[ \Delta \varepsilon_r^c = \left( \frac{\varepsilon_{eq}}{\sigma_{eq}} \right) \left[ \sigma_r - \frac{1}{2} (\sigma_\theta + \sigma_z) \right] \quad (6.27) \]

\[ \Delta \varepsilon_\theta^c = \left( \frac{\varepsilon_{eq}}{\sigma_{eq}} \right) \left[ \sigma_\theta - \frac{1}{2} (\sigma_r + \sigma_z) \right] \quad (6.28) \]

\[ \Delta \varepsilon_z^c = \left( \frac{\varepsilon_{eq}}{\sigma_{eq}} \right) \left[ \sigma_z - \frac{1}{2} (\sigma_r + \sigma_\theta) \right] \quad (6.29) \]

The equivalent stress for the porous fuel is given in Ref. [5] as follows:

\[ \sigma_{eq} = \left[ \frac{1}{2} (\sigma_r - \sigma_\theta)^2 + (\sigma_\theta - \sigma_z)^2 + (\sigma_z - \sigma_r)^2 + 3\alpha_c (\sigma_r + \sigma_\theta + \sigma_z + 3P_p)^2 \right]^{1/2} \quad (6.30) \]
(σ_r + σ_p + σ_z + 3P_p) is the net effective hydrostatic stress applied to the open pores. Note that the gas plenum pressure is equal to the internal pressure of the open pores. α_c is the open pore compressibility factor given as follows [5]:

$$\alpha_c = \begin{cases} 
0.0 & \varepsilon_{sw}^{opn} = 0.0 \\
\frac{1}{6} \left( \varepsilon_{sw}^{opn} \right)^{1.5} & 0 < \varepsilon_{sw}^{opn} < 0.1 \\
\frac{1}{6} & 0.1 < \varepsilon_{sw}^{opn} 
\end{cases}$$

(6.31)

Note that α_c equals zero for the cladding region.

The equivalent creep strain rate for the fuel is given as follows [26]:

$$\dot{\varepsilon}_{eq} = \begin{cases} 
T < 923.15 \text{ K} & (5 \times 10^3 \sigma_{eq} + 6 \times \sigma_{eq}^{4.5}) \times \exp(-26170 / T) \\
T \geq 923.15 \text{ K} & (0.08 \times \sigma_{eq}^{3} \times \exp(-14350/T)) 
\end{cases} \text{ (1/sec)}$$

(6.32)

The plastic behavior of the fuel is modeled with the “perfectly plastic” approach. If the fuel exceeds the yield stress (Appendix-A), the strain rate increases so much that the fuel stays at the yield stress level. Note that it is unlikely for the fuel to enter and stay in this region during the steady state operation because fuel creep is very effective in relaxing the stresses.

The thermal and irradiation creep equations which are used for the HT9 cladding material in FEAST are given in Appendix-A.

6.9. Swelling

The fuel swelling strain (ε^s) is given by

$$\varepsilon_{fuel}^s = \frac{1}{3} \left[ \left( \frac{\Delta V}{V} \right)_{\text{Solid FP}} + \left( \frac{\Delta V}{V} \right)_{\text{Closed Bubble}} + \left( \frac{\Delta V}{V} \right)_{\text{Open Porosity}} - \left( \frac{\Delta V}{V} \right)_{\text{Hot Pressing}} \right]$$

(6.33)

Fuel swelling is isotropic within the fuel. Hence, each direction share one-third of the total swelling. One-third of the total swelling of fuel is given by Eq.6.31. Swelling due to solid fission product accumulation is taken into account by an empirical relation dependent on burnup (Eq-2.37). The gaseous fission product swelling term is related to the size and concentration of the fission-gas bubbles calculated by the fission gas release and swelling model together with open porosity.
The hot-pressing contribution to fuel swelling is negative inasmuch as porosity is removed by this process as a result of fuel clad mechanical interaction. When the initial gap space between the fuel and the cladding is filled with the swollen fuel slug, further gas swelling is restrained by the cladding. The volume of the existing open pores decreases so that further buildup of the fission products is accommodated. Fuel Clad Mechanical Interaction remains at a low level as long as enough open porosity is available. The mechanism is assumed to be creep-dependent as given by Eq-6.34.

\[
\Delta \varepsilon^{opn} = 9 \alpha_e (\sigma_r + \sigma_\theta + \sigma_z + 3P_v) \frac{\Delta \varepsilon_{eq}}{\sigma_{eq}} \quad (6.34)
\]

The compressibility factor given in Equation-6.31 rapidly drops when the open pore concentration is below 5%.

In the cladding the swelling strain is due solely to void formation.

\[
\varepsilon_s^{clad} = \frac{1}{3} \left( \frac{\Delta V}{V} \right)^{\text{Void Swelling}} \quad (6.35)
\]

However, swelling is not observed for HT9 cladding before a very high fast-neutron damage is reached (100 dpa at 400 °C). For EBR-II conditions the corresponding burnup value is of the order of 20 at %, which is beyond the scope of the analysis given in this report.

### 6.10. Anisotropic Slug Deformation

The empirical approach given in Ref. [5] is adopted to model anisotropic deformation of the metal fuel slug in FEAST.

After the fuel slug comes into contact with the cladding, further axial growth is restrained. However, slug deformation prior to slug-cladding contact is anisotropic. This is due to the formation of large radial cracks in the brittle ternary fuel. Tearing at the grain or phase boundaries in the peripheral region of the slug also occurs due to anisotropic irradiation growth of \(\alpha\)-U crystals. The latter effect is more important in U-Zr fuels, while the former dominates in U-Pu-Zr fuels. To incorporate these effects, the effective fuel slug radius is defined:

\[
r_{\text{eff}} = r_o + dr_{\text{slug}} + dr_{\text{crack}} = r_{\text{slug}} + dr_{\text{crack}} \quad (6.36)
\]

\(r_o\) is the as-fabricated slug radius and \(dr_{\text{slug}}\) is the radial strain increment due to thermal expansion, elasticity, creep/plasticity, closed bubble, open pore and solid fission product swelling. The increment \(dr_{\text{crack}}\) is due to the cracks and also the tearing. After the slug comes into contact with the cladding, the swelling of the fuel is accommodated by the closure of the tears and cracks. This process prevents the FCMI stress from growing. During this stage of contact, the area of the contact interface continues to increase without significant FCMI stress, while the slug sticks to the cladding.
According to this description, the fuel/cladding contact condition can be divided into three time intervals:

(I) \( r_{\text{eff}} < r_i \): no restraint by the cladding (no contact)

(II) \( r_{\text{slug}} < r_i = r_{\text{eff}} \): axial restraint by the cladding, no radial restraint.

(III) \( r_i = r_{\text{slug}} \): both axial and radial restraint by cladding

Where \( r_i \) is the inner radius of the cladding.

\[
d r_{\text{crack}} = f_{\text{crack}} \times r_0 \quad \text{(6.37)}
\]

where \( r_0 \) is the initial gap width between the fuel and cladding. The anisotropy factor, \( f_{\text{crack}} \), is given in Figure-6.3, which is calculated based on references [15], [27] and [28] as a function of Plutonium content and \( q / D_o \) (average linear power divided by the diameter of the slug). Note that the value of \( f_{\text{crack}} \) ‘saturates’ above 19 wt % Plutonium and 790 W/cm² \( q / D_o \) value.

![Figure-6.3: Anisotropy Factor](image)

Table-6.1 shows several experimental data for axial fuel elongation. FEAST predictions are in reasonable agreement with the experimental data.
Table-6.1: Slug Axial Elongation

<table>
<thead>
<tr>
<th>Fuel Composition</th>
<th>Fuel Smear Density (%)</th>
<th>( \frac{q}{D_o} ) (W/cm²)</th>
<th>Axial Elongation (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>U-10Zr</td>
<td>76 [28]</td>
<td>790</td>
<td>6.2</td>
</tr>
<tr>
<td>U-19Pu-10Zr</td>
<td>76 [28]</td>
<td></td>
<td>1.5</td>
</tr>
<tr>
<td>U-10Zr</td>
<td>72 [27]</td>
<td>830</td>
<td>8.5</td>
</tr>
<tr>
<td>U-8Pu-10Zr</td>
<td>72 [27]</td>
<td></td>
<td>6.5</td>
</tr>
<tr>
<td>U-19Pu-10Zr</td>
<td>72 [27]</td>
<td></td>
<td>2.5</td>
</tr>
<tr>
<td>U-10Zr</td>
<td>75 [15]</td>
<td>650</td>
<td>8</td>
</tr>
<tr>
<td>U-8Pu-10Zr</td>
<td>75 [15]</td>
<td></td>
<td>5.8</td>
</tr>
<tr>
<td>U-19Pu-10Zr</td>
<td>75 [15]</td>
<td></td>
<td>6.5</td>
</tr>
</tbody>
</table>

6.11. Verification of the Mechanical Analysis Module against the Analytical Solution for the Radial Distribution of Thermal Stresses

To verify the accuracy of the numerical algorithm that solves Eq. 6.11, the FEAST predictions were compared to the close analytical solution for a very simple case. Consider an infinitely long cylinder fuel pin of radius \( R \) operating at linear power, \( q' \). Creep and swelling strains are assumed to be zero. Assuming the material properties such as thermal conductivity, \( k \), thermal expansion coefficient, \( \alpha \), Young’s Modulus, \( E \), and Poisson’s ratio, \( \nu \), are constant as given in Table-6.2, the radial, hoop and axial stresses become [12]:

\[
\sigma_r = -\frac{\alpha E q'}{16\pi(1-\nu)k} \left[ 1 - \left( \frac{r}{R} \right)^2 \right]
\]  
(6.38)

\[
\sigma_\theta = -\frac{\alpha E q'}{16\pi(1-\nu)k} \left[ 1 - 3 \left( \frac{r}{R} \right)^2 \right]
\]  
(6.39)

\[
\sigma_z = -\frac{\alpha E q'}{8\pi(1-\nu)k} \left[ 1 - 2 \left( \frac{r}{R} \right)^2 \right]
\]  
(6.40)

Table-6.2: Approximate metal fuel properties

<table>
<thead>
<tr>
<th>Fuel Properties</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \alpha ) ( \degree C^{-1} )</td>
<td>2E-05</td>
</tr>
<tr>
<td>E (GPa)</td>
<td>150</td>
</tr>
<tr>
<td>( \nu )</td>
<td>0.3</td>
</tr>
<tr>
<td>k (W/mK)</td>
<td>25</td>
</tr>
<tr>
<td>( q' ) (kW/m)</td>
<td>40</td>
</tr>
</tbody>
</table>
Figure-6.4, 6.5 and 6.6 show the comparison of the FEAST results and the analytical solution of the radial variation of thermal stresses. The agreement is very good.

Figure-6.4: Radial stress distribution in radial direction

Figure-6.5: Hoop stress radial distribution
7. Validation of the FEAST Code

To validate the FEAST code, its predictions are compared to the irradiation database available from the EBR-II reactor experience, and to the predictions of the ALFUS and LIFE-METAL codes. The EBR-II test assemblies designated as X430 [28], X425 [5], [27], [29] and X447 [19], [25] are used for the validation exercise as sufficient information is available for these assemblies.

Some metal fuel rods are currently being irradiated in the PHENIX reactor in France under the auspices of Japan’s CRIEPI. The irradiation history has been reported up to 7.2 at % burnup [30]. These data are also used in the validation of the FEAST code.

There also exists a Russian report on metal fuels [31]; however, it contains no original irradiation data.

7.1. X430 Benchmark

Table-7.1 shows the fuel composition and geometry for the X430 benchmark. The peak assembly burnup is 11.9 at %. The coolant outlet temperature and peak linear heat rate as functions of burnup (i.e., the irradiation history) are the input required to run FEAST. Figure-7.1 is the irradiation history of the rod T-654. The thermo-mechanical behavior is predicted by FEAST for this particular rod and for four other high-burnup rods for which a similar irradiation history was assumed.
Table-7.1: X430 fuel data

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel Composition</td>
<td>U-19Pu-10Zr</td>
</tr>
<tr>
<td>Cladding Material</td>
<td>HT-9</td>
</tr>
<tr>
<td>Fuel slug radius (mm)</td>
<td>2.86</td>
</tr>
<tr>
<td>Clad inner radius (mm)</td>
<td>3.28</td>
</tr>
<tr>
<td>Clad outer radius (mm)</td>
<td>3.68</td>
</tr>
<tr>
<td>Fuel Active Length (cm)</td>
<td>34.3</td>
</tr>
<tr>
<td>Fuel Smear Density (%)</td>
<td>76.1</td>
</tr>
<tr>
<td>Plenum to Fuel Ratio</td>
<td>1.4</td>
</tr>
</tbody>
</table>

Figure-7.1: Irradiation history of T-654.

Figure-7.2 shows the average axial power profile given for EBR-II, and is used for all X430 rods.

Figure-7.2: Axial Power Profile

The following relation between the neutron flux and the volumetric heat generation rate is assumed in order to match the neutron fluence data reported in Ref. [32].
\[ \phi = Cq'''' \]  
\[ \phi = \text{Neutron Flux (n/cm}^2\text{s)} \]  
C=840000  
\[ q'''' = \text{Volumetric Heat Generation Rate (W/m}^3\) \]

In Figure-7.3 the fission gas release behavior of the T-654 fuel rod is shown, and compared to the reported peak fission gas release at the end of life [28]. The agreement is very satisfactory. Figure-7.3 also shows generic data for U-19Pu-10Zr at lower burnup from Figure 2.1.

![Figure-7.3: Fission Gas Release Behavior of T-654 Fuel Rod.](image)

Figure-7.4 shows the swelling behavior of the T-654 fuel rod. The fuel hot spot (located at 93% of the fuel slug length) touches the clad at \(~1\) at % burnup (Figure-7.4(b)). However, the fuel located at 50% of the fuel slug length, which is cooler, is not radially restrained by the clad until it reaches 3.5 at % (Figure-7.4(a)). Therefore, temperature has a significant effect on the swelling behavior of the metal fuel, as expected.

![Figure-7.4 (a) Swelling at 50 %, (b) Swelling at 93 % of the fuel slug length for T-654 Fuel Rod.](image)
The fuel/clad contact pressure starts to increase after the fuel becomes radially restrained. As can be seen in Figure-7.5, FCMI is practically negligible at the hot spot of the fuel slug, thanks to the very high fuel creep rate at these temperatures. On the other hand, FCMI in the fuel cooler section becomes non-negligible shortly after the fuel becomes radially restrained. This is due to two effects; first, the lower temperature makes the fuel less compliant (i.e., compressing the open pores requires higher stresses); second, the somewhat high linear heat rate generates more solid fission products, which makes the fuel even stiffer.

![Figure-7.5: Contact and plenum pressure for T-654 Fuel Rod](image)

Note that the oscillations in the contact stress are directly related to the creep properties of the metal fuel. The creep rate of the gamma phase is two orders of magnitude higher than that of the alpha and beta phases. When the phase boundary moves the compressibility of the fuel changes drastically and oscillations arise.

In parallel with the rise in contact pressure, the peak cladding strain rises as shown in Figure-7.6(a). Figure-7.6(b) shows the cladding strain axial distribution at the End of Life. Since irradiation creep dominates within the operating history, the peak cladding strain occurs at the peak power location.
Finally, note that the maximum cladding wastage reported in Ref. [28] is of the order of 20 microns and the FEAST prediction is 29 microns; therefore the agreement is again reasonable.

Comparison of Predicted and Measured Peak Cladding Strain

Experimental data for peak cladding strain are available for both low- and high-burnup cases.

Table-7.2 shows the experimental and predicted cladding strain data at low burnup. FEAST appears to underestimate considerably the cladding strain at these conditions. However, the low-burnup experimental data reported here are unusually high and are not consistent with the low-burnup cladding strain values reported in many other sources. A brief discussion of this issue is given next.

Table-7.2: X430 assembly peak cladding strain at low burnup

<table>
<thead>
<tr>
<th>Fuel Rod ID</th>
<th>Burnup (at %)</th>
<th>Experimental Data</th>
<th>FEAST Prediction</th>
<th>Relative Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>T-654</td>
<td>7.4</td>
<td>0.28</td>
<td>0.16</td>
<td>-43</td>
</tr>
<tr>
<td>T-655</td>
<td>7.2</td>
<td>0.38</td>
<td>0.14</td>
<td>-63</td>
</tr>
<tr>
<td>T-659</td>
<td>7.4</td>
<td>0.28</td>
<td>0.17</td>
<td>-39</td>
</tr>
<tr>
<td>T-660</td>
<td>7.2</td>
<td>0.41</td>
<td>0.16</td>
<td>-61</td>
</tr>
</tbody>
</table>

The Evidence for low Burnup HT-9 cladding creep behavior

Figure-7.7 shows the clad strain of HT9 cladding [6]. The fuel composition is U-10Zr. At 7 at % the cladding strain should not exceed about 0.2 % whereas the experimental values for X430 are well in excess of 0.2 %.
Figure-7.7: U-10Zr/HT9 cladding strain behavior (fuel smear density is ~75 %) [6]

Figure-7.8 shows a typical behavior of U-19Pu-10Zr fuel given by Ref. [1]. At 7 at %, the expected cladding strain is virtually zero for HT9 cladding.

Figure-7.8: U-19Pu-10Zr/HT9 clad strain data (72 % smear density) [1]

Figure-7.9 and 7.10 show other cladding strain data for U-19Pu-10Zr given in Ref. [5]. Cladding strains at 5 at % burnup are relatively low even for 85 % smear density.
Figure-7.9: U-19Pu-10Zr/HT9 clad strain data (72 % smear density) [5]
It seems that the clad strains predicted by FEAST for fuel rods at low burnup are consistent with the trends described in most sources in the literature. However, this is clearly an area that warrants further investigation.

On the other hand, the FEAST predictions match reasonably well the cladding strain values at high burnup, as shown in Table-7.3.

Table-7.3: X430 assembly peak cladding strain at high burnup

<table>
<thead>
<tr>
<th>Fuel Rod ID</th>
<th>Burnup (at %)</th>
<th>Experimental Data</th>
<th>FEAST Prediction</th>
<th>Relative Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>T-654</td>
<td>11.6</td>
<td>0.97</td>
<td>0.87</td>
<td>-10.3</td>
</tr>
<tr>
<td>T-655</td>
<td>11.8</td>
<td>0.86</td>
<td>0.93</td>
<td>8.1</td>
</tr>
<tr>
<td>T-659</td>
<td>11.7</td>
<td>1.17</td>
<td>1.04</td>
<td>-11.1</td>
</tr>
<tr>
<td>T-660</td>
<td>11.9</td>
<td>1.03</td>
<td>1.19</td>
<td>15.5</td>
</tr>
</tbody>
</table>
7.2. X425 Benchmark

Table-7.4 shows the X425 fuel data. The irradiation history for X425 assembly unfortunately is not available in the open literature. Therefore, it was approximated by the X430 irradiation history as follows. The peak coolant exit history of the X425 assembly is assumed to be identical to that of the X430 assembly, as they were irradiated at same time and their locations in the core were very close to each other. Then, assuming a constant mass flow rate and knowing the initial peak linear heat rate given in Table-7.4, the power history given in Figure-7.11 was generated.

Table-7.4: X425 Fuel Data

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel Composition</td>
<td>U-19-Pu-10Zr</td>
</tr>
<tr>
<td>Clad Material</td>
<td>HT-9</td>
</tr>
<tr>
<td>Fuel slug radius (mm)</td>
<td>2.16</td>
</tr>
<tr>
<td>Clad inner radius (mm)</td>
<td>2.54</td>
</tr>
<tr>
<td>Clad outer radius (mm)</td>
<td>2.92</td>
</tr>
<tr>
<td>Fuel Smear Density (%)</td>
<td>72.4</td>
</tr>
<tr>
<td>Fuel Active Length (cm)</td>
<td>34.3</td>
</tr>
<tr>
<td>Plenum to Fuel Ratio</td>
<td>1.0</td>
</tr>
<tr>
<td>Peak Linear Heat Rate (kW/m)</td>
<td>40</td>
</tr>
<tr>
<td>Peak Clad Temperature (°C )</td>
<td>590</td>
</tr>
</tbody>
</table>

Figure-7.11: Approximate Irradiation History of X425 assembly

The axial power profile given in Figure-7.2 has been adopted for X425 as well. The fast flux is again calculated by means of Equation-7.1.

In Figure-7.12, the fission gas release for the X425 peak fuel rod is shown. Comparing it with Ref. [27] which states that the fission gas release for the peak fuel rod of this assembly is 80 % at the end of life, the agreement is excellent. Figure-7.3 also shows generic data for U-19Pu-10Zr at lower burnup from Figure 2.1.
Figure-7.12: Fission Gas Release Behavior of the X425 Fuel Rod

Figure-7.13 shows the swelling behavior of the X425 peak fuel rod. The fuel touches the clad at the hot spot at ~2 at % burnup (Figure-13 (b)). Due to X425 lower linear heat rate compared to X430, the fuel temperature and thus the swelling rates are somewhat lower. The fuel located at 36 % of the fuel slug length is not radially restrained by the clad at up to 5 at % (Figure-7.13(a)).

Here too, the contact pressure starts to increase after the fuel becomes radially restrained. As can be seen in Figure-7.14, FCMI is negligible in the hot section of the fuel slug, and more significant in the cooler section of the fuel slug.
The cladding strain increases rapidly after 10 at % burnup as given in Figure-7.15.

The cladding strain profile at 15.8 at % peak burnup predicted by FEAST is compared to the ALFUS predictions and the experimental data in Figure-7.16. Both codes give reasonable results, with FEAST predicting the correct bottom-peaked profile and a closer peak clad strain.
Figure 7.16: Axial variation of cladding strain (peak burnup is 15.8 at %)

Table 7.5 gives a comparison of the FEAST, ALFUS, and also LIFE-METAL predictions with respect to the experimental data. It is important to note that the spectacular agreement of LIFE-METAL with the experimental data is due to the fact that X425 (and X441) were used for calibration of the various empirical coefficients in that code.

<table>
<thead>
<tr>
<th>Peak Burnup (at %)</th>
<th>Experimental Data</th>
<th>FEAST</th>
<th>ALFUS [5]</th>
<th>LIFE-METAL [33]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Cladding Strain (%)</td>
<td>Relative Error (%)</td>
<td>Cladding Strain (%)</td>
<td>Relative Error (%)</td>
</tr>
<tr>
<td>10.4</td>
<td>0.25</td>
<td>0.2</td>
<td>-20.0</td>
<td>-0.37</td>
</tr>
<tr>
<td>15.8</td>
<td>0.98</td>
<td>1.02</td>
<td>4.0</td>
<td>-0.86</td>
</tr>
</tbody>
</table>

7.3. X447 Benchmark

Table 7.6 gives the fuel specifications for X447 assembly and Fig. 7-17 shows the irradiation history.

Table 7.6: X447 Fuel Data

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel Composition</td>
<td>U-10Zr</td>
</tr>
<tr>
<td>Clad Material</td>
<td>HT-9</td>
</tr>
<tr>
<td>Fuel slug radius (mm)</td>
<td>2.16</td>
</tr>
<tr>
<td>Clad inner radius (mm)</td>
<td>2.54</td>
</tr>
<tr>
<td>Clad outer radius (mm)</td>
<td>2.92</td>
</tr>
<tr>
<td>Fuel Smear Density (%)</td>
<td>75.0</td>
</tr>
<tr>
<td>Fuel Active Length (cm)</td>
<td>34.3</td>
</tr>
<tr>
<td>Plenum to Fuel Ratio</td>
<td>1.4</td>
</tr>
<tr>
<td>---------------------</td>
<td>-----</td>
</tr>
<tr>
<td>Peak Linear Heat Rate (kW/m)</td>
<td>33</td>
</tr>
<tr>
<td>Peak Clad Temperature (C)</td>
<td>660</td>
</tr>
</tbody>
</table>

**Irradiation History:**

![Graphs showing peak linear heat rate and coolant outlet temperature vs. peak burnup](image.png)

Figure-7.17: DP04 fuel rod irradiation history

The axial power profile given in Figure-7.2 and the fluence correlation for EBR-II given in Eq-7.1 are again adopted in the analysis.

**Fission Gas Release**

The fission gas release at the end of life for the X447 fuel assembly is reported by Ref. [25] to be between 72-76 %. The FEAST prediction for the peak fuel rod is 75 %. The agreement is satisfactory. Figure-7.3 also shows generic data for U-19Pu-10Zr at lower burnup from Figure 2.1.
The FEAST-predicted cladding strain for the DP-04 fuel rod matches well with the experimental cladding strain data, as shown in Figure 7-19.

Fast reactor metal fuel rods containing minor actinides (MAs) and rare earths (REs) have been irradiated in the fast reactor PHENIX. The fuel specifications are given in Table-7.7.

<table>
<thead>
<tr>
<th>Fuel</th>
<th>U-19Pu-10Zr/U-19Pu-10Zr-5MA/U-19Pu-10Zr-5MA-5RE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clad</td>
<td>CW 15-15Ti Steel</td>
</tr>
<tr>
<td>Pin length (mm)</td>
<td>1793</td>
</tr>
<tr>
<td>Outer cladding diameter (mm)</td>
<td>6.55</td>
</tr>
</tbody>
</table>
The irradiation history of the metal fuel samples is given in Figure-7.20 [30]. Note that the total neutron flux was reported whereas the fast flux (>0.1 MeV) is actually needed for the irradiation creep calculation. According to Ref. [34] the PHENIX reactor cladding receives 18 dpa per cycle. Since three cycles were completed, the flux term is converted into dpa so that the cladding dose at the end of the irradiation is 54 dpa. The axial power profile given in Figure-7.21 was assumed to be unchanged during the irradiation.

![Figure-7.20(a): Total Peak Neutron Flux](image1)

![Figure-7.20(b): Peak Linear Power](image2)

![Figure-7.21: Axial Power profile](image3)

**Irradiation Creep**

The irradiation creep of CW 15-15Ti steel is given by following correlation [35]
where

\[ \varepsilon_{\theta}(\text{creep}) = \frac{3}{4} A(dpa^{-1} MPa^{-1}) \times \sigma_{\theta}(MPa) \times \phi t(dpa) \]  

(7.2)

\( \phi t \): The dose,
\( \varepsilon_{\theta}(\text{creep}) \): The circumferential creep strain component (total deformation minus one-third volume swelling), and
\( \sigma_{\theta} \): The average hoop stress

\( A = \) Creep Modulus (Figure-7.22)

Figure-7.22: Creep Modulus

The correlation given in Eq. (7.2) is given only for the \( \theta \)-component of the strain. According to the benchmark cases for X430, X425 and X447 assemblies the z-component of the creep strain remains negligibly small compared to the r- and \( \theta \)-components. As a consequence, the r-component of the irradiation creep strain is assumed to be the opposite of the \( \theta \)-component and the z-component is assumed to be zero in this analysis.

Note that thermal creep of this material is assumed to be negligible within the temperature range of interest [30].

**Swelling**

The temperature- and dose-dependent swelling behavior is given in Figure-7.23. A best fit of this data was performed in order to obtain the swelling strain at each time interval of the calculation. Since the maximum dose is 54 dpa, no swelling is expected for clad temperatures above 500 °C (Figure-7.23).
Figure-7.24 shows the simplified swelling behavior of the clad material as a function of dose, given the clad temperature. Given the temperature of a cladding node, Table-1 can be used as a look-up table to obtain the corresponding Point-1, Point-2 and Point-3 depicted in Figure-7.24. Having obtained the swelling behavior of the cladding, Eq-7.3 gives the swelling rate.

Figure-7.23: Swelling behavior of CW 15-15Ti
Figure-7.24: Simplified swelling behavior of the clad as a function of dose.

Table-1: Fitting Points

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Point-1 (dpa, swelling (%))</th>
<th>Point-2 (dpa, swelling (%))</th>
<th>Point-3 (dpa, swelling (%))</th>
</tr>
</thead>
<tbody>
<tr>
<td>460</td>
<td>(45,0)</td>
<td>(52,0.3)</td>
<td>(60,1.4)</td>
</tr>
<tr>
<td>500</td>
<td>(60,0)</td>
<td>(73,0.75)</td>
<td>(81,2.0)</td>
</tr>
</tbody>
</table>

\[
\Delta \varepsilon_s = \varepsilon_s(\phi(t + dt)) - \varepsilon_s(\phi(t))
\]  

(7.3)

\(\Delta \varepsilon_s\): Clad swelling within the time interval \(dt\)

\(\phi(t)\): Dose at time \(t\) (dpa)

**Results**

The fuel swelling predictions at peak axial power location are given in Figure-7.25, and the code-to-code agreement is rather good. In Figure-7.26 it is shown that FEAST somewhat underestimates the contact pressure with respect to ALFUS predictions. The axial elongations shown in Figure-7.27 agree reasonably well. The discrepancy in cladding strain predictions shown in Figure-7.28 could be related to the lower predicted contact pressure of the fuel element.
Figure-7.25(a) ALFUS prediction

Figure-7.25(b): FEAST prediction

Figure-7.26(a) ALFUS prediction

Figure-7.26(b): FEAST prediction
8. Conclusion

In this study a thermo-mechanical analysis code (named FEAST) has been developed to analyze the irradiation behavior of metal alloy fuels. Modeling of this fuel is challenging as it requires simulation of complex phenomena such as fission gas release, fuel swelling, irradiation and thermal creep, and fuel restructuring. Moreover, most material properties in the fuel change significantly with burnup and phase transitions during the irradiation. The code attempts to use mechanistic models were possible, to facilitate future extrapolation beyond the existing irradiation database with reasonable confidence.

A comparison of the new code against EBR-II experimental data shows that the agreement of FEAST and experimental data is quite satisfactory. The code is able to predict axial fuel swelling, peak cladding strain and fission gas release as a function of burnup reasonably well. A code-to-code benchmark was also performed using the latest PHENIX irradiation data. The results show that FEAST’s and the Japanese code ALFUS predictions agree on axial fuel swelling and total fuel swelling; however, there are some discrepancies in the cladding strain predictions.
9. Future Work

- A mechanistic diffusion-based model for Fuel Clad Chemical Interaction will be incorporated into the code.
- An intergranular creep-fracture model will be incorporated into the code to predict failure during transients.
- The transient capabilities of FEAST will be validated against furnace tests.

Appendix-A

A.1. Cladding Mechanical Properties

A.1.1. Young’s Modulus, Shear Modulus and Poisson’s Ratio

\[ E = 2.137 \times 10^5 - 102.74T \text{ (MPa)} \]
\[ G = 8.964 \times 10^4 - 53.78T \text{ (MPa)} \]
\[ \nu = \frac{E}{2G} - 1 \]

The unit of temperature is Celsius.

A.1.2. Thermal Expansion [24]

\[ \alpha \Delta T = -0.2191 + 5.678 \times 10^{-4} T + 8.111 \times 10^{-7} T^2 - 2.576 \times 10^{-10} T^3 \]

T: Temperature (K)
\( \alpha \Delta T \): Thermal Expansion (%)

A.1.3. Irradiation Creep

\[ \dot{\varepsilon}_i = \left[ B_o + A \exp\left(-\frac{Q}{RT}\right) \right] \phi \bar{\sigma}^{1.3} \]

\( \dot{\varepsilon}_i \): Equivalent Strain rate (%/sec)
\( B_o = 1.83 \times 10^{-4} \)
\( A = 2.59 \times 10^{14} \)
\( Q = 73000 \text{ (Cal/g-mol)} \)
\( R = 1.987 \text{ (Cal/g-mol-K)} \)
\( T = \text{temperature (K)} \)
\( \phi = \text{Neutron Flux (n/cm}^2/\text{s)} \)
\( \bar{\sigma} = \text{Equivalent Stress} \)
A.1.4. Thermal Creep

Thermal Creep has three components. They are primary, steady-state (secondary) and tertiary creep.

\[
\dot{\varepsilon}_T = \dot{\varepsilon}_{TP} + \dot{\varepsilon}_{TS} + \dot{\varepsilon}_{TT}
\]

\[
\dot{\varepsilon}_{TP} = \left[ C_1 \exp\left(-\frac{Q_1}{RT}\right) + C_2 \exp\left(-\frac{Q_2}{RT}\right) + C_3 \exp\left(-\frac{Q_3}{RT}\right) + C_4 \exp\left(-\frac{Q_4}{RT}\right) \right] \frac{C_5 \exp\left(-\frac{Q_5}{RT}\right) C_6 \exp(-C_7 t)}{\sigma}
\]

\[
\dot{\varepsilon}_{TS} = C_7 \frac{C_8 \exp\left(-\frac{Q_8}{RT}\right)}{\sigma^2} \quad \text{and} \quad \dot{\varepsilon}_{TT} = 4C_9 \exp\left(-\frac{Q_9}{RT}\right) \sigma^{10} t^3
\]

The values for the constants in these equations are:

\begin{align*}
C_1 &= 13.4 \\
C_2 &= 8.43 \times 10^{-3} \\
C_3 &= 4.08 \times 10^{18} \\
C_4 &= 1.6 \times 10^{-6} \\
C_5 &= 1.17 \times 10^9 \\
C_6 &= 8.33 \times 10^9 \\
C_7 &= 9.53 \times 10^{21} \\
Q_1 &= 15027 \\
Q_2 &= 26451 \\
Q_3 &= 89167 \\
Q_4 &= 83142 \\
Q_5 &= 108276 \\
Q_6 &= 282700 \\
R &= 1.987 \\
T &= \text{Temperature, K} \\
\sigma &= \text{Equivalent Stress (MPa)} \\
\dot{\varepsilon}_T &= \text{Effective Thermal Creep Strain (%/s)}
\end{align*}

A.2 Fuel Mechanical Properties

According to Ref. [3] the fuel Poisson’s Ratio is similar to that of the HT9 cladding.
A.2.1. Thermal Expansion Coefficient

The thermal expansion coefficient depends on the phases present in the fuel.

\[ \alpha = \begin{cases} 1.76 \times 10^{-5} & T < T_3 \\ \frac{T - T_3}{T_6 - T_3} \times 1.76 \times 10^{-5} & T_3 < T < T_6 \\ \frac{T - T_3}{T_6 - T_3} (2.01 \times 10^{-5} - 1.76 \times 10^{-5}) + 1.76 \times 10^{-5} & T \geq T_6 \end{cases} \]

\( T \): Temperature (K)
\( \alpha \): Thermal expansion coefficient (1/°C)
\( T_3 \): \( \alpha + \delta \rightarrow \beta + \gamma \) phase transition temperature
\( T_6 \): \( \beta + \gamma \rightarrow \gamma \) phase transition temperature


Similarly to the thermal expansion coefficient, the modulus of elasticity depends on the phases present.

\[ E = \begin{cases} 56 - 0.1158 \times (T - T_3) & T < T_3 \\ 20 - 0.1273 \times (T - T_3) & T_3 \leq T < T_6 \\ 31 - 0.08 \times (T - T_6) & T \geq T_6 \end{cases} \]

\( E \): Modulus of Elasticity (GPa)
\( T \): Temperature (°C)
\( T_3 \): \( \alpha + \delta \rightarrow \beta + \gamma \) phase transition temperature
\( T_6 \): \( \beta + \gamma \rightarrow \gamma \) phase transition temperature

A.2.3. Yield Strength

Using Ref. [9] and [36] the following relation has been derived for metallic fuel.

\[ \sigma_y = \begin{cases} 0.04 \times (T_6 - T) + 10 & T \geq T_6 \\ 0.08 \times (T_6 - T) + 10 & T < T_6 \end{cases} \] MPa
Appendix-B

A line-by-line input description of the FEAST code is given in Table-B.1 and a sample input file is shown after the table. The input file mimics that of the popular oxide fuel performance code FRAPCON, to facilitate use of FEAST by FRAPCON users. The input file format will be improved further to let the user specify a burnup-dependent axial power profile and neutron–flux-to-dose conversion factor.

FEAST Input File Description

Table-B.1

<table>
<thead>
<tr>
<th>Line Number</th>
<th>Description</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Title</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td># of time nodes</td>
<td>im</td>
</tr>
<tr>
<td>3</td>
<td># of axial nodes</td>
<td>na</td>
</tr>
<tr>
<td>4</td>
<td># of radial nodes within the fuel slug</td>
<td>nrf (six is recommended)</td>
</tr>
<tr>
<td>5</td>
<td># of radial nodes within the clad</td>
<td>nrc (&gt;2 is recommended)</td>
</tr>
<tr>
<td>6</td>
<td>Plenum to fuel ratio</td>
<td>ptof</td>
</tr>
<tr>
<td>7</td>
<td>Fuel outer radius (m)</td>
<td>rfo</td>
</tr>
<tr>
<td>8</td>
<td>Clad inner radius (m)</td>
<td>rci</td>
</tr>
<tr>
<td>9</td>
<td>Clad outer radius (m)</td>
<td>rco</td>
</tr>
<tr>
<td>10</td>
<td>Wire radius (m)</td>
<td>rw</td>
</tr>
<tr>
<td>11</td>
<td>Fission gas release model (1 is mechanistic model, 2 is empirical model)</td>
<td>fgr (1 is recommended, 2 can be used for comparison purposes)</td>
</tr>
<tr>
<td>12</td>
<td>Plutonium weight fraction</td>
<td>xpu</td>
</tr>
<tr>
<td>13</td>
<td>Zirconium weight fraction</td>
<td>xzr</td>
</tr>
<tr>
<td>14</td>
<td>Initial fill gas pressure (Pa)</td>
<td>fpgav</td>
</tr>
<tr>
<td>15</td>
<td>Bond sodium above the fuel level (m)</td>
<td>bonds</td>
</tr>
<tr>
<td>16</td>
<td>Fuel slug total length (m)</td>
<td>totl</td>
</tr>
<tr>
<td>17</td>
<td>Coolant pressure (Pa)</td>
<td>pco</td>
</tr>
<tr>
<td></td>
<td>Coolant inlet temperature (°C)</td>
<td>tcin</td>
</tr>
<tr>
<td>---</td>
<td>--------------------------------</td>
<td>--------</td>
</tr>
<tr>
<td>19</td>
<td>Axial Power distribution (normalized to one.)</td>
<td>qf(i), i= 1,na</td>
</tr>
<tr>
<td>20</td>
<td>Burnup (at %)</td>
<td>burnup(i), i= 1,im</td>
</tr>
<tr>
<td>21</td>
<td>Average Linear Heat Rate (kW/m)</td>
<td>qmpy(i), i=1,im</td>
</tr>
<tr>
<td>22</td>
<td>Coolant Outlet Temperature (°C)</td>
<td>tco(i), i=1,im</td>
</tr>
</tbody>
</table>

**Sample Input**

"FEAST: metal fuel code"

im= 26
na= 7
nrf= 6
nc= 4
ptof= 1.4
rfo= 2.858e-03
rci= 3.277e-03
rco= 3.683e-03
rw= 0.71e-03
fgr= 1
xpu= 0.19
xzr= 0.10
fgpav= 0.84E5
bonds= 6.35e-03
totl= 0.343
pec= 1.0e5
tcin= 370.0
qf= 0.952,1.062,1.116,1.115,1.056,0.939,0.760
burnup= 0.0,0.014,0.023,0.024,0.035,0.041,0.052,
0.052,0.061,0.065,0.067,0.067,0.068,0.072,0.073,
0.078,0.081,0.091,0.092,0.092,0.095,0.095,0.104,0.104,0.111,0.116
qmpy= 15.1,15.1,14.7,14.0,14.0,14.9,13.3,
10.7,11.8,11.9,10.5,12.3,12.3,11.8,11.5,
11.2,11.2,11.2,10.6,10.9,11.0,10.9,10.6,10.6,10.7,10.8
tcout= 559.0,559.0,553.0,547.0,541.0,557.0,534.0,
509.0,522.0,522.0,505.0,527.0,526.0,518.0,516.0,
514.0,514.0,516.0,510.0,514.0,514.0,511.0,510.0,510.0,512.0,512.0
References


[34] www.nea.fr/html/pt/docs/iem/lasvegas04/10_Session_IV/S4_01.pdf
