MOOSE Simulation Project: Part 1

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1 Introduction

This project involved using the MOOSE[3] (Multiphysics Object Oriented Simulation Environment) simulation framework to model the temperature profile of a fuel pellet within a fuel rod. Specifically, steady-state and transient temperature profiles with both constant thermal conductivity and temperature-dependent thermal conductivity were modeled. The simulation object used here is a 2-D representation of one half of a fuel rod in order to easily model how heat conducts radially from the inside of the fuel pellet to the outer cladding. The axial (Z) and radial (R), dimensions for each element were given as seen in Figure 1. The materials for each element were not given, but decided to use uranium dioxide UO_2 as fuel, helium (He) as my gap and Zirconium (Zr) as my cladding as they are commonly used materials in fuel rods. [1]

1.1 Simulation Setup

1.2 Mesh

The coordinate system 'RZ' was applied to account for the 2-D axisymmetric geometry that is needed for this particular problem where a the shape of a fuel rod is considered. Although the systems with constant thermal conductivity are 1 dimensional problems, 2 dimensions are useful when applying a temperature-dependent thermal conductivity which solves variations in the R and Z directions. Since heat within a fuel rod is generated from the fuel pellet, then conducted radially outward through multiple materials, the resolution in the radial direction needs to be higher than those in the axial direction where material is uniform and heat transfer is less complex. The resolution is enhanced by increasing the number of points in the radial (nx) and axial (ny) directions. My selection for the nx and ny were determined by running a range of simulations with different nx and ny values. The temperature profiles of these simulations were then compared to the analytical temperature profile which was calculated in python. As seen in Figure 2, having an nx=400, ny=4 and nx=600, ny=6 gave a temperature profile close to that of the analytical approach. I chose to use nx=400 and ny=4 resolution for mesh since the temperature profile was

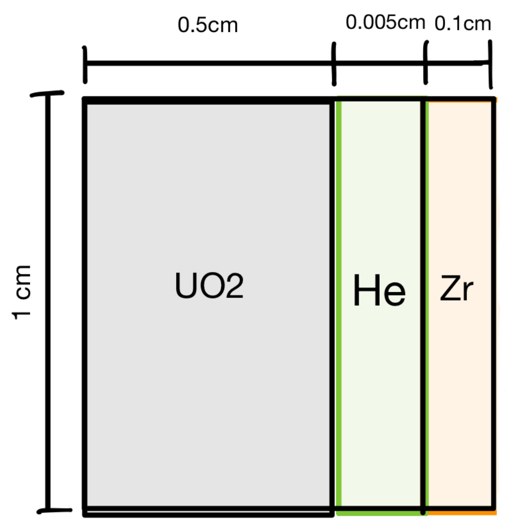

Figure 1: Schematic of the 2-D fuel rod model being simulated and studied where UO_2 is the fuel, He is the gap, and Zr is the cladding.

close to the analytical results without exceeding their temperature values. Additionally, for the transient systems, a time derivative kernel is implemented into the heat conduction equation to vary temperature with time.

Within the Mesh, the material boundaries were specified as subdomains. The material specific boundaries used within the mesh are seen in Figure 1. This includes the radial and axial length in centimeters of each material subdomain in the overall fuel rod simulation object.

1.3 Variables and Functions

The heat conduction equations, which solve for temperature as a function of space and time in all of the systems, are solved using the first order finite element approximation. The heat conduction equations do differ between steady state 1 and transient 2 systems however, since temperature varies with time in the transient systems. The transient heat conduction equation also requires the heat capacity and density of each material as these properties effect the heating and cooling rates for of each material.

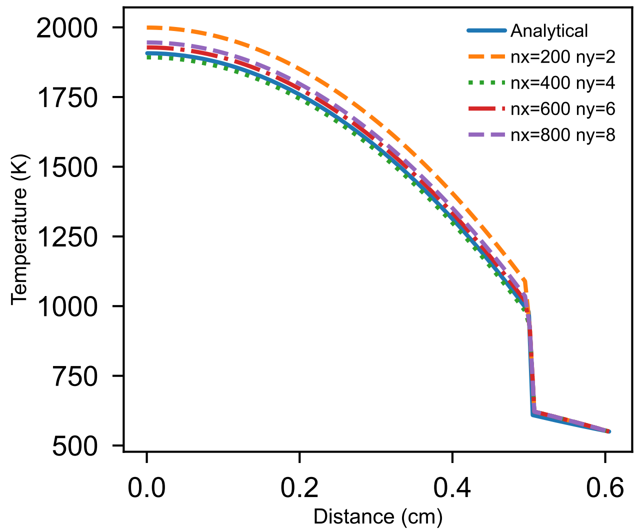

Figure 2: Comparison of steady state temperature profiles of systems with varying mesh resolutions to the analytically solved temperature profile. All temperature profiles are holding thermal conductivity constant.

$$0 = \nabla \cdot (k\nabla T) + Q \tag{1}$$

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k\nabla T) + Q \tag{2}$$

The applied heat source is represented by the Volumetric Heat Rate (VHR) which calculates the amount of heat generated through the length of the material (or fuel rod). The VHR for the steady state systems is constant (350 W/m^2) and represents a uniform heat source. The VHR for the transient systems 3 is modeled by a Gaussian function that varies with time since this system is time dependent. This function represents a heat generation rate that peaks at $t = 20\,\mathrm{s}$ and decays over time.

$$\mathrm{VHR}(t) = 350 \times \exp\left(\frac{-(t-20)^2}{2}\right) + 350 \tag{3}$$

1.4 Materials

For my materials, I used UO_2 as fuel, He as my gap, and Zr as a cladding, since these are all commonly used reactor materials. The densities, heat capacities, and thermal conductivities for each material were found in literature [4] [2] [5] and declared within each material so they could be used to calculate the heat conduction equations.

Material	k (W/cm·K)	ρ (g/cm³)	c_p (J/g·K).
UO_2	0.03	10.98	0.33
(Helium)	0.0015	$0.1786\ \times 10^{-3}$	5.19
(Zirconium)	0.17	6.5	0.35

Table 1: Materials and Their Properties Used in Simulation

For the temperature-dependent thermal conductivity systems we use equation 4 for the fuel, equation 5 for the gap, and equation 6 for the cladding.

$$k_{\text{fuel}}(T) = \frac{100}{7.5408 + 17.629\frac{T}{1000} + 3.6142\left(\frac{T}{1000}\right)^2 + 6400\left(\frac{T}{1000}\right)^{5/2}\exp\left(\frac{-16.35}{T/1000}\right)} \tag{4}$$

$$k_{\text{gap}}(T) = 16 \times 10^{-6} \cdot T^{0.79} \tag{5}$$

$$k_{\text{cladding}}(T) = 8.8527 + 7.0820\times 10^{-3}\cdot T + 2.5329\times 10^{-6}\cdot T^2 + 2.9918\times 10^3\cdot \frac{1}{T} \tag{6}$$

1.5 Boundary Conditions

Different boundary conditions were applied to the left and right sides of the model. The right side, where the outer cladding is, uses the Dirichlet Boundary condition. The Dirichlet 7 Boundary holds a specified temperature value constant at the boundary which is consistent with the outer surface of our cladding that is held at a constant temperature of 550K. The constant temperature is used to mimic the coolant surrounding a fuel rod in a reactor. The left side of the system/center of the fuel pellet, uses the Neumann 8 boundary condition. The Neumann boundary condition makes the heat flux zero at the specified boundary to maintain radial symmetry. Since the radial axis is symmetric at this location, this a zero heat flux boundary is appropriate. The Neumann boundary condition is also applied to the top and bottom of the system to ensure that the transfer of heat is isolated along the length of the rod.

$$u = g \quad \text{on } \partial\Omega_D \tag{7}$$

$$\frac{\partial u}{\partial n} = h \quad \text{on } \partial\Omega_N \tag{8}$$

2 Executioner

For the executioner, steady state or transient was applied, depending on the system type being simulated. For transient systems, an iterative time stepper was added to adjust the time step based on the simulation rather than using a constant time step value.

3 Results

From figure 3, we can see that the curve of the analytical and modeled constant thermal conductivity curves are very similar. Both have peaks of 1800K at the centerline temperature and decrease in temperature as you move from inside the pellet out towards the helium gap. The sharp drop in temperature around 0.5cm occurs right at the helium gap then slowly decreases down to 550K where it reaches the outer cladding. The steady state temperature for temperature dependent thermal conductivity system shows a similar trend but with a lower temperature profile through the fuel, starting at 1750K but still finishing around 550K at the outer cladding. This behavior suggests that reducing the effective thermal conductivity at higher temperatures lowers the overall heat flux through the material, resulting in a higher overall temperature profile compared to the constant thermal conductivity system.

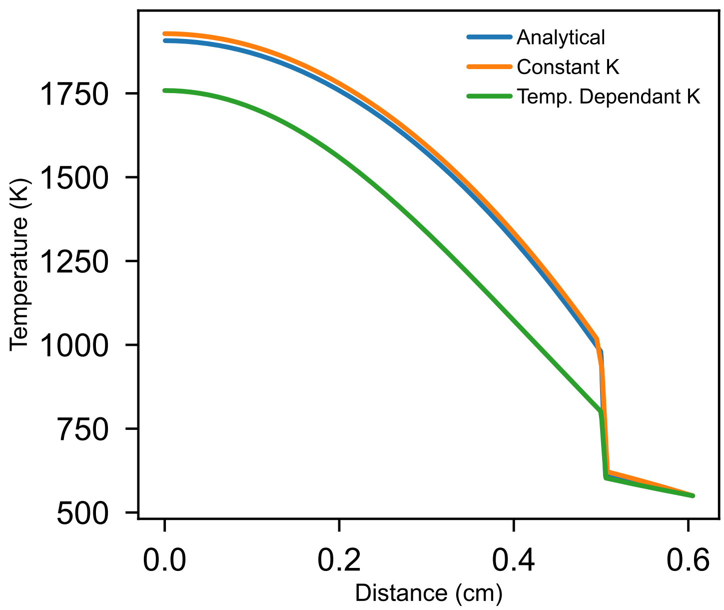

Figure 3: Temperature profile for three steady-state modeling approaches: (1) an analytical solution, (2) a numerical solution with constant thermal conductivity (K), and (3) a numerical solution with temperature-dependent thermal conductivity.

Figure 4 shows the centerline temperature over a specified time interval of 0 to 100 seconds. For both constant and time dependent thermal conductivity systems, the temperatures increases from 0K to 1600K in the first 20 seconds. At 23 seconds the centerline temperature sharply increases to a max temperature of 1971.3K for the constant thermal conductivity model and 2005.3K for the temperature dependent thermal conductivity model. Both curves then exhibit minor dips in temperature. It is worth noting that the constant thermal conductivity curve dips 100K less than the temperature dependent thermal conductivity curve. For the remainder of time (23 to 100 seconds), both curves settle to a constant centerline temperature of 1758K. This tells us that at higher temperatures the temperature-dependent thermal conductivities drive a quicker initial rise in the temperature, but as time goes on, the thermal conductivity on the system has little effect on the thermal equilibration.

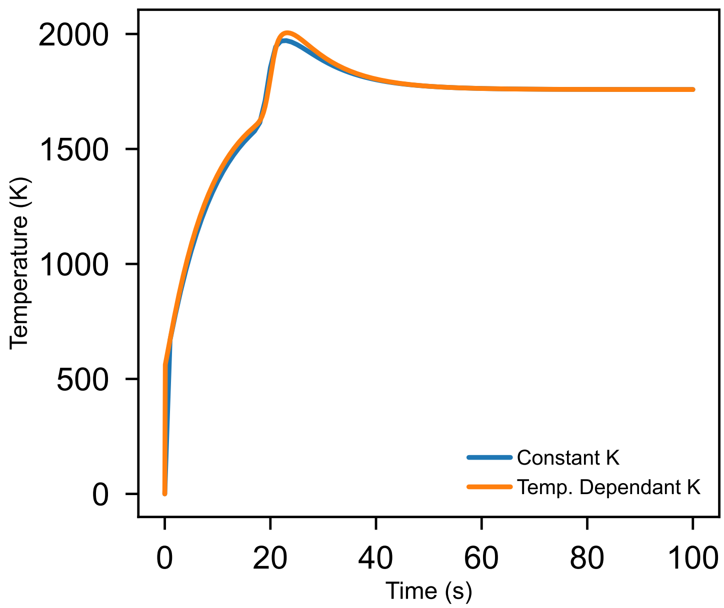

Figure 4: Centerline temperature over time of transient systems.

4 Conclusions

In this project, MOOSE was utilized to simulate the temperature profile of a fuel pellet within a fuel rod and demonstrate the signifigance of thermal conductivity on both steady-state and transient thermal behavior. By comparing constant and temperature-dependent thermal conductivity models, it was observed that in steady-state conditions, a temperature-dependent thermal conductivity leads to a higher overall temperature due to reduced heat flux. In transient systems, it results in a more rapid increase in centerline temperature, though its influence is little to none after approximately 30 seconds as the system approaches thermal equilibrium. These findings highlight the critical role of thermal conductivity in reactor fuel performance.

References

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