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NE 533 MOOSE Completed Project

Overview: The MOOSE project described herein is presented in three parts. The first part solves the thermal profile in a single fuel pellet for a steady state and transient condition and compares the results to the analytical solution. The second part solves for the steady state axial temperature profile in a fuel rod. The third part assesses the impact of expansion phenomena on gap closure.

Part One: I determined the temperature profile of a fuel pellet analytically and computationally, and found the maximum centerline temperature of a fuel pellet thermal transient with a constant and temperature dependent thermal conductivity.

For these problems, the fuel pellet has a radius of 0.5 centimeters, a gap thickness of 0.005 cm, and a cladding thickness of 0.01 cm. Additionally, the fuel pellet has a linear heating rate of 350 W/cm2, and the outer surface temperature of the cladding is 550 K. Figure 1 below shows a 2D cross-section of the fuel pellet.

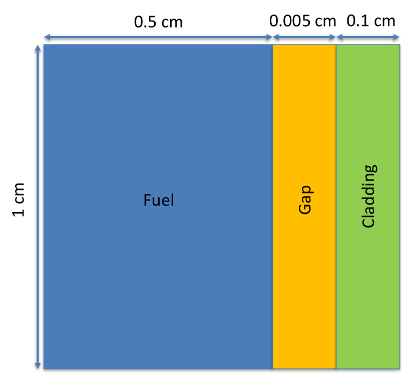

Figure 1. Fuel pellet 2D cross-section.

I selected to use a fuel thermal conductivity of 0.03 W/cm-K and a cladding thermal conductivity of 0.15 W/cm-k consistent with the first in class exercise. This allowed me to compare my answers to previously completed work.

Steady State Temperature Profile:

a. Analytical:

Temperature increases/decreases across non-heat-generating materials increases/decreases linearly to satisfy the constant heat flux condition for a steady state system. The total increase in temperature over a material can be calculated by assessing the temperature change across the whole thickness of the material. Equation 1 below shows the relationship of temperature as a function of cladding thickness and cladding heat conductivity. Equation 2 applies it for this problem and finds an inner cladding wall temperature of 557.43K.

$$T_{CI} = \frac{LHR}{2\pi R_f}\frac{t_C}{k_C} + T_{CO} \quad \text{(Eq. 1)}$$

$$T_{CI} = \frac{350\frac{W}{cm^2}}{2\pi(0.5\ cm)}\frac{0.1\ cm}{0.15\frac{W}{cm^2\cdot K}} + 550K = 624.27K \quad \text{(Eq. 2)}$$

Similarly for the gap, a heat increase/decrease can be calculated. However, the thermal conductivity of the gap depends on the gas temperature that fills it. For this problem, I assumed that the fuel was at the beginning of life and the gap is pure helium gas. The thermal conductivity of helium is defined in Equation 3. In Equation 4, I used the cladding inner wall temperature to set the thermal conductivity of the gas because it results in the lowest thermal conductivity, hence the most conservative heat increase across the gap. This ensures the highest centerline temperature is calculated, which results in the least margin to thermal requirements. Equations 5 and 6 define and apply the heat increase/decrease across the gap.

$$k_g = 16 \cdot 10^{-6} \cdot T^{0.79}\frac{W}{cm^2\cdot K} \quad \text{(Eq. 3)}$$

$$k_g = 16 \cdot 10^{-6} \cdot (557.43K)^{0.79} = 2.36 \cdot 10^{-3}\frac{W}{cm^2\cdot K} \quad \text{(Eq. 4)}$$

$$T_{FO} = \frac{LHR}{2\pi R_f}\frac{t_g}{k_g} + T_{CI} \quad \text{(Eq. 5)}$$

$$T_{FO} = \frac{350\frac{W}{cm^2}}{2\pi(0.5\ cm)}\frac{0.005\ cm}{2.36\cdot 10^{-3}\frac{W}{cm^2\cdot K}} + 624.27K = 860.3K \quad \text{(Eq. 6)}$$

Finally the temperature increase across the fuel can be determined. The temperature increase/decrease across the fuel is not linear because the fuel is generating heat. This relationship is defined in Equation 7. Equation 8 solves for the centerline temperature.

$$T_F(r) = \frac{LHR}{4\pi k_f}(1 - \frac{r^2}{R_f^{\ 2}}) + T_{FO} \quad \text{(Eq. 7)}$$

$$T_F(0\ cm) = \frac{350\frac{W}{cm^2}}{4\pi(0.03\frac{W}{cm^2\cdot K})}(1 - \frac{0^2}{(0.5)^2}) + 860.3K = 1788.7K \quad \text{(Eq. 8)}$$

The temperature increase/decrease across the three materials can then be combined to show the thermal profile of the fuel-cladding system.

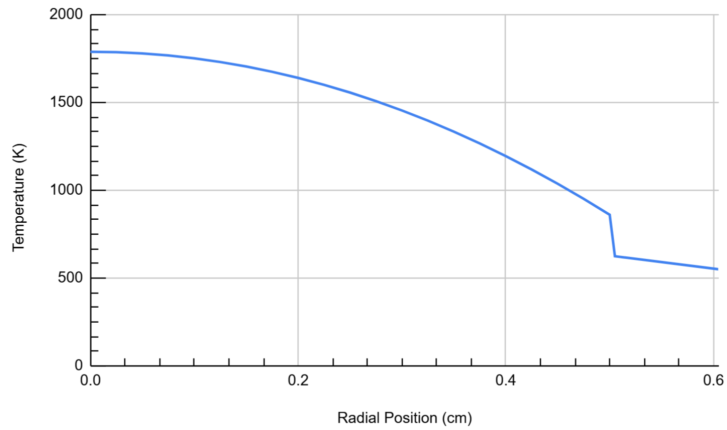

Figure 2. Analytical fuel-cladding system temperature profile.

b. Computed: This same problem can be solved computationally using the finite element method with the heat equations. I used a MOOSE simulation for this problem as well and the results were nearly identical to the analytical solution. Figure 3 visualizes this similarity where the analytical and computed solutions are practically identical.

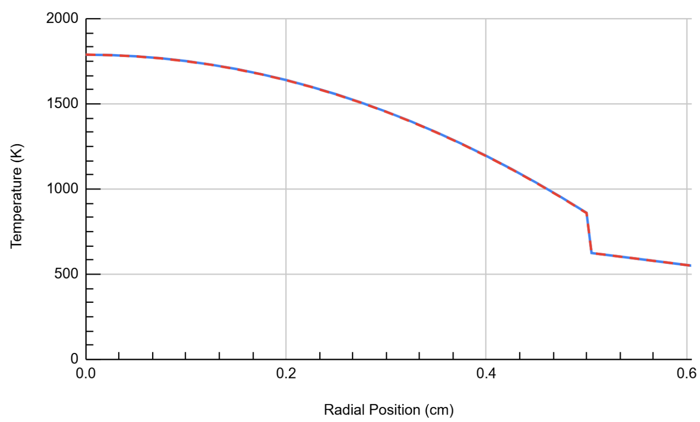

Figure 3. Analytical solution (blue) compared with the computed solution (red).

Transient Solution: The steady-state computational MOOSE input file can easily be modified to solve for the temperature response of the fuel-cladding system when power is spiked in the fueled region. For this problem, I investigated a power spike in the fueled region which doubled the linear heat rate at 20 seconds using Equation 9 below.

$$LHR = 350 \cdot (1 + e^{-\frac{(t-20)^2}{2}})\frac{W}{cm^2} \quad \text{(Eq. 9)}$$

a. Constant Fuel Thermal Conductivity: I made the following changes to the steady state MOOSE input file to generate a transient response. Note, the LHR constant is converted to a volumetric heat generation rate as previously described. The MOOSE simulation determined that the maximum centerline temperature for the fuel was 2055.03K at 21.8 seconds.

b. Temperature Dependent Fuel Thermal Conductivity: I then performed the same assessment again, but I added temperature dependence to the fuel thermal conductivity. I used Equation 10, which was provided in class, and changed the material property for the fuel in the MOOSE input file as shown below.

$$k_f(T) = \left[\frac{100}{7.5408+17.629\cdot\frac{T}{1000}+3.6142(\frac{T}{1000})^2} + \frac{6400}{(\frac{T}{1000})^{5/2}} \cdot e^{\frac{-16.45}{\frac{T}{1000}}} \right] \cdot 10^{-2} \frac{W}{cm\cdot K} \qquad \text{(Eq. 10)}$$

The MOOSE simulation determined that the maximum centerline temperature for the fuel when the thermal conductivity changed as a function of temperature was 2113.72K at 22.5 seconds.

<u>Mesh Justification</u>: For the model in part 2, I selected 20 nodes within the fuel, 20 nodes in the gap, and 4 nodes in the cladding. I chose the number of nodes to keep a consistent temperature increase between nodes to avoid missing subtle temperature variation effects, but minimize run time. A higher resolution solution could be performed if desired.

<u>Part Two</u>: For the second part of the NE 533 MOOSE project, I determined the temperature profile of the cladding inner surface, fuel surface, and fuel centerline computationally, and found the axial location of peak centerline temperature.

For these problems, I increased the fuel pellet height to 1 meter and set the inlet coolant temperature to 500 Kelvin. Figure 5 below shows a 2D cross-section of the fuel rod.

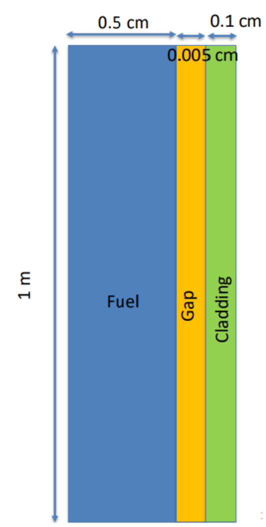

Figure 5. Fuel pellet 2D cross-section.

<u>Model Changes To Add Coolant Flow As A Factor</u>: To meet the problem statement for the second part of this assignment, I modified my boundary condition to account for a cooling flow in the channel. In the first part of the assignment, I was directed to set a constant cladding outer temperature of 550 K. I accomplished this using the following assumptions and steps:

1. Function Derivation: I used a FunctionDirichletBC boundary condition, which requires a function that defines the condition as a function of t, x, y, and z, instead of a DirichletBC boundary condition which sets a fixed value condition. To define that function I used the convective heat transfer equation derived in class.To implement this, I determined the temperature rise in the channel and then shaped it to match the integrated heat rise over the channel as shown in Equation 11.

$$T_{OC}(z) = \frac{LHR^{o} cos\left(\frac{\pi}{2\cdot\gamma}\left(\frac{z}{z_o}-1\right)\right)}{2\pi R_f h_{cool}} + \frac{\dot{q}\pi R_f^2 core_{height}}{v(rod_{pitch}^2 - \pi rod_{radius}^2)\rho C_v}\frac{sin\left(\frac{\pi}{2\cdot\gamma}\left(\frac{z}{z_o}-1\right)\right) + sin\left(\frac{\pi}{2\cdot\gamma}\right)}{2\cdot sin\left(\frac{\pi}{2\cdot\gamma}\right)} + T_i \quad \text{(Eq. 11)}$$

2. Variable Definitions: Realistic variables were then defined based on scaling common Westinghouse AP 1000 reactor parameters to match this sized reactor. These values could be modified to match a specific design to assess core thermal performance. SI units were used for this simulation to simplify calculations.

a. Given parameters: fuel radius (0.5 cm), gap thickness (0.005 cm), clad thickness (0.1 cm), core height (1 m), LHR (350 W/cm), and inlet temperature (500 K) were given.

b. Calculated parameters: Rod diameter (0.605 cm) was computed geometrically and volumetric heat production rate (445.6 W/cm3) can be calculated using Equation 12.

$$Q_{ave} = \frac{LHR}{\pi R_f^2} \quad \text{(Eq. 12)}$$

c. Assumed parameters:

i. Material Thermal Conductivities: I selected to use a gap thermal conductivity of 0.00236 W/cm-K and a cladding thermal conductivity of 0.15 W/cm-K consistent with the first in class exercise. Additionally, I used the fuel thermal conductivity correlation as a function of temperature as described in class (Eq. 13).

$$k_0 = \frac{100}{7.5408_{17.629T} + 3.6142T^2} + \frac{6400}{T^{5}/_{2}} exp\left(\frac{-16.35}{T}\right) \quad \text{(Eq. 13)}$$

ii. Rod Pitch: I used the ratio of rod pitch to rod diameter (1.326) from reference (1) to scale the rod pitch for this problem. Rod pitch was 1.60446 cm.

iii. Coolant Average Velocity: I scaled the coolant average velocity for this problem to match the mass flow rate per rod per unit power from the reference (1) AP 1000 reactor to the power generated by a rod in this assignment. This resulted in an average coolant velocity of 1.264 m/s. For reference, this is roughly a quarter of the average coolant velocity of the AP 1000 reactor. However, it results in the same 80 K temperature rise over the height of the core as desired.

iv. Water Heat Transfer Coefficient: For this problem, I used a common heat transfer coefficient of 30 kW/m2-K as stated in reference (2) for light water reactors. More specific heat transfer coefficients can be calculated using the Dittus-Bölter correlation, but that approach was beyond the scope of this assignment.

v. Core pressure and average temperature: I matched the 2250 psia core pressure of the AP 1000 reactor from reference (3). I used an average temperature of 550 Kelvin to set water properties for the whole channel because there is a 80 Kelvin temperature rise across the channel in an AP 1000 reactor as stated in reference (1). The temperature of 550 Kelvin, while not the exact average temperature, was convenient to use with a steam table. Ultimately, I used a water property calculation, reference (4), to determine the water properties shown in Table I.

Table I. Water material properties for the selected reactor condition.

Property	Value	Unit
medium :	water, fluid	
pressure :	155.1375	[bar]
temperature :	276.85	[Celsius]
density :	769.71815384007	[kg / m^3]
dynamic viscosity :	9.7661703428876E-5	[Pa s]
kinematic viscosity :	0.12687982340243	[10^{-6} m^2 / s]
specific inner energy :	1196.5505899213	[kJ / kg]
specific enthalpy :	1216.7056946471	[kJ / kg]
specific entropy :	3.0101860744483	[kJ / kg K]
specific isobar heat capacity : cp	5.0268704880304	[kJ / kg K]
specific isochor heat capacity : cv	3.0768769263483	[kJ / kg K]
thermal conductivity :	0.60123176341873	[W / m K]
speed of sound :	1094.9450982938	[m / s]

Results: Using the equations and assumptions described above, the MOOSE model produced a temperature profile that was consistent with my expectations as described below:

a. Cladding Surface Temperature Profile: The temperature profile for the inner cladding surface varies semi-parabolically from 580 K to a peak of 665 K at 0.86 m before falling to 660 K as shown in Figure 6.

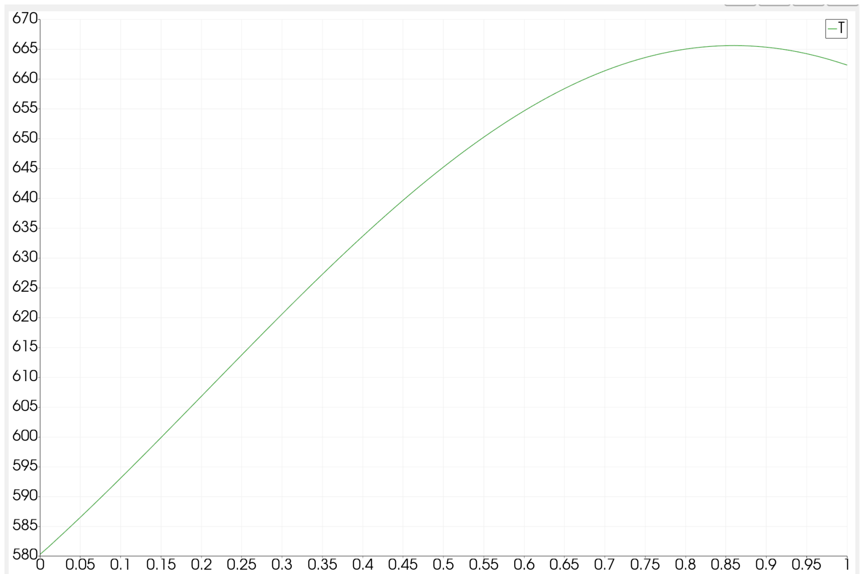

Figure 6. Inner cladding surface temperature (K) as a function of axial position (m).

b. Fuel Surface Temperature Profile: The temperature profile for the fuel surface varies semi-parabolically from 815 K to a peak of 900 K at 0.86 m before falling to 895 K as shown in Figure 7. This shows a 235 K temperature increase across the 0.005 cm gap between the cladding and fuel. This is larger than expected, but is reasonable given the low thermal conductivity of helium at the beginning of life.

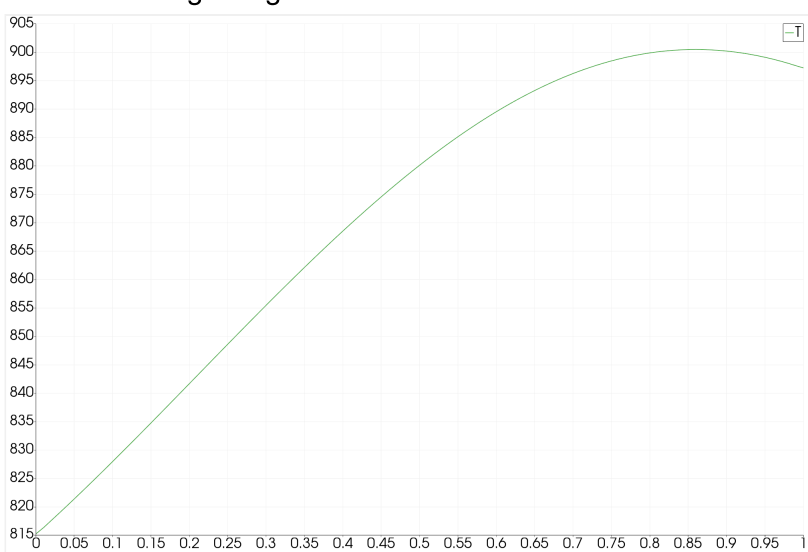

Figure 7. Fuel surface temperature (K) as a function of axial position (m).

c. Fuel Centerline Temperature Profile: The temperature profile for the fuel centerline varies semi-parabolically from 1790 K to a peak of 1950 K at 0.86 m before falling to 1945 K as shown in Figure 8. This shows a temperature rise of 975 K at the bottom of the core and rise of 1050 K at the peak core power. This is the only material in the model that shows a non-constant temperature rise axial, which is due to the variable thermal conductivity of the fuel set up in the first part of this MOOSE assignment.

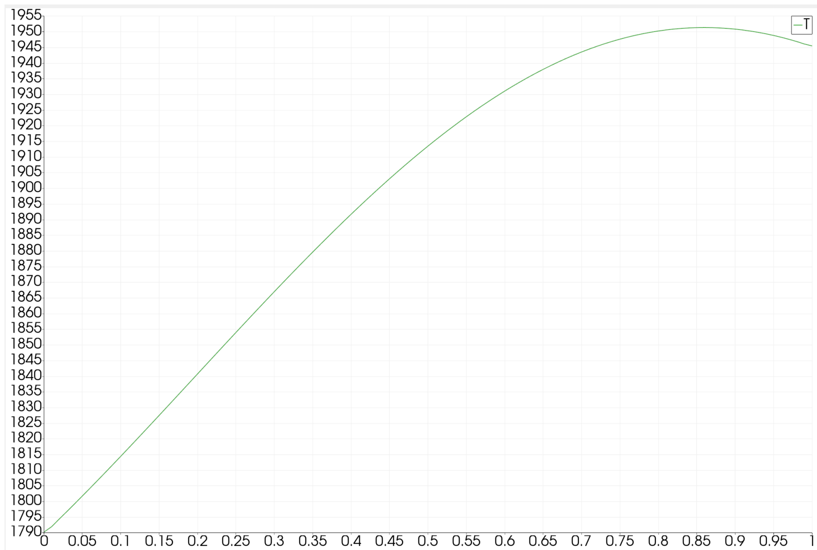

Figure 8. Fuel Centerline Temperature (K) as a function of axial location (m).

d. Axial Location of Peak Centerline Temperature: As shown in Figure 4, the location of peak centerline temperature in the fuel is 0.86 m above the bottom of the core. At this location, the fuel is 1950 K. At this height, the cladding temperature is the highest, because the coolant temperature in the channel has increased to store the heat generated from the fuel.

Part Three: For the third part of the NE 533 MOOSE project, I returned to the 1 cm tall pellet in the first part, but added expansion phenomena to measure gap change over time and performed a cracking analysis based on my end results.

Expansion Physics: To determine gap size as a function of burnup I added the following expansion phenomena:

a. Solid Mechanics Properties: To add in geometric change effects, the elastic modulus and poisson's ratio must be provided. I used the values from Lecture 5. Fuel has an elastic modulus of 200 GPa and a poison's ratio of 0.345. The cladding has an elastic modulus of 80 GPa and a poisson's ratio of 0.41. For the gap, I assigned an elastic modulus of 1e-10 to make it fully pliable.

b. Thermal Expansion: Thermal expansion captures the increase in size due to heating from an initial temperature. Equation 14 captures this phenomena. For this project, I assumed a 300K starting temperature since that is approximately room temperature. For the thermal coefficient expansion, I used the values presented in lecture six in class, 11e-6 for fuel and 7.1e-6 for clad.

$$\epsilon_0 = (T - T_0)\alpha I \qquad \text{(Eq. 14)}$$

c. Densification: Fuel pellets are not fully dense when they are manufactured. As a result, the pellets densify, or contract, as the void space in the pellet is consumed when at a raised temperature. Equation 15 captures this phenomena. For this project, I assumed values from lecture 10. So the pellet is initially 99% dense ($\Delta\rho_0$), burnup densification stops at 5 MWD/kgU (β_D), and the densification coefficient is as described in Equation 16.

$$\epsilon_D = \Delta\rho_0 \left(e^{\frac{\beta \ln 0.01}{C_D \beta_D}} - 1 \right) \qquad \text{(Eq. 15)}$$

C_D = 7.235 − 0.0086 (T − 25) for T < 750C
CD = 1 for T ≥ 750C (Eq. 16)

d. Fission Product Induced Swelling: As fuel is depleted, fission products build up in the fuel. Fission products are either solid or gaseous. As a result, the swelling from each type of fission product is capture using a different equation, with gaseous products being temperature dependent while solid products are not. Equation 17 defines the solid fission product strain, and Equation 18 defines the gaseous fission product strain. For this project, I assumed that the fuel density is 10.97 g/cc like used in Lecture 12. This density changes initially in service as the fuel densifies, but a constant value was picked here for simplicity.

$$\epsilon_{sfp} = 5.577 \times 10^{-2} \rho\beta \qquad \text{(Eq. 17)}$$

$$\epsilon_{gfp} = 1.96 \times 10^{-28} \rho\beta (2800 - T)^{11.73} e^{-0.0162(2800-T)} \, e^{-17.8\rho\beta} \qquad \text{(Eq. 18)}$$

e. Boundary Conditions: Boundaries must be applied to solve the problem. For this project I constrained both bottom and top surfaces in the Z direction, which assumes an infinitely long pellet, similar to how fuel in a rod would be constrained. I constrained the left boundary in the R direction since this problem has radial symmetry about the left boundary. Finally I assumed that the cladding expanded about its midplane because it would be pinned at both ends, forcing the thermal expansion of the cladding to expand out into the coolant channel and fuel-clad gap slightly. To implement this in code I halved the cladding thickness and applied a right boundary R direction constraint. This required me to increase the fixed temperature boundary from 550K to 582K to take the temperature rise across the outer half of the cladding into account.

<u>Updated Thermal Conductivity</u>: In Part One, I modeled fuel thermal conductivity as a function of temperature. In Part Three, I also added the impact of burnup to fuel thermal conductivity as well using the Equations 19 - 24 below.

$$k = (1 - R_f(T))k_{ph1}(T, \beta) + R_f(T)k_{ph2}(T, \beta) + k_{el}(T)$$

$$R_f(T) = \frac{1}{2}\left(1 + \tanh\left(\frac{T - 900}{150}\right)\right)$$

$$k_{ph1} = \frac{1}{(9.592 \times 10^{-2} + 6.14 \times 10^{-3}\beta - 1.4 \times 10^{-5}\beta^2 + (2.5 \times 10^{-4} - 1.81 \times 10^{-6}\beta)T}$$

$$k_{ph2} = \frac{1}{(9.592 \times 10^{-2} + 2.6 \times 10^{-3} \cdot \beta + (2.5 \times 10^{-4} - 2.7 \times 10^{-7}\beta)T}$$

$$k_{el} = 1.32 \times 10^{-2} \, e^{1.88 \times 10^{-3} T}$$

Gap Closure: Using the updated model, the change in gap size as a function of depletion is plotted in Figure 9. For my project, I ran the steady state solution at multiple depletions and recorded the resulting gap size. MOOSE is also capable of performing multiple steady state solutions in sequence using a transient executioner, but I elected not to use that approach. Surprisingly, the gap closes when the reactor is initially critical. The gap size increases as the core depletes because the fuel densifies. This densification is overcome by fission product buildup at 3 MWd/kgU. This is before the densification completes at 5 MWd/kgU. The fission product buildup and swelling then closes the gap again at 12.3925 MWd/kgU.

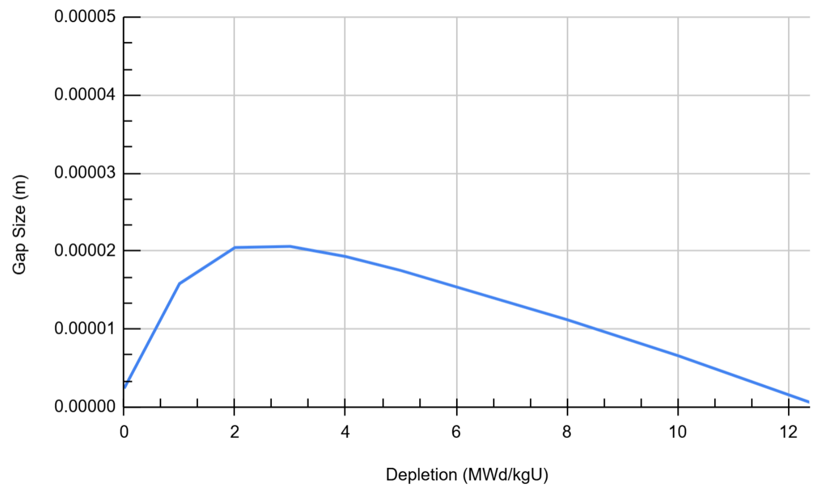

Figure 9. Gap size as a function of depletion.

Fuel Displacement: The same mesh data used to plot gap size can be used to plot the fuel displacement as a function of burnup as well (Figure 10). Like the gap model, the fuel starts out in contact with the cladding. The fuel then contracts as it densifies, reaching a minimum displacement of 0.002682 cm at 3 MWd/kgU. Eventually the pellet surface returns to the cladding surface at 12.3925 MWd/kgU having expanded by 0.004682 cm.

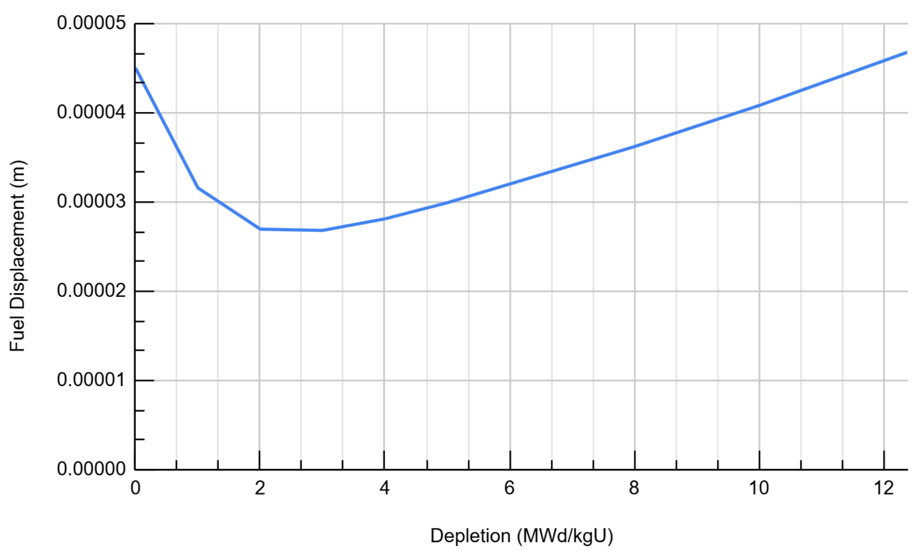

Figure 10. Fuel displacement as a function of depletion.

Stress State: The stress state of the fuel pellet also changes with depletion. For my project, I measured the vonMises stress of the pellet to understand the stress state of the pellet relative to failure. My simulations showed that the stress was highest at the center of the pellet as plotted in Figure 11 below. Notably there is an increase in stress as the pellet densifies in the beginning of life peaking at 5 MWd/kgU. The stress state then reduces as the pellet expands.

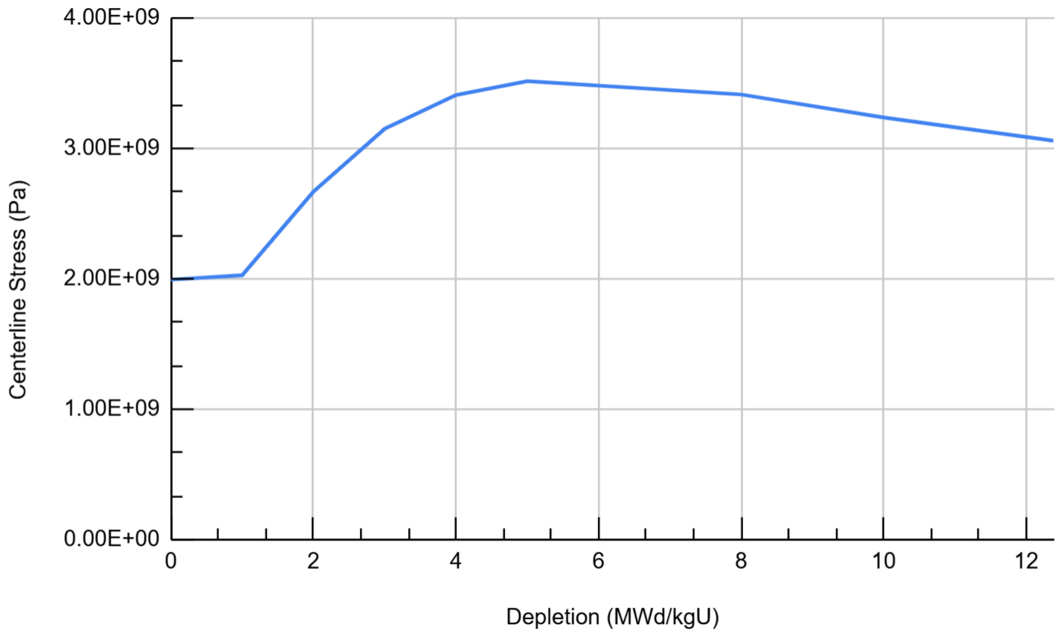

Figure 11. Centerline VonMises stress as a function of depletion.

Pellet Cracking: A separate way to evaluate pellet performance relative to stress states is to calculate its failure radius. Equation 11 defines the hoop stress based on thermal expansion. Since the fuel starts in contact with the cladding surface and then returns to contact using fission products, I chose to assess the initial thermal expansion state to assess crack formation since once a crack forms the stress in the pellet is relieved. Consistent with Lecture 6, I chose a yield stress of 130 MPa. From the simulation output file I found a temperature rise of 628 K, a radius of 0.504503 cm.

$$\sigma_{\theta\theta}(\eta) = -\frac{\alpha E \Delta T}{4(1-\nu)} \left(1 - 3\left(\frac{r}{R_f}\right)^2\right) \quad \text{(Eq. 25)}$$

Solving for the radius where the stress equals the yield stress results in cracking 0.179301 cm into the pellet, or 35.5% into the pellet.

References

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