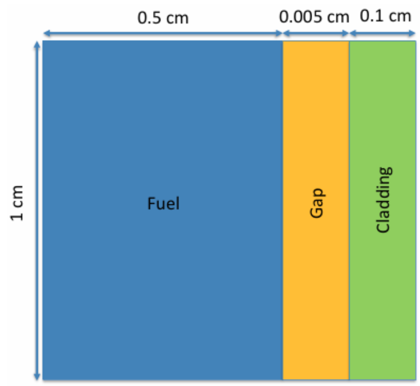
MOOSE Project, Parts 1 & 2

Part 1

In this first part of the project, we were given the dimensions of a fuel system (pellet, gap, cladding) and asked to solve for the temperature profile. A diagram of the system is illustrated below.



There were 5 ways with which to solve this problem:

1. Analytical steady-state solution, constant LHR, constant material properties
2. FEM steady-state solution, constant LHR, constant material properties
3. FEM transient solution, time-dependent LHR, constant material properties
4. FEM steady-state solution, constant LHR, temperature-dependent material properties
5. FEM transient solution, time-dependent LHR, temperature-dependent LHR

All FEM solutions were performed using the MOOSE program. Input and output files for all FEM solutions are attached in this submission.

Guidance for setting up the problem was as follows:

- Assume reasonable values for material properties
- Outer cladding constant temperature: 550 K
- Constant Linear Heat Rate (LHR): 350 W/cm
- Time-dependent LHR: 350*EXP(-(t-20)^2/2) + 350 W/cm
- Determine transient solution for up to t = 100

Constant material properties were found through various resources and are given below.

Material	Thermal Conductivity, k (W/cm*K)	Specific Heat, C_p (J/g*K)	Density (g/cm^3)
UO_2 (Fuel)	0.03	0.33	10.98
He gas (Gap)	0.00152	5.193	0.1785
Zr (cladding)	0.23	0.35	6.511

Properties for the fuel and cladding were found in NE 533 Lecture 3. Properties for the gap were found at Helium - Thermal Conductivity.

The only equations used to solve for temperature-dependent material properties are those given for the thermal conductivity of the fuel pellet, and the thermal conductivity of the gap (assuming the gap remains pure He gas) and are given in NE 533 Lecture 8 and Lecture 3, respectively. Those equations are presented for both below in W/cm*K.

$$k_f = \frac{\left(\frac{100}{7.5408 + 17.629t + 3.6142t^2} + \frac{6400}{t^{\frac{5}{2}}} \exp\left[-\frac{16.35}{t}\right]\right)}{100}$$

Where t = T / 1000, and

$$k_g = 16 \times 10^{-6} T^{0.79}$$

Solution #1- Analytical

The following equations were used to solve the steady-state temperature profile of the fuel system from the outside of the cladding to the fuel centerline. Subscripts denote the type of material (fuel, gap, cladding), and the radius/thickness of the materials are given in the diagram. The temperatures at each boundary were calculated, and the profile from the edge to the centerline of the pellet was modeled.

$$T_{IC} = \frac{LHR}{2\pi R_f} \times \frac{t_c}{k_c} + T_{OC}$$

$$T_s = \frac{LHR}{2\pi R_f} \times \frac{t_g}{k_g} + T_{IC}$$

$$T_o = \frac{LHR}{4\pi k_f} + T_s$$

$$T(r) = \frac{LHR}{4\pi k_f}\left(1 - \frac{r^2}{R_f^2}\right) + T_s$$

Boundary	Location (cm)	Temperature (K)
Outer Cladding	0.605	550
Inner Cladding	0.505	615.5
Surface of Fuel	0.5	983.7
Centerline of Fuel	0	1912.1

Solution #2- FEM, steady-state, constant properties

There are six parts to each MOOSE input file:

- Mesh
- Variables
- Kernels
- BCs
- Executioner
- Outputs

All six of these parts will be described in this section. Since some of these parts will be repeated for the input files of other solutions, it is not necessary to cover them multiple times. This solution most closely correlates to the analytical solution, with a peak centerline temperature of about 1900K.

Mesh

Individual meshes were generated using *GeneratedMeshGenerator* that had the dimensions of each block outlined. Each block was assigned a subdomain ID using *SubDomainIDGenerator*. The blocks were stitched together at the interfaces using *StitchedMeshGenerator*. Meshes were split into 150x1, 10x1, and 100x1; the size of the meshes was varied to determine proper size for reasonable resolution. The coordinate type was changed from the default x-y system to the axisymmetric r-z system, with symmetry around the default y-axis.

```
[system]
    type = StitchedMeshGenerator
    inputs = 'pellet_id gap_id clad_id'
    stitch_boundaries_pairs = 'right left; right left'
    prevent_boundary_ids_overlap = false
[]
```

Variables

The variable was set as temperature, and an initial condition of 550 K was set because it made sense.

Kernels

The function *ADHeatConduction* was used to model the heat conduction of this closed system using automatic differentiation. The function *HeatSource* was required to add the volumetric heat generation rate, given to us in the problem as LHR. The LHR given was divided by the cross-sectional area of the pellet to give the value seeked.

BCs

There were two boundary conditions to be used in this problem. The centerline temperature of the fuel is at a peak, thus the derivative of temperature here is 0. This is reflected in the function *NeumannBC*. The outside of the cladding is held at 550 K, and is modeled using *DirichletBC*.

Materials

Three subsets of materials were chosen and their properties (i.e. thermal conductivity) were defined using *ADGenericConstantMaterial* as is done with most materials with constant properties.

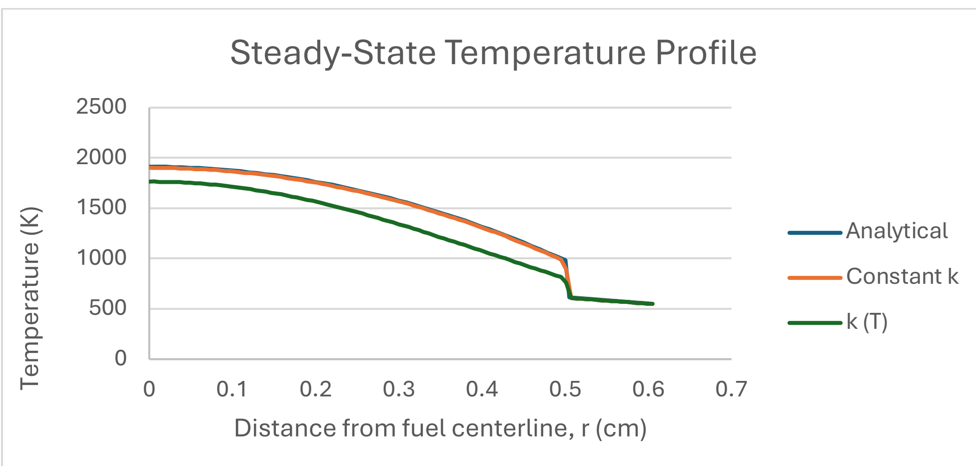
Executioner

Since this was a steady-state solution, the function for the executioner was chosen as *Steady* with a Newton solve type as is common with other steady-state solutions in MOOSE. The 'petsc' lines were artifacts of other steady-state solutions observed online.

```
[Executioner]
    type = Steady       # Steady state problem
    solve_type = NEWTON # Perform a Newton solve, uses AD to compute Jacobian terms
    petsc_options_iname = '-pc_type -pc_hypre_type' # PETSc option pairs with values below
    petsc_options_value = 'hypre boomeramg'
[]
```

Outputs

The outputs to this input file were an exodus file that could simulate the solution in a program like Paraview, and a csv file that utilized the post processor built in. The Vector Post Processor *LineValueSampler* takes the data (temperature) of a line from one point to another (fuel centerline to cladding in middle of system). The 1D steady-state temperature profile of the fuel system for the analytical solution, the constant properties solution, and the temperature dependent properties solution can be seen below.



Solution #3- FEM, transient, constant properties

The parts of this solution identical to Solution #2 are: Variables, BCs, and Outputs. The max peak centerline temperature is a bit higher, almost 2100 K.

Mesh

The mesh was changed to be much rougher to make the computations easier (50x1, 5x1, 10x1).

Kernels

A kernel was added to include the time-dependence of heat conduction, *ADHeatConductionTimeDerivative*. The time-dependent formula for LHR in *HeatSource* was written out for the pellet.

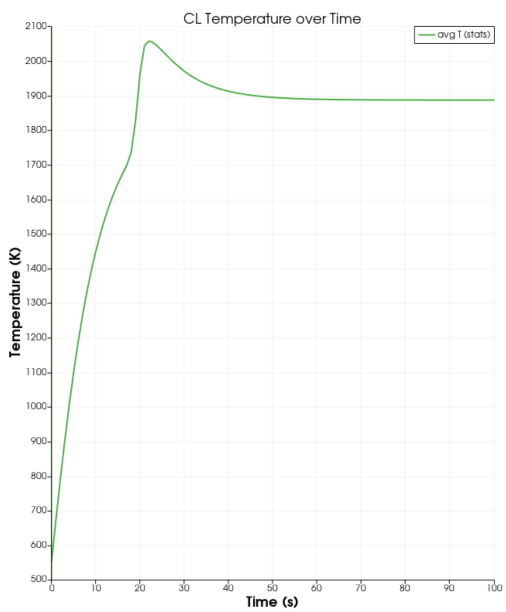
Materials

Materials were still defined using *ADGenericConstantMaterial*, but additional properties (specific heat, density) were required to run the time derivative.

Executioner

The type for this problem was changed from Steady to Transient. The solve type used was PJFNK. The time step dt was chosen as 1 to get individual time steps. Therefore, from 0 to 100 is 100 steps. The non-linear relative tolerance and the non-linear absolute tolerance were both set at 1E-10. The linear tolerance was set at 1E-5, and a steady-state detection function was added in.

The fuel centerline temperature over time was plotted in Paraview and can be seen below.



Solution #4- FEM, steady-state, changing properties

The Mesh, Variables, BCs, and Outputs are identical to Solution #2. However, the max peak centerline temperature for this solution was only around 1760 K as reflected in the first plot. This is due to the changing value of thermal conductivity with temperature of the material.

Kernels

The only change is that the heat conduction function was changed from *ADHeatConduction* to just *HeatConduction*, since no AD materials were used.

Materials

The materials were changed from *ADConstantGenericMaterial to ParsedMaterial* for the fuel and gap, and *GenericConstantMaterial* for the cladding. *ParsedMaterial* was used for materials whose thermal conductivity changed with temperature, and the cladding was changed to reflect a non-AD heat conduction kernel.

Executioner

Instead of a steady-state solver, a transient solver was used with a time step of 1. The tolerances given in Solution #3 were also used here.

Solution #5- FEM, transient, changing properties

The Mesh has the same size elements as the other transient solution. The Variables, BCs, and Outputs are similar to Solution #2. The Executioner is the same as Solution #3.

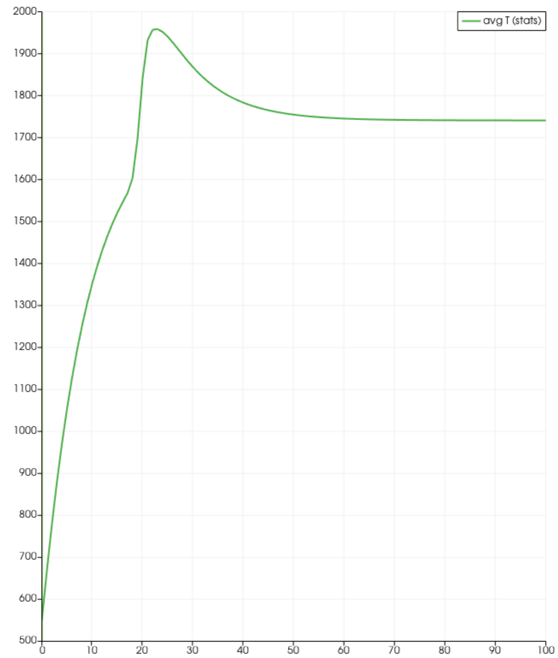
Kernels

The same functions were used as in Solution #3 except they were converted from AD-functions to their non-AD form.

Materials

ParsedMaterial and *GenericConstantMaterial* were used as in Solution #4. However, both functions would have to be used for the fuel and the gap since they had both constant properties and changing properties that were required for the time derivative function.

The fuel centerline temperature over time was plotted in Paraview and can be seen below.



Part 2

In the second part of the project, the dimensions of the fuel system were changed. The system is now 1 m (100 cm) tall. The materials have material properties dependent on the temperature. The LHR changes as a function of axial elevation, and the outer cladding temperature changes with the two relationships below:

$$LHR\left(\frac{z}{Z_0}\right) = LHR^0 \cos\left[1.2 * \left(\frac{z}{Z_0} - 1\right)\right]$$

$$T_{cool} = \frac{1}{1.2}\frac{Z_0 * LHR^0}{\dot{m}C_{pw}}\left[\sin(1.2) + \sin\left(1.2\left(\frac{z}{Z_0} - 1\right)\right)\right] + T_{cool}^{in}$$

Values for LHR^0 and T^{in}_{cool} are 350 W/cm and 500 K, respectively.

Part 2 Solution- Steady State, k(T), LHR(z), T_{cool}(z)

Mesh

The Mesh was stitched just like the other solutions. A mesh convergence study was done to determine the proper amount of finite elements to get a converging solution with reasonable resolution. The mesh sizes are 100x200, 10x200, and 50x200.

Variables

The initial condition was set for 500 K.

Kernels

Since this is a steady-state problem, only the heat conduction and heat source kernels are used. However, the heat source function is changed to be dependent on the axial elevation as above, in this case that is the y-coordinate.

BCs

The BCs are the same as in previous solutions except the Dirichlet BC value for the outer cladding has changed to a function that is dependent on axial LHR and axial elevation. The mass flow rate of 0.25 kg/s and heat capacity of water of 4200 J/kg*K are built in to the function.

Materials

Ther materials are built the same way as they are in Solution #4.

Executioner

The same executioner is used as is in Solution #4.

Outputs

The outputs to this are an exodus file for simulation, and a csv file with a post processor built in to generate axial temperature profiles for the fuel centerline, fuel surface, and inner cladding as seen below.