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NE 533 MOOSE Project Part 1

Problem Set Up: For the first part of the NE 533 MOOSE project, 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 centimeters, and a cladding thickness of 0.01 centimeters. Additionally, the fuel pellet has a linear heating rate of 350 Watts per squared centimeter, and the outer surface temperature of the cladding is 550 Kelvin. Figure 1 below shows a 2D cross-section of the fuel pellet.

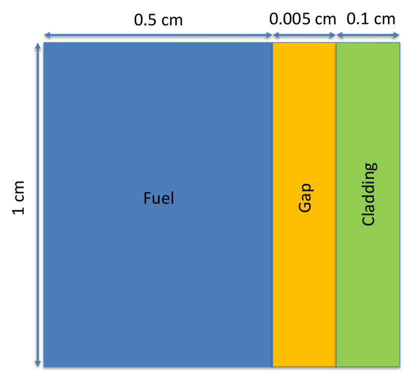


Figure 1. Fuel pellet 2D cross-section.

I selected to use a fuel thermal conductivity of 0.03 Watts per centimeter Kelvin and a cladding thermal conductivity of 0.15 Watts per centimeter Kelvin consistent with the first in class exercise. This allowed me to compare my answers to previously completed work. Alternative thermal conductivity values could be used in future assignment parts.

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.

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

$$T_{CI} = \frac{350\ \frac{W}{cm^2}}{2\pi(0.5\ cm)} \frac{0.01\ cm}{0.15\frac{W}{cm^2 \cdot K}} + 550K = 557.43K \qquad \text{(Eq. 2)}$$

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.

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

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

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

$$T_{FO} = \frac{350\ \frac{W}{cm^2}}{2\pi(0.5\ cm)} \frac{0.005\ cm}{2.36 \cdot 10^{-3} \frac{W}{cm^2 \cdot K}} + 557.43K = 793.46K \qquad \text{(Eq. 6)}$$

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.

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

$$T_F(0\ cm) = \frac{350\frac{W}{cm^2}}{4\pi(0.03\frac{W}{cm^2 \cdot K})}\left(1 - \frac{0^2}{(0.5)^2}\right) + 793.46K = 1721.86K \qquad \text{(Eq. 8)}$$

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

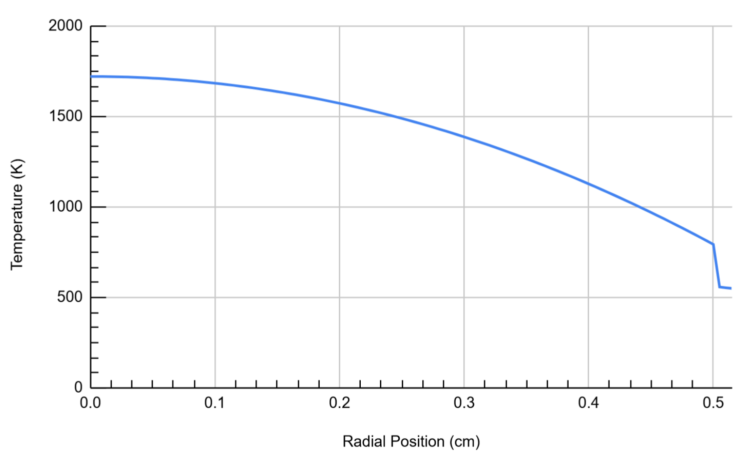


Figure 2. Analytical fuel-cladding system temperature profile.

b. Computed: This same problem can be solved computationally using the finite element method with the heat equations. For this project, I used MOOSE, which is an open-source software for solving coupled physics problems. MOOSE uses input files to generate the problem geometries and material properties, and define the problem to be solved. Below is how I constructed the input file for this problem.

i. Mesh Generation and Material Properties: Below are the mesh and materials properties used for this simulation. I created a GeneratedMeshGenerator for each submaterial to control the number of elements in each material region. Then I stitched the meshes together using the StitchedMeshGenerator because MOOSE only takes in one mesh for this calculation. Then I added in material blocks, or definitions, to each subregion to ensure the correct material property is applied. For the materials, I used the same value for the computed case as the analytical case to aid in solution comparison.

```
[Mesh]
  [fuelMesh]
    type = GeneratedMeshGenerator
    dim = 2
    xmin = 0
    xmax = 0.5
    ymin = 0
    ymax = 1
    nx = 200
    ny = 1
  []
  [gapMesh]
    type = GeneratedMeshGenerator
    dim = 2
    xmin = 0.5
    xmax = 0.505
    ymin = 0
    ymax = 1
    nx = 20
    ny = 1
  []
  [cladMesh]
    type = GeneratedMeshGenerator
    dim = 2
    xmin = 0.505
    xmax = 0.515
    ymin = 0
    ymax = 1
    nx = 200
    ny = 1
```

```
  []
  [cmbn]
    type = StitchedMeshGenerator
    inputs = 'fuelMesh gapMesh cladMesh'
    stitch_boundaries_pairs = 'right left; right left'
  []
  [fuelBlock]
    type = SubdomainBoundingBoxGenerator
    input = cmbn
    block_id = 1
    block_name = 'fuel'
    bottom_left = '0 0 0'
    top_right = '0.5 1 0'
  []
  [gapBlock]
    type = SubdomainBoundingBoxGenerator
    input = fuelBlock
    block_id = 2
    block_name = 'gap'
    bottom_left = '0.5 0 0'
    top_right = '0.505 1 0'
  []
  [cladBlock]
    type = SubdomainBoundingBoxGenerator
    input = gapBlock
    block_id = 3
    block_name = 'clad'
    bottom_left = '0.505 0 0'
    top_right = '0.515 1 0'
  []
  coord_type = RZ
  rz_coord_axis = Y
[]

[Materials]
  [fuelMaterial]
    type = HeatConductionMaterial
    thermal_conductivity = 0.03
    block = 'fuel'
  []
  [gapMaterial]
    type = HeatConductionMaterial
    thermal_conductivity = 0.00236
    block = 'gap'
```

```
  []
  [cladMaterial]
    type = HeatConductionMaterial
    thermal_conductivity = 0.15
    block = 'clad'
  []
[]
```

ii. Kernel, Variables, and Boundary Conditions: The Kernal declares what type of physics needs to be applied to the problem and the linked variable for the engine. I also included the heat source physics here as well. Note, the value of the heat source is the volumetric heat generation rate. This value is calculated by dividing the linear heat rate by pi and the fuel radius. The variable T is declared for use in the kernel. Then I applied the fixed boundary condition of 550K to the cladding outside wall per the problem instructions.

```
[Kernels]
  [heat_conduction]
    type = HeatConduction
    variable = T
  []
  [heat_source]
    type = HeatSource
    variable = T
    value = 445.63384
    block = 'fuel'
  []
[]

[Variables]
  [T]
  []
[]

[BCs]
  [t_right]
    type = DirichletBC
    variable = T
    value = '550'
    boundary = 'right'
  []
[]
```

iii. Executioner and Output: Finally the executioner defines the solution type for the engine to calculate. In this case, I wanted the steady state solution. The Outputs block is also declared so the results can be viewed using a data visualizer like ParaView.

```
[Executioner]
  type = Steady
[]

[Outputs]
  exodus = true
[]
```

Results: The MOOSE computation for this input file was nearly identical to the analytical solution. Table I below shows agreement to within a few tenths of a degree, and Figure 3 visualizes this similarity where the analytical and computed solutions are practically identical.

Table I. Analytical and Computed Comparison

| Radial Position (cm) | Analytical (K) | Computed (K) |
|---|---|---|
| 0.515 | 550 | 550 |
| 0.505 | 557.43 | 557.28 |
| 0.5 | 793.46 | 792.14 |
| 0.25 | 1489.76 | 1488.72 |
| 0 | 1721.86 | 1722.47 |

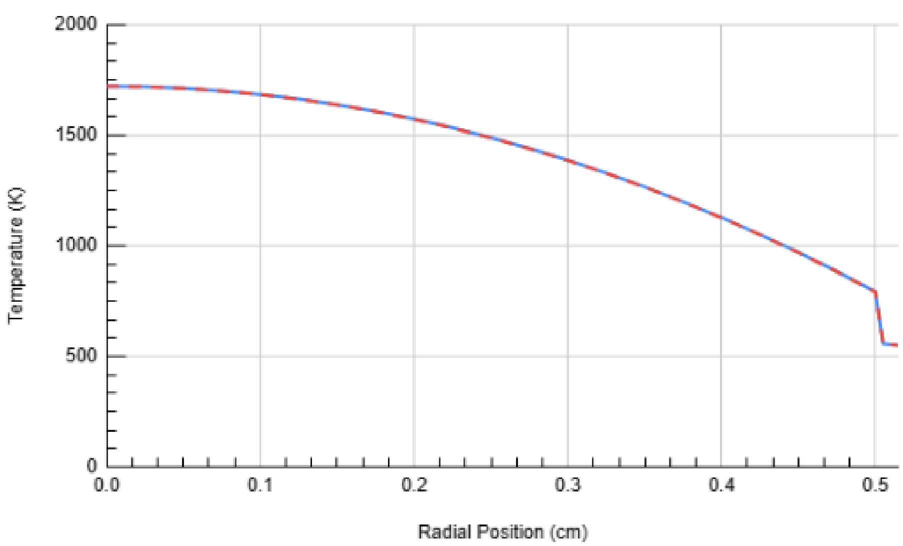


Figure 3. Analytical solution (blue) compared with the computed solution (red).

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.

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

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.

```
[Executioner]
  type = ~~Steady~~Transient
  end_time = 55
  dt = 0.1
[]

[Kernels]
  [heat_conduction]
    type = HeatConduction
    variable = T
  []
  [heat_source]
    type = HeatSource
    variable = T
    ~~value = 445.63384~~
    function = '445.63384*exp(-1*((t-20)^2)/2)+445.63384'
    block = 'fuel'
  []
[]
```

The MOOSE simulation determined that the maximum centerline temperature for the fuel was 2055.03K at 21.8 seconds. However, I was not able to model to converge out to 100 seconds per the instructions. I could only get convergence through 55 seconds per the instructions. The transient subsides a little after 20 seconds so the interesting information is captured.

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.

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

```
[Materials]
  [fuelMatCond]
    type = ParsedMaterial
    property_name = 'thermal_conductivity'
    coupled_variables = T
    expression =
'((100)/(7.5408+17.629*T/1000+3.6142*(T/1000)^2)+(6400)/((T/1000)^(5/2))*exp((-16.45
)/(T/1000)))*10^(-2)'
    block = 'fuel'
  []
  [fuelDensityCp]
    type = GenericConstantMaterial
    prop_names = 'density specific_heat thermal_conductivity_dT'
    prop_values = '10.97 0.26 0' # g/cm3  J/gK
    block = 'fuel'
  []
  [gapMaterial]
    type = HeatConductionMaterial
    thermal_conductivity = 0.00236
    specific_heat = 5.19 # J/gK
    block = 'gap'
  []
  [gapDensity]
    type = GenericConstantMaterial
    prop_names = 'density'
    prop_values = 0.0000857 # g/cm3
    block = 'gap'
  []
  [cladMaterial]
    type = HeatConductionMaterial
    thermal_conductivity = 0.15
    specific_heat = 0.285 # J/gK
    block = 'clad'
  []
  [cladDensity]
    type = GenericConstantMaterial
    prop_names = 'density'
    prop_values = 6.56 # g/cm3
    block = 'clad'
  []
[]
```

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. However, I was not able to model to converge out to 100 seconds per the instructions. I could only get convergence through 30 seconds per the instructions. The transient subsides a little after 20 seconds so the interesting information is captured.