MOOSE Project Part 1

Hongsup Oh

1 Introduction

In MOOSE project part 1, we need to analyze the heat transfer in a fuel system, which includes the fuel pellet, gap, and cladding. The coolant is not considered. The fuel pellet has a radius of 0.5 [cm], the gap is 0.005 [cm] thick, the cladding is 0.1 [cm] thick, and all components have a height of 1.0 [cm], as shown in Figure 1.

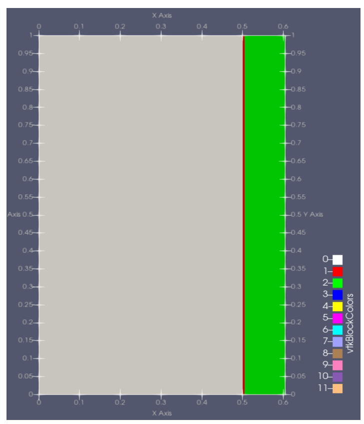


Figure 1: Geometry of the Fuel System: Fuel Pellet (Gray), Gap (Red), and Cladding (Green)

The strong form of the governing equation to be solved in this project is given by:

$$\rho c_p \frac{\partial T(\mathbf{x})}{\partial t} = \nabla \cdot (k \nabla T(\mathbf{x})) + \dot{q}, \quad \mathbf{x} \in \Omega. \tag{1}$$

The boundary condition is:

$$T(\mathbf{x}) = g_D, \quad \mathbf{x} \in \partial\Omega_D. \tag{2}$$

In the MOOSE framework, Equation 1 must be transformed into its weak form, and a residual function must be formulated to obtain the temperature field (T) by minimizing Equation 3.

$$r(T) = \int_\Omega \psi_i \rho c_p \frac{\partial T}{\partial t} d\Omega + \int_\Omega \nabla \psi_i \cdot k \nabla T d\Omega - \int_\Omega \psi_i \dot{q} d\Omega - \int_\Gamma \psi_i (k \nabla T) \cdot n d\Gamma \tag{3}$$

Equation 3 can be represented by Equation 4 where $(\cdot)$ denotes the kernel and $< \cdot >$ represents the boundary condition [1, 2]:

$$r(T) = \left(\psi_i, \rho c_p \frac{\partial T}{\partial t}\right)_\Omega + (\nabla \psi_i, k \nabla T)_\Omega - (\psi_i, \dot{q})_\Omega - \langle \psi_i, (k \nabla T) \cdot n \rangle_\Gamma \tag{4}$$

Equation 3 is solved using the Newton-Raphson method:

$$J(T_i) \delta T_{i+1} = -r(T_i) \tag{5}$$

where solving Equation 5 yields δT_{i+1}, which is then used to update according to:

$$T_{i+1} = T_i + \delta T_{i+1} \tag{6}$$

The primary objective of this project is to create an input file. In the mesh block, the fuel domain, including the fuel pellet, gap, and cladding, is designed. In the variable block, the temperature field (T) is defined as a variable. In the kernel block, the kernel functions from Equation 4 are implemented. In the material block, material properties such as thermal conductivity (k) are specified. In the boundary and initial conditions block, the prescribed boundary and initial conditions are defined. Finally, in the executioner block, the Newton solver is chosen as the nonlinear solver (Equation 3), while LU decomposition is used as the linear solver (Equation 5) [1, 2].

The project report focuses on presenting the results from MOOSE and is structured into five sections: steady-state with constant k, steady-state with temperature-dependent k, transient with constant k, transient with temperature-dependent k, and conclusion.

2 Steady-state with a constant k

The input and output files for this section are **project1_steady.i** and **project1_steady_out.e**, respectively. In this section, we solve the steady-state thermodynamic problem, assuming constant thermal conductivities for the fuel pellet (k_f), gap (k_g), and cladding (k_c). The governing equation is:

$$\nabla \cdot (k \nabla T(\mathbf{x})) + \dot{q} = 0, \quad \mathbf{x} \in \Omega. \tag{7}$$

The boundary condition is:

$$T(\mathbf{x}) = g_D, \quad \mathbf{x} \in \partial\Omega_D. \tag{8}$$

where $\dot{q} = 350$ W/cm^2 and $g_D = 550$ K. The fuel pellet is composed of UO_2, the cladding is made of Zr, and the gap is filled with He. Their thermal properties are summarized in Table 1.

Table 1: The thermal conductivity.

k_f [W/cm-K]	k_g [W/cm-K]	k_c [W/cm-K]
0.03	0.00256	0.17

Equation 7 is solved using the Newton nonlinear solver with LU decomposition. The fuel geometry is uniformly meshed with a grid size of $n_x = 800$ and $n_y = 100$. The resulting temperature field in the fuel domain is presented in Figure 2a. The temperature gradually decreases from the centerline to the outer cladding. The centerline temperature profile is depicted in Figure 2b, while the analytical solution is shown in Figure 2. Both plots exhibit a similar trend.

3 Steady-state with a temperature dependent k

The input and output files for this section are **project1_steady_k_time_dependent.i** and **project1_steady_k_time_dependent_out.e**, respectively. In this section, we solve the steady-state thermodynamic problem, assuming that the thermal conductivities of the fuel pellet ($k_f(T)$), gap ($k_g(T)$), and cladding ($k_c(T)$) depend on temperature. The governing equation is:

$$\nabla \cdot (k(T) \nabla T(\mathbf{x})) + \dot{q} = 0, \quad \mathbf{x} \in \Omega. \tag{9}$$

The boundary condition is:

$$T(\mathbf{x}) = g_D, \quad \mathbf{x} \in \partial\Omega_D. \tag{10}$$

(a) The temperature (T) field in the fuel domain.

(b) The temperature profile at y is 0.5 cm.

(c) The temperature profile from the analytical solution.

Figure 2: The result of steady-state problem with a constant k.

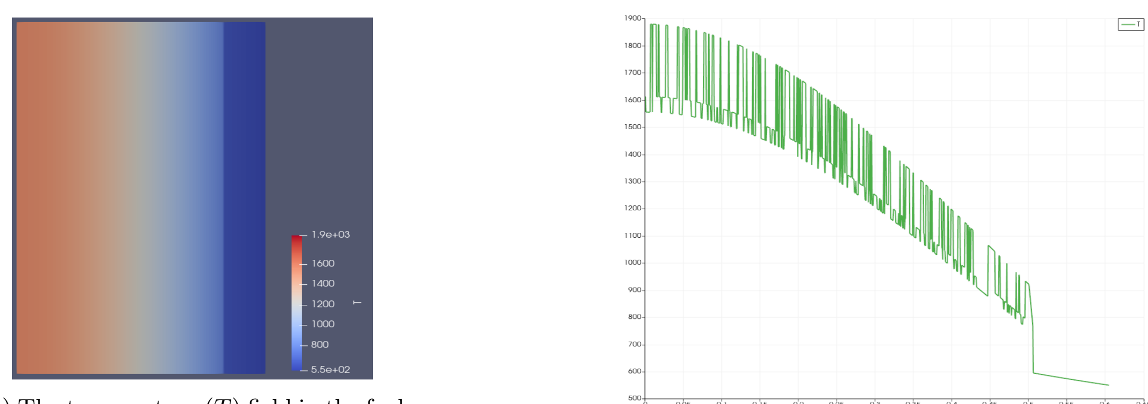
where $\dot{q} = 350$ W/cm^2 and $g_D = 550$ K. The fuel pellet is composed of UO_2, the cladding is made of Zr, and the gap is filled with He. Their thermal conductivities are defined as follows:

$$k_f(T) = \frac{0.01}{0.041 + (2.81e-4)T + (9.88e-9)T^2}, \tag{11}$$

$$k_g(T) = (2.28e-3) + (7.058e-7)T, \text{ and} \tag{12}$$

$$k_c(T) = 0.1098 + (1.4e-4)T - (5e-8)T^2. \tag{13}$$

Equation 11 to 13 represent the thermal conductivity of the fuel pellet, gap, and cladding, respectively. Equation 9 is solved using the Newton nonlinear solver with LU decomposition. The fuel geometry is uniformly meshed with a grid size of $n_x = 800$ and $n_y = 100$. The resulting temperature field in the fuel domain is presented in Figure 3a. The centerline temperature profile is depicted in Figure 3b. The centerline temperature rises relative to the case with constant thermal conductivity.



(a) The temperature (T) field in the fuel domain.

(b) The temperature profile at y is 0.5 cm.

Figure 3: The result of steady-state problem with a temperature dependent k.

4 Transient with a constant k

The input and output files for this section are **project1_transient.i** and **project1_transient_out.e**, respectively. In this section, we solve the transient thermodynamic problem, assuming constant thermal conductivities for the fuel pellet (k_f), gap (k_g), and cladding (k_c). The governing equation is:

$$\rho c_p \frac{\partial T(\mathbf{x})}{\partial t} = \nabla \cdot (k \nabla T(\mathbf{x})) + \dot{q}(\mathbf{x}), \quad \mathbf{x} \in \Omega. \tag{14}$$

The boundary condition is:

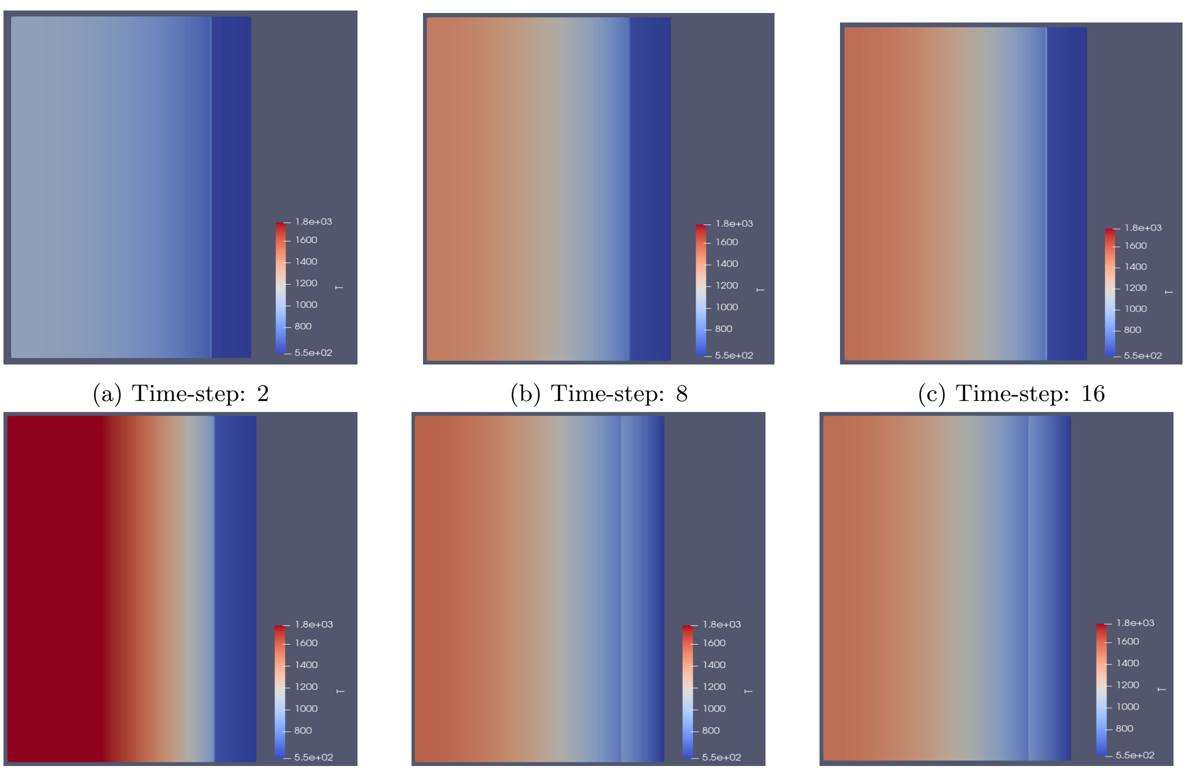
$$T(\mathbf{x}) = g_D, \quad \mathbf{x} \in \partial\Omega_D. \tag{15}$$

where $\dot{q}(t) = 350 * \exp(-(t-20)^2/2) + 350$ W/cm^2 and $g_D = 550$ K. The fuel pellet is composed of UO_2, the cladding is made of Zr, and the gap is filled with He. Their thermal properties are summarized in Table 2.

Table 2: The thermal conductivity.

k_f [W/cm-K]	k_g [W/cm-K]	k_c [W/cm-K]
0.03	0.00256	0.17

Equation 14 is solved using the Newton nonlinear solver with LU decomposition. The fuel geometry is uniformly meshed with a grid size of $n_x = 400$ and $n_y = 100$. Steady-state solution is achieved at time = 76. The results are shown in Figure 4.



(a) Time-step: 2

(b) Time-step: 8

(c) Time-step: 16

(d) Time-step: 20

(e) Time-step: 28

(f) Time-step: 76

Figure 4: Constant k: The evolution of temperature field over time-steps.

The maximum temperature of each time step is represented in Figure 5 and Table 3. The evolution trend of the maximum temperature reflects the exponential function of $\dot{q}$. It goes up from time step 2 to 20, with big jumps around step 17, then starts going down at step 20 and stays steady after that.

Table 3: The maximum temperature at each time step.

Time-step	2	6	10	14	18	22	26	30	34	38
Temperature [K]	1053.98	1541.033	1696.966	1745.33	1828.60	2166.35	1898.176	1807.802	1779.603	1770.88
Time-step	42	46	50	54	58	62	66	70	74	76
Temperature [K]	1768.185	1767.35	1767.095	1767.015	1766.99	1766.98	1766.98	1766.98	1766.98	1766.98

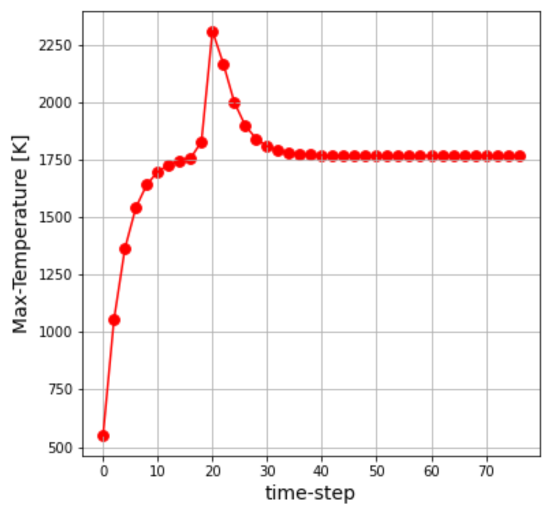


Figure 5: The evolution of maximum temperature over time-steps.

5 Transient with a temperature dependent k

The input and output files for this section are **project1_transient_k_time_dependant.i** and **project1_transient_k_time_dependant_out.e**, respectively. In this section, we solve the transient thermodynamic problem, assuming that the thermal conductivities of the fuel pellet ($k_f(T)$), gap ($k_g(T)$), and cladding ($k_c(T)$) depend on temperature. The governing equation is:

$$\rho c_p \frac{\partial T(\mathbf{x})}{\partial t} = \nabla \cdot (k(T)\nabla T(\mathbf{x})) + \dot{q}(\mathbf{x}), \quad \mathbf{x} \in \Omega. \tag{16}$$

The boundary condition is:

$$T(\mathbf{x}) = g_D, \quad \mathbf{x} \in \partial\Omega_D. \tag{17}$$

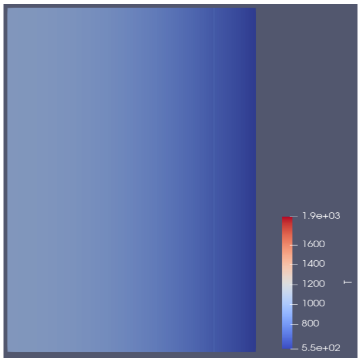
where $\dot{q}(t) = 350 * \exp(-(t-20)^2/2) + 350\ \mathrm{W/cm^2}$ and $g_D = 550$ K. The fuel pellet is composed of UO_2, the cladding is made of Zr, and the gap is filled with He. Their thermal conductivities are defined as follows:

$$k_f(T) = \frac{0.01}{0.041 + (2.81e-4)T + (9.88e-9)T^2}, \tag{18}$$

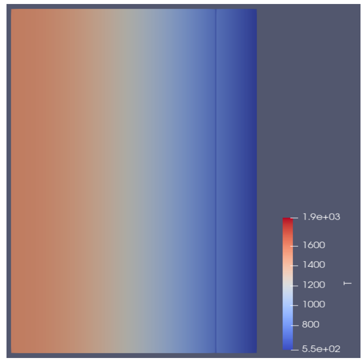
$$k_g(T) = 2.28e-3 + (7.058e-7)T, \text{ and} \tag{19}$$

$$k_c(T) = 0.1098 + (1.4e-4)T - (5e-8)T^2. \tag{20}$$

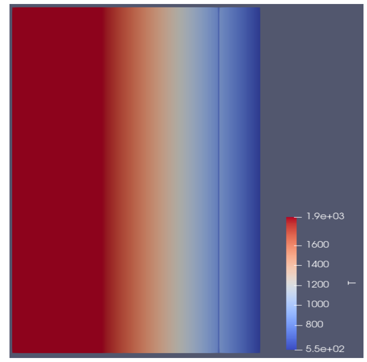
Equation 18 to 20 represent the thermal conductivity of the fuel pellet, gap, and cladding, respectively. Equation 16 is solved using the Newton nonlinear solver with LU decomposition. The fuel geometry is uniformly meshed with a grid size of $n_x = 400$ and $n_y = 100$. Steady-state solution is achieved at time = 81.5 (115 iterations). The results are shown in Figure 6.



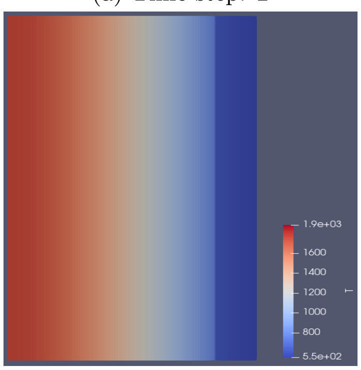
(a) Time-step: 2



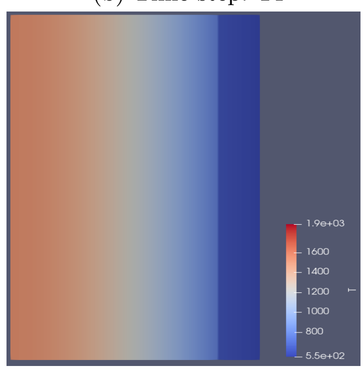
(b) Time-step: 14



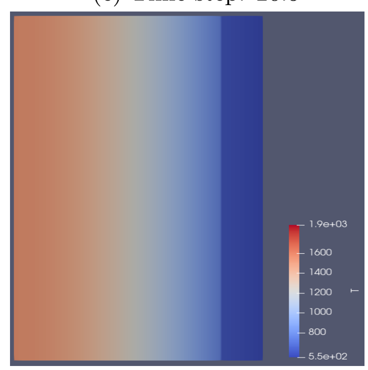
(c) Time-step: 20.5



(d) Time-step: 25.5



(e) Time-step: 40.5



(f) Time-step: 81.5

Figure 6: The evolution of temperature field over time-steps.

The maximum temperature of each time step is represented in Figure 7. The evolution trend of the maximum temperature reflects the exponential function of $\dot{q}$. It goes up from time step 2 to 20, with big jumps around step 17, then starts going down at step 20 and stays steady after that.

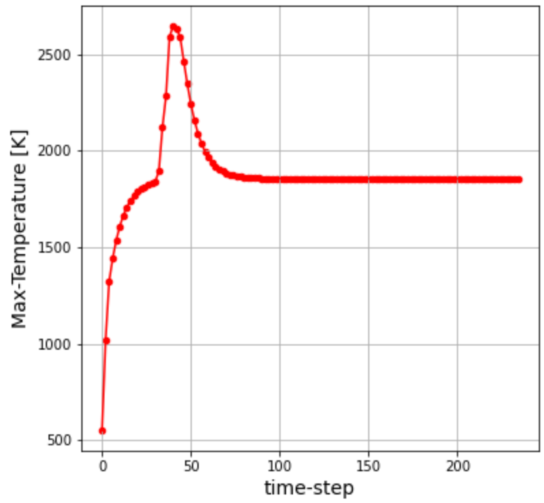


Figure 7: The evolution of maximum temperature over time-steps.

6 Conclusion

In MOOSE Project 1, we solve steady-state and transient thermodynamic problems using both constant and temperature-dependent thermal conductivity, k. Given the simplicity of the problem, a direct solver (LU decomposition) was selected over an iterative method for the linear system. In all cases, the temperature field decreases from the centerline to the outer surface of the cladding. For the steady-state problem with constant k, the temperature profile closely matches the analytical solution. However, when k is temperature dependent, the centerline temperature increases slightly. In the transient case, the maximum temperature rises exponentially until approximately timestep 20, then decreases before reaching a steady state. Convergence is slower when k is temperature-dependent; for instance, with constant k, the solver converges in fewer iterations, whereas with temperature-dependent k, 115 iterations are required.

References

[1] D. Gaston, C. Newman, G. Hansen, and D. Lebrun-Grandie. Moose: A parallel computational framework for coupled systems of nonlinear equations. *Nuclear Engineering and Design*, 239(10):1768–1778, 2009.

[2] Idaho National Laboratory. Moose: Multiphysics object oriented simulation environment, 2024. Accessed: 2024-02-28.