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X Appendix D: Simulations

For this project, team members learned COMSOL Multiphysics at Dr. Hutter's recommendation, and used the software to construct and run simulations on the thermal performance. These simulations fell into three major groups: simulations of heat transfer across a PEC alone, simulations of heat dissipation by the heat sink and fan combo, and simulations of heat transfer through the sensor stack. Each of these groups served their own purpose in terms of constraint validation, as will be discussed in their sections below.

The first group of simulations was undertaken to replicate the simulation provided by INL (seen in Figure X-A), confirming that we agreed with their analysis and that our setup of the program was correct. The team's simulation of a similar geometry, in Figure X-B, demonstrates a series of temperature isosurfaces consistent with those provided. Additionally, as mentioned in the Simulation section of the paper, a "derived values: surface max" inspection of the top surface allows us to view the rate of temperature change and compare it to experimental results.

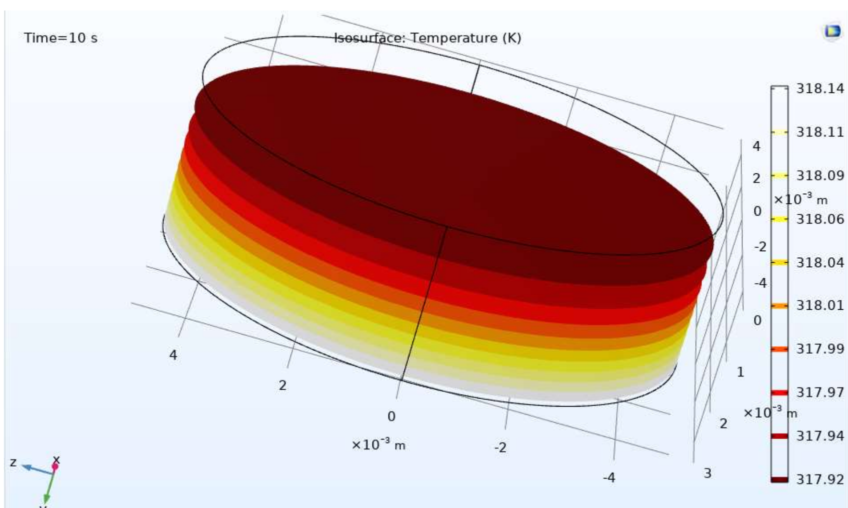


Figure X-A. Thermal Simulation of a 0.008m Diameter Pyroelectric Crystal with a 0.003m Thickness. Courtesy of INL

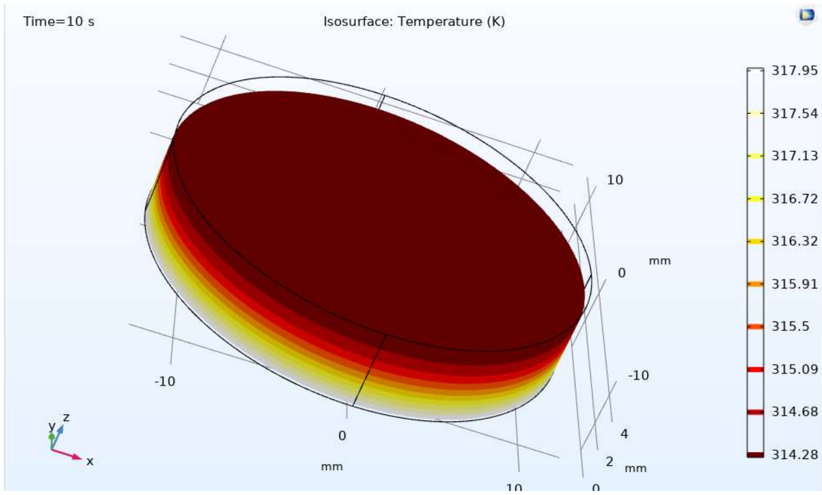


Figure X-B. Thermal Simulation of a 0.02m Diameter Pyroelectric Crystal with a 0.004m Thickness

The next group of simulations utilized the “Heat Transfer in Solids and Fluids” and “Laminar Flow” modules paired through the “Nonisothermal Flow” multiphysics module. A stripped down assembly of the heat sink and peltier were placed into an air volume, with a channel for the fan’s output to be applied. These simulations were conducted through a steady state analysis due to computation restriction and the intensity of fluid flow simulations. With this group of simulations, the primary goal was to validate the math done to choose the heat sink, by proving that it could actually dissipate 30W of heat (our worst case scenario).

The first task required was the construction of the simulation. The build components and final construction can be found below in Figure X-C. The second step was developing a mesh for the simulation. Mesh quality is analyzed in a number of ways, but the primary two relevant for this simulation was the avoidance of thin features and the skewness of the mesh, or how close each element was to equilateral. While the “course” mesh generation setting passed all requirements, it does provide slightly different results when compared to the “normal” mesh generation simulation. Plots of the skewness of both meshes can be found in Figure X-D.

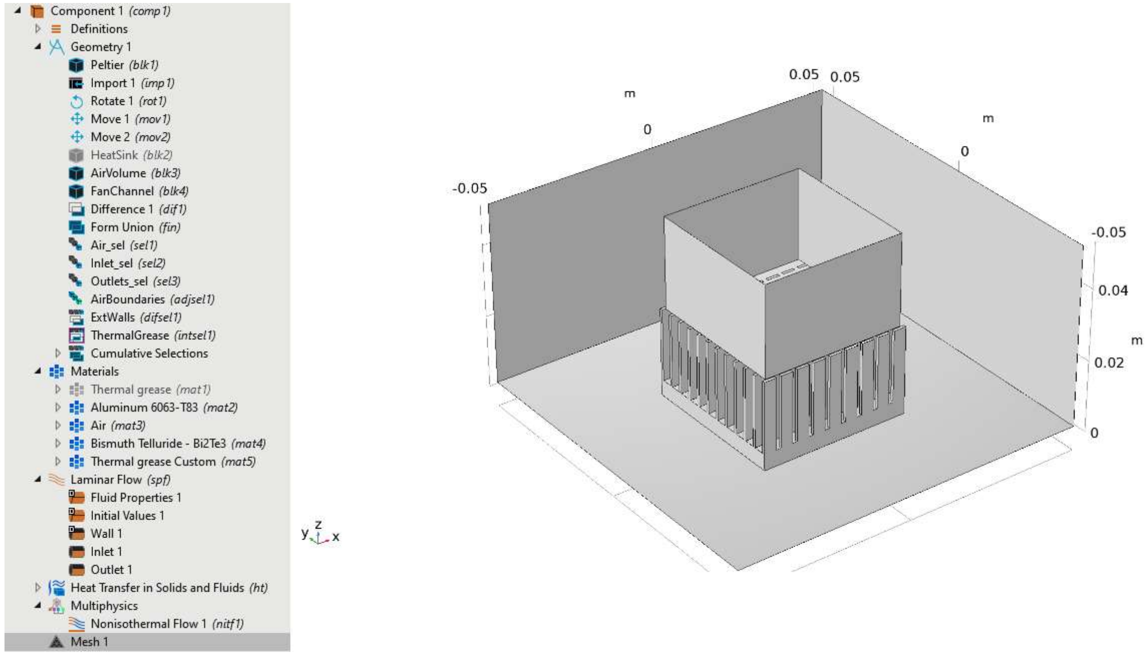
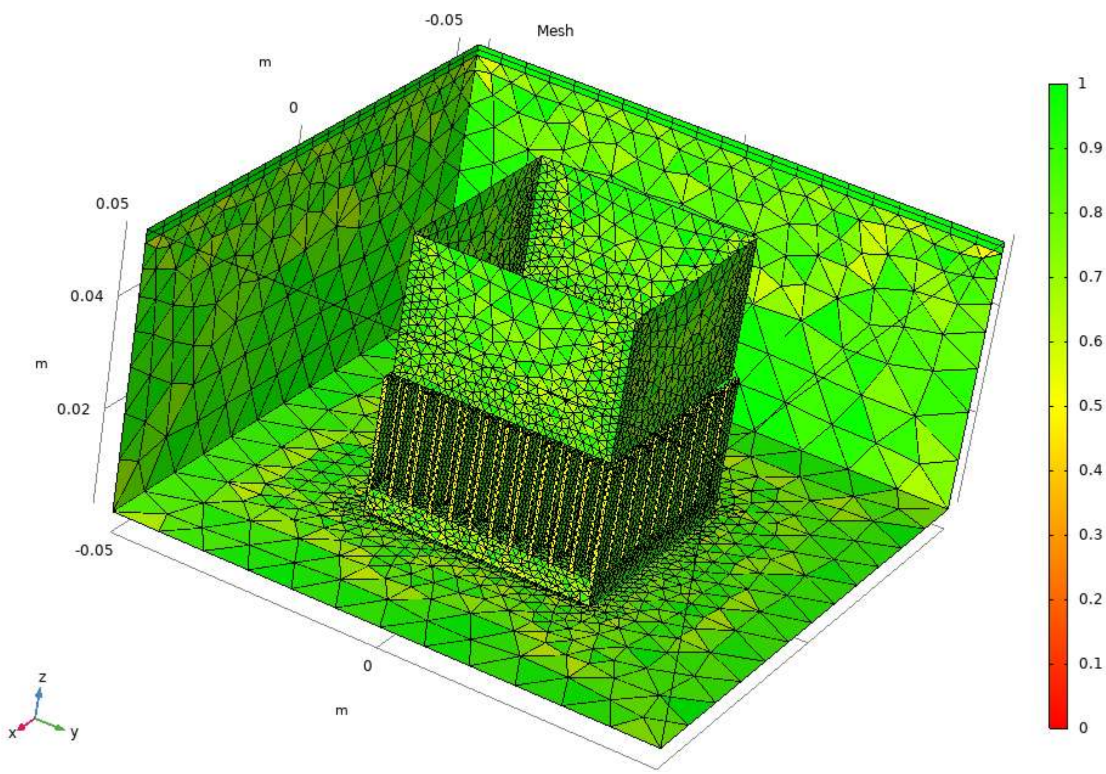


Figure X-C. Build Components (Left) and Simulation Setup (Right) for Steady State Heat Sink Simulation



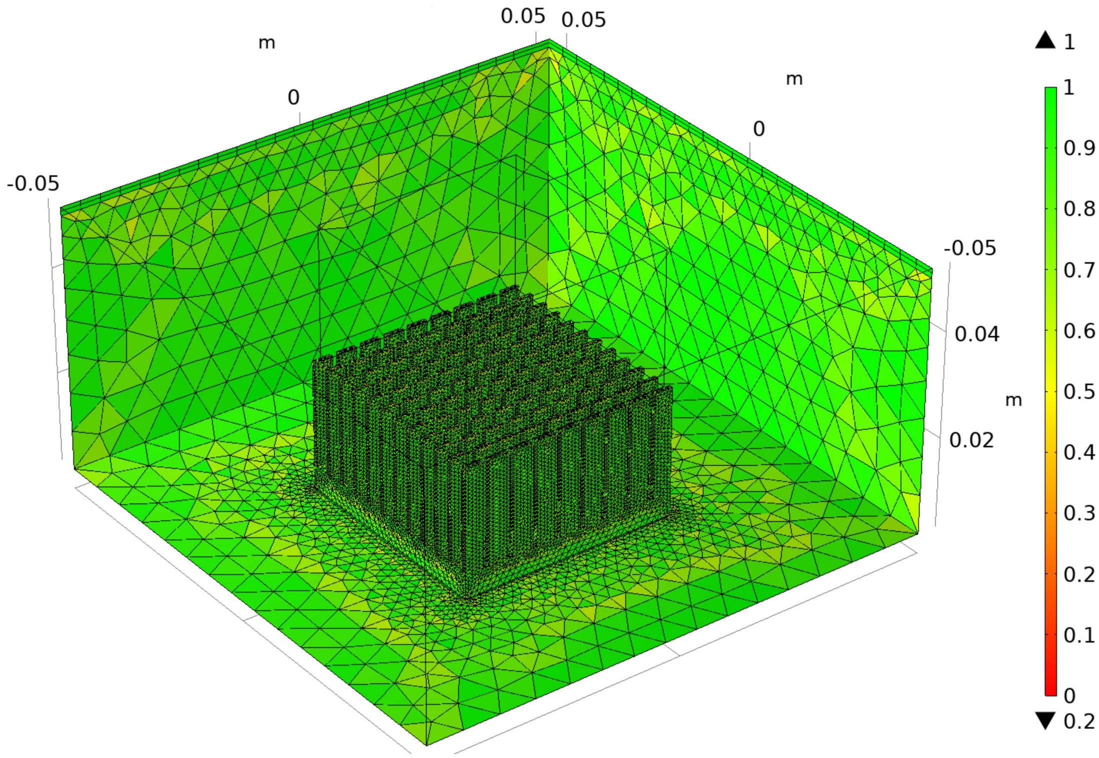
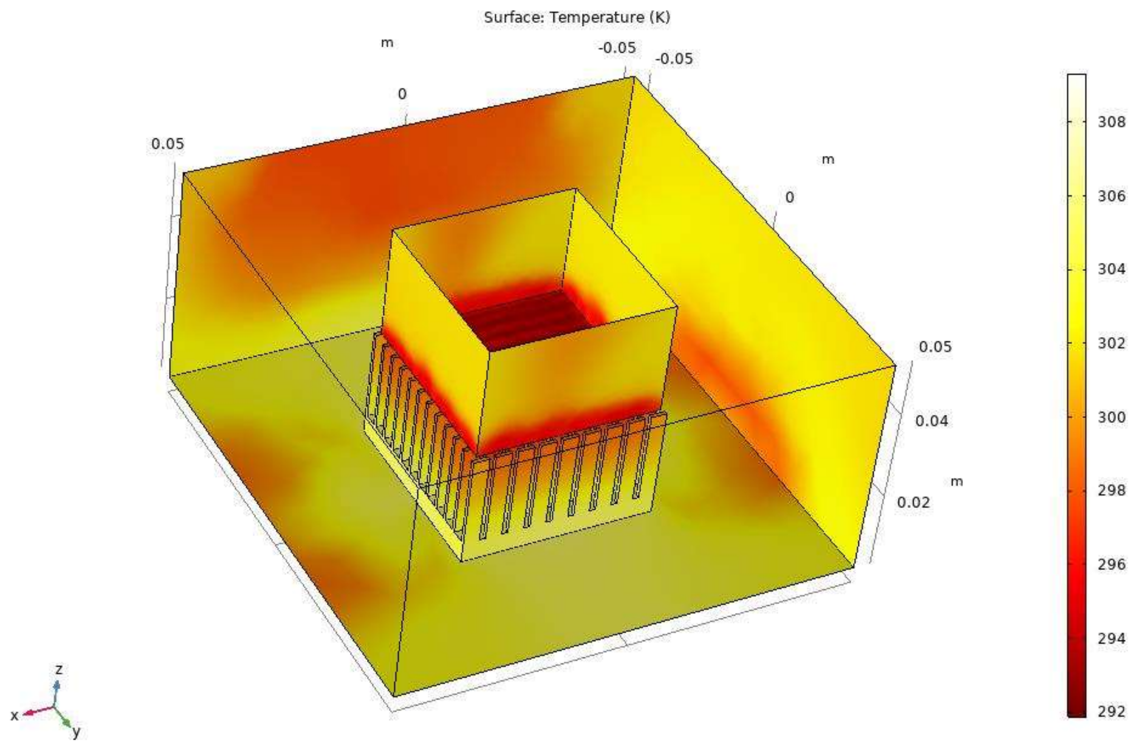
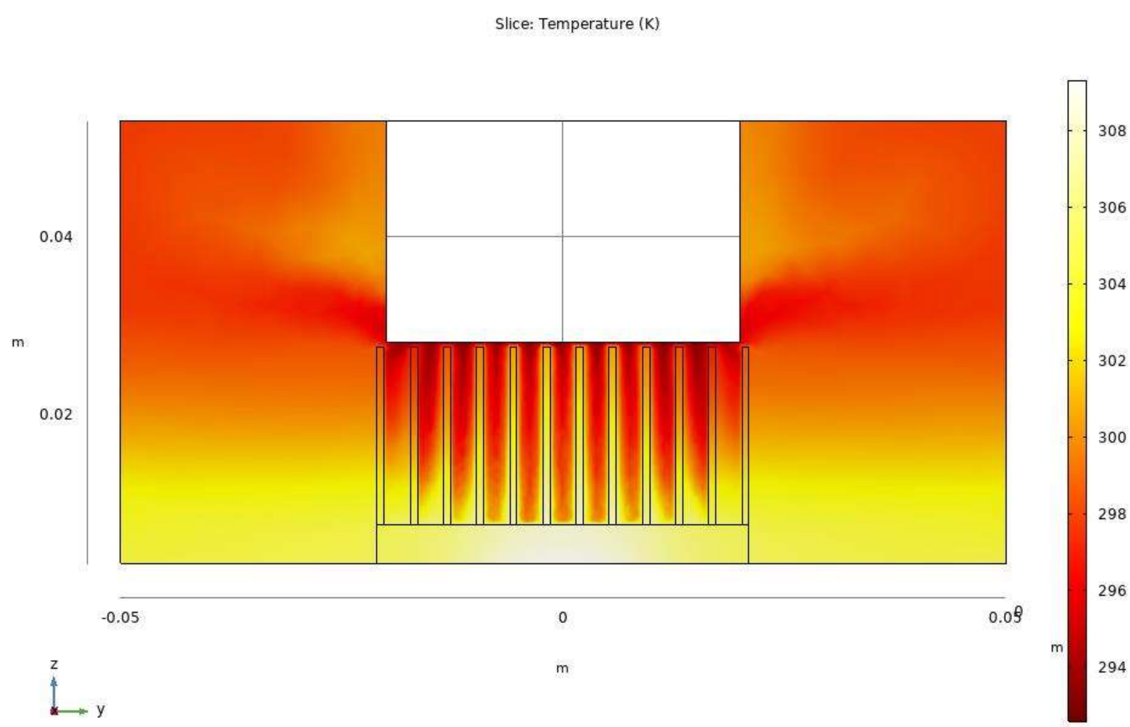
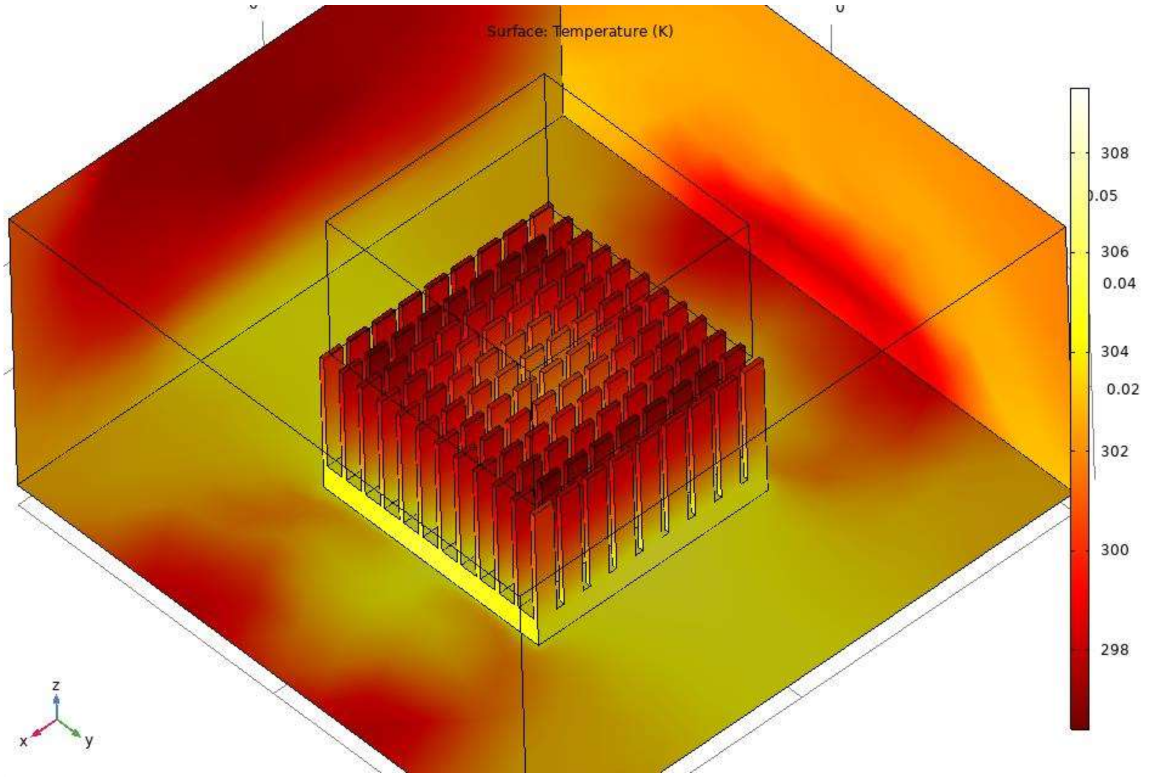


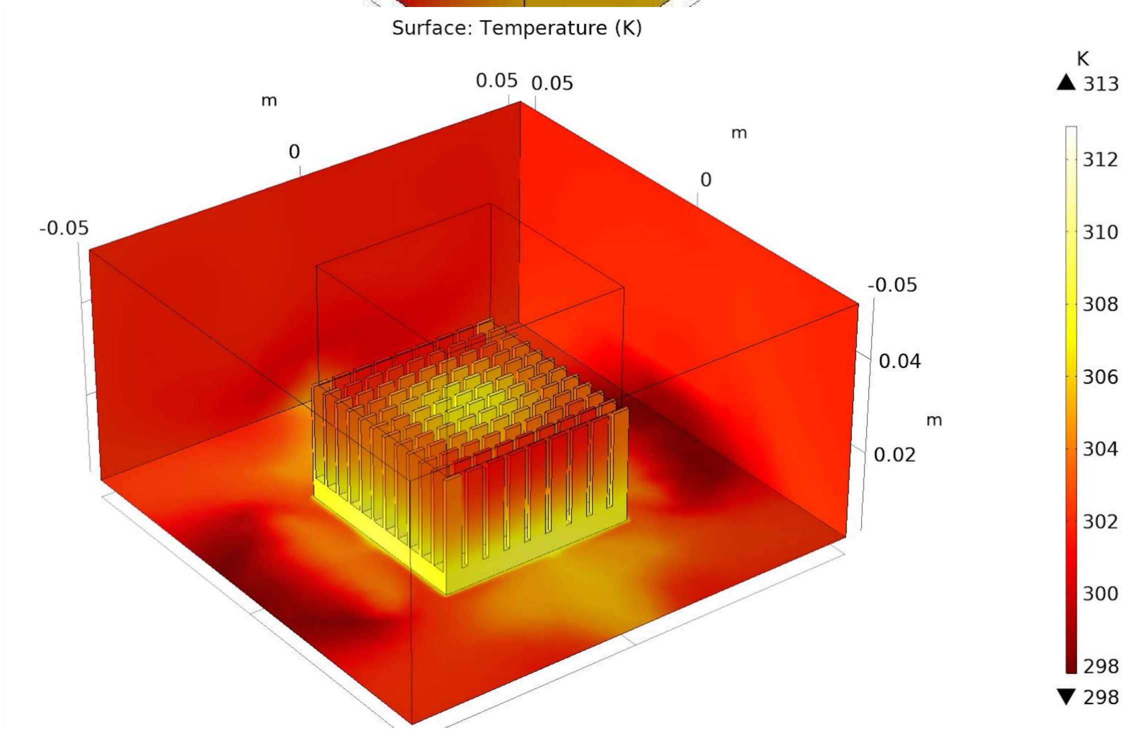
Figure X-D. Plot of Mesh Skewness for Steady State Heat Sink Simulation, Course (Top) and Normal (Bottom) Mesh Settings.

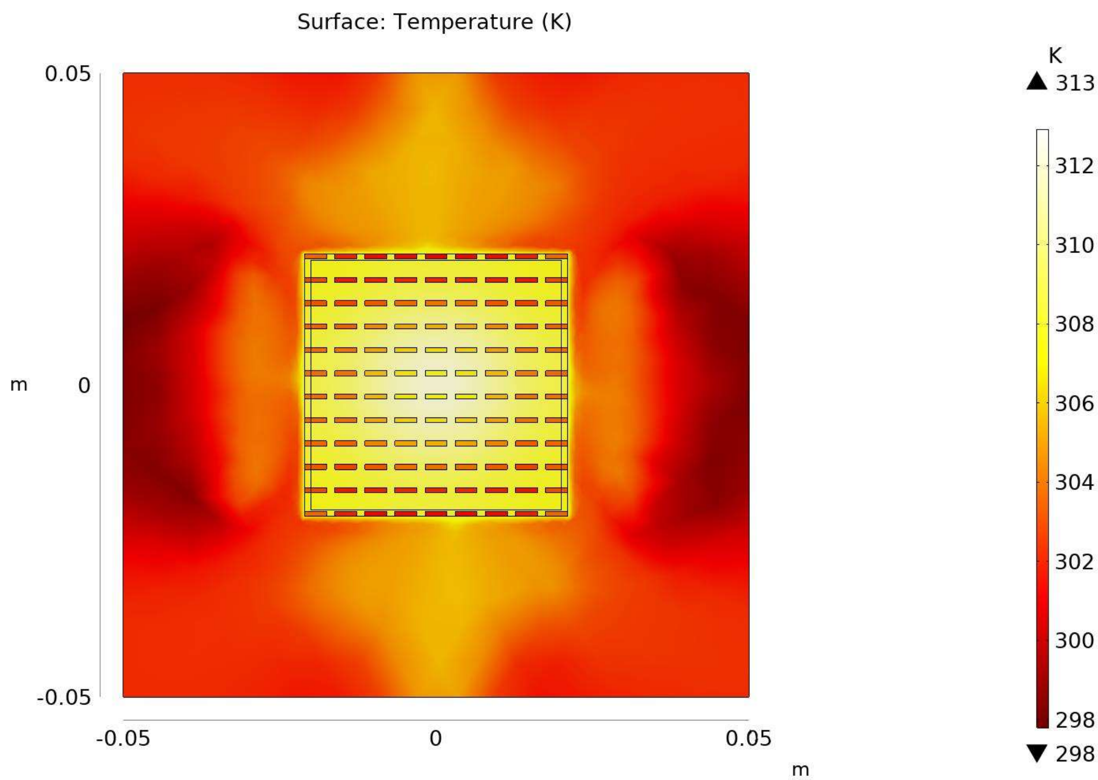
With meshing done, the next task was running and analyzing the simulation, ultimately to determine if the heat sink would be adequate. The primary tools for this are Isosurface and Surface temperature plots. While the two detail levels output slightly different results, they generally agree that the heat sink had a maximum temperature delta of roughly 20 ◦K, well within the peltier's ability to continue to pump heat. Surface maps of the temperature can be seen below in Figure X-E. Additionally, as best demonstrated by the isosurface plots found in Figure X-F, that zone of maximum heat is very small, and localized to directly above the peltier.


Surface: Temperature (K)
m
-0.05
-0.05
0
0.05
m
0
0.05
0.04
m
0.02
308
306
304
302
300
298
296
294
292
z
x
y


Slice: Temperature (K)
0.04
m
0.02
-0.05
0
0.05
m
m
308
306
304
302
300
298
296
294
z
y


Surface: Temperature (K)
308
0.05
306
0.04
304
0.02
302
300
298
z
x
y


Surface: Temperature (K)
m
0.05
0.05
0
m
0
-0.05
-0.05
0.04
m
0.02
K
▲ 313
312
310
308
306
304
302
300
298
▼ 298



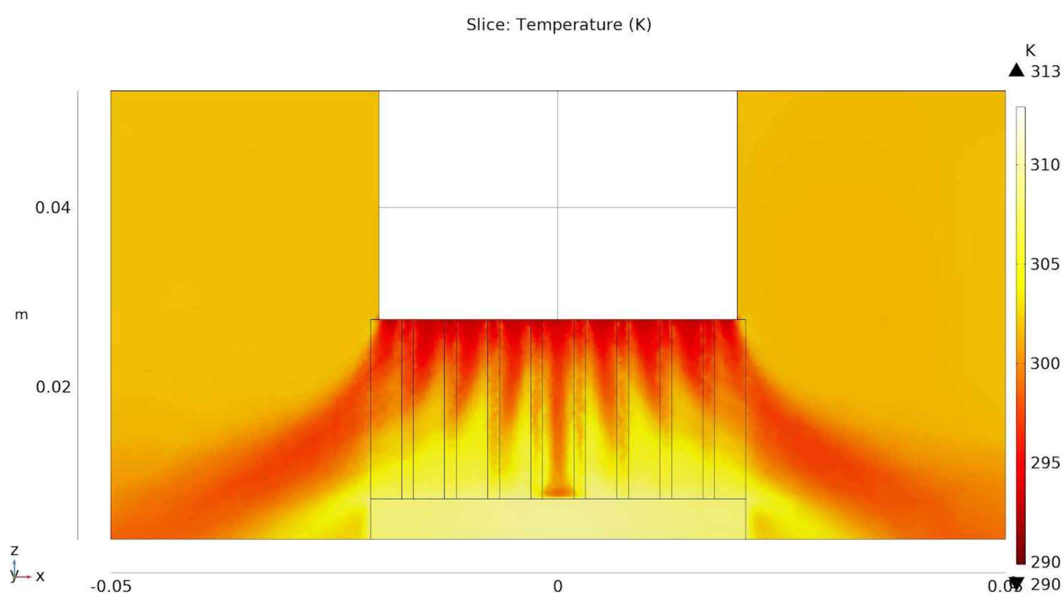
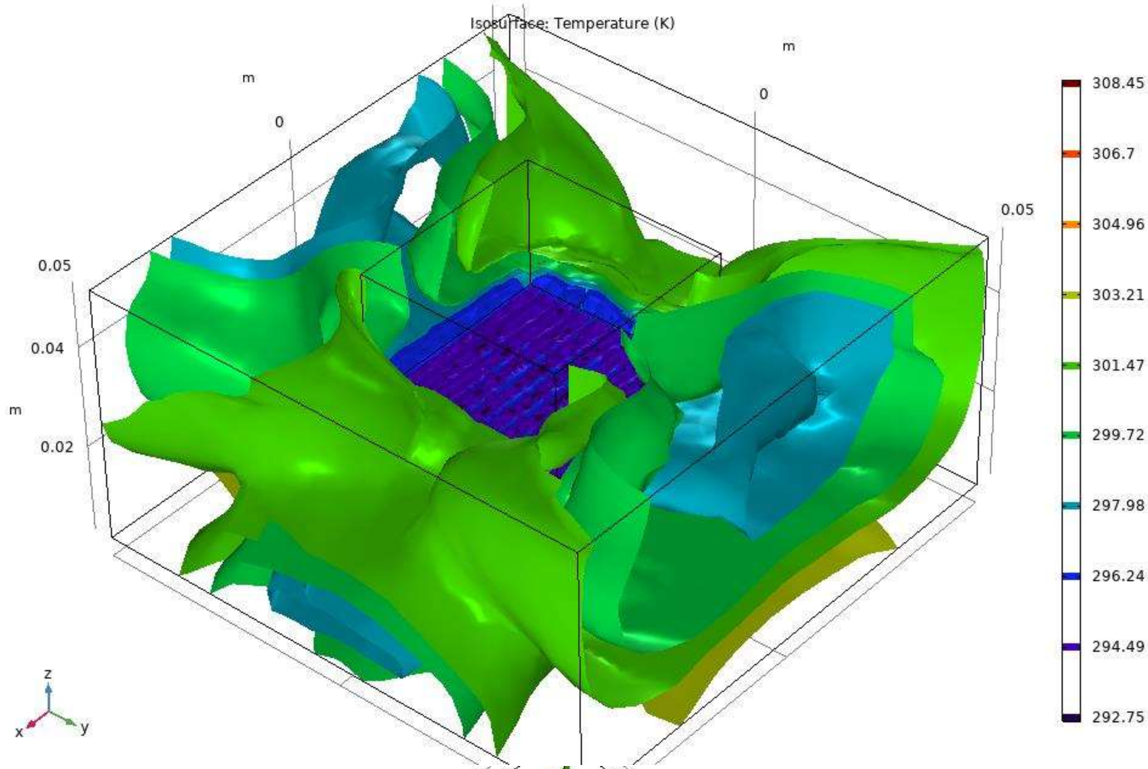
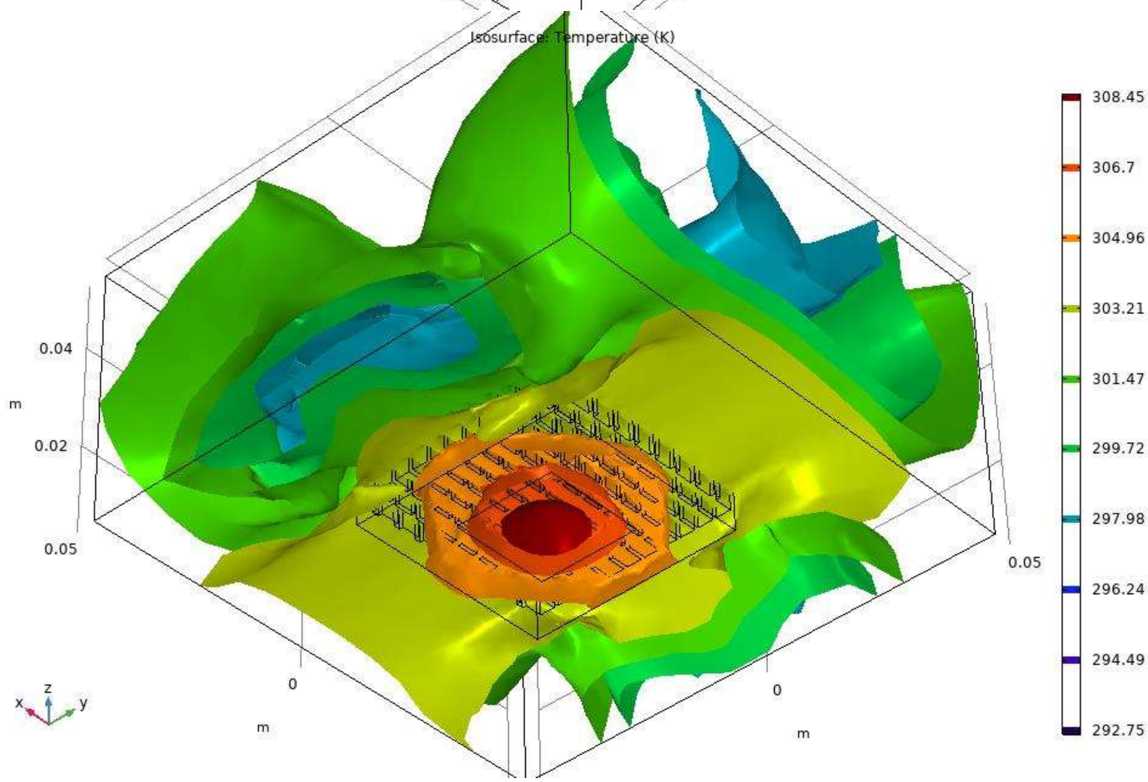


Figure X-E. Plot of Surface Temperature in Steady State Heat Sink Simulation, Course (Top 3) and Nirmal (Bottom 3) Meshes


Isosurface: Temperature (K)
m
0
0.05
0.04
0.02
z
x
y
308.45
306.7
304.96
303.21
301.47
299.72
297.98
296.24
294.49
292.75


Isosurface: Temperature (K)
0.04
m
0.02
0.05
0
z
x
y
308.45
306.7
304.96
303.21
301.47
299.72
297.98
296.24
294.49
292.75

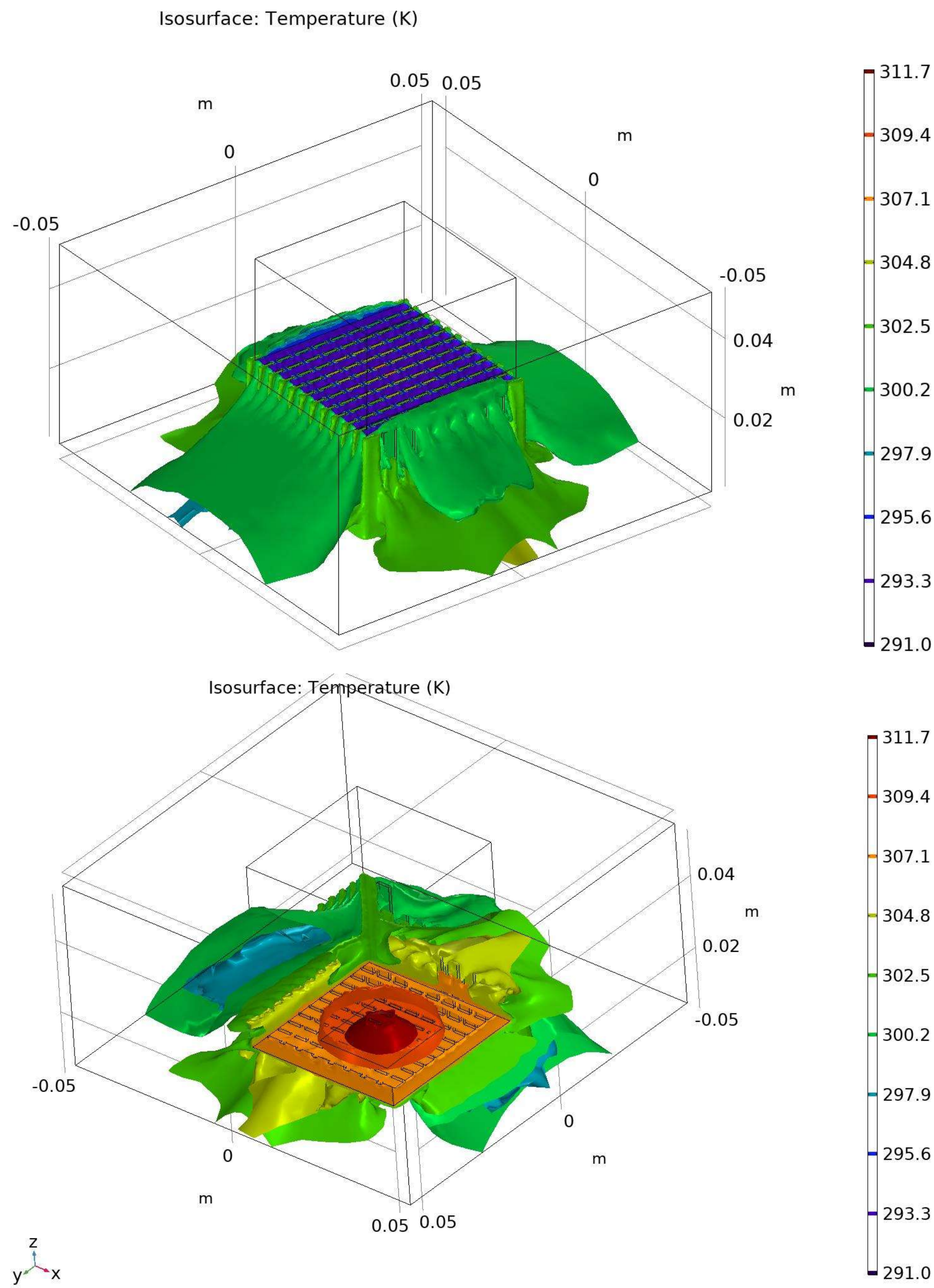
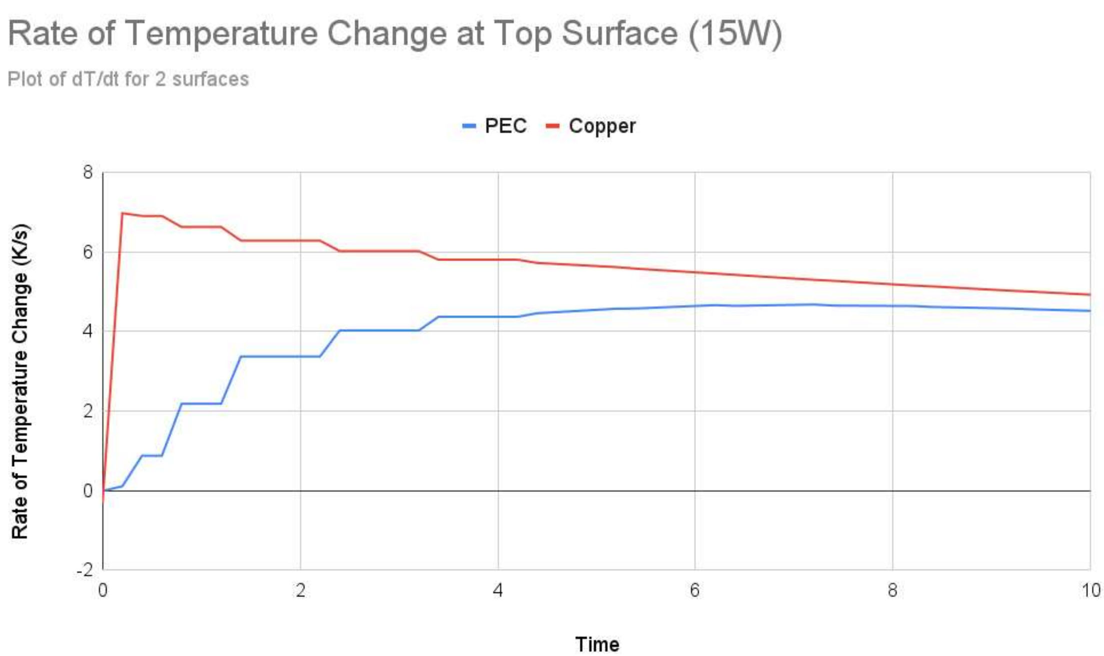


Figure X-F. Plot of Temperature Isosurfaces for Steady State Heat Sink Simulation, Course (Top 2) and Normal (Bottom 2) Meshes

The third and final group of simulations was a “Heat Transfer in Solids and Fluids” time dependent simulation of the full sensor stack north of the peltier. This simulation is particularly important for the accuracy of test results, as how the PEC heats directly impacts the ionization energy and thus results. The top surface of the PEC needs to be exposed, but as a result a thermistor cannot be placed on that surface to monitor temperature. Both the prior prototype and ours rely on the copper sheet as a “good enough” approximation of the heat in the PEC, and the python program that controls heating works from that data. This simulation allows us to investigate that assumption directly, with the opportunity to use this information to improve the program.

While the actual simulation plots can be found in Figure X-H, the more important plots are found below in Figure X-G. These line charts plot the rate of temperature change across the top surface of the copper and the top surface of the PEC at a constant power input (15 or 5 Watts, respectively) from the peltier. In a 10 second test, the PEC spends the first 3 seconds of the trial significantly out of step with the temperature rate being reported by the copper, and therefore the thermistor. This is very important information to take into account when running tests, and indicates that something similar to a soft “preheat” may help prime the PEC to keep pace with the copper sheet during heating.



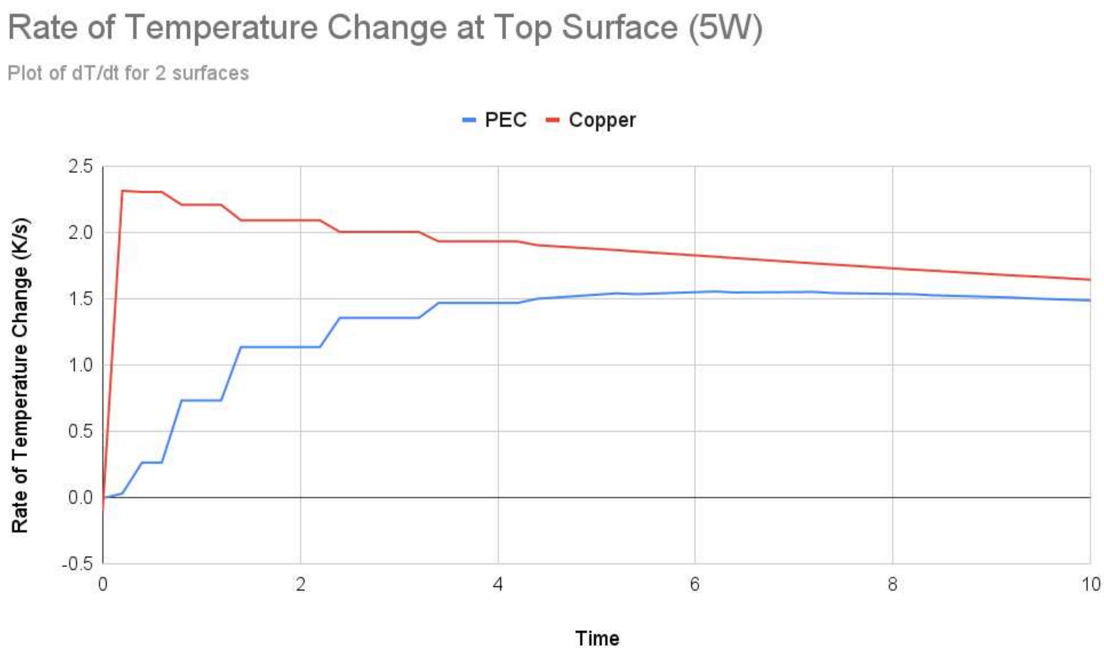
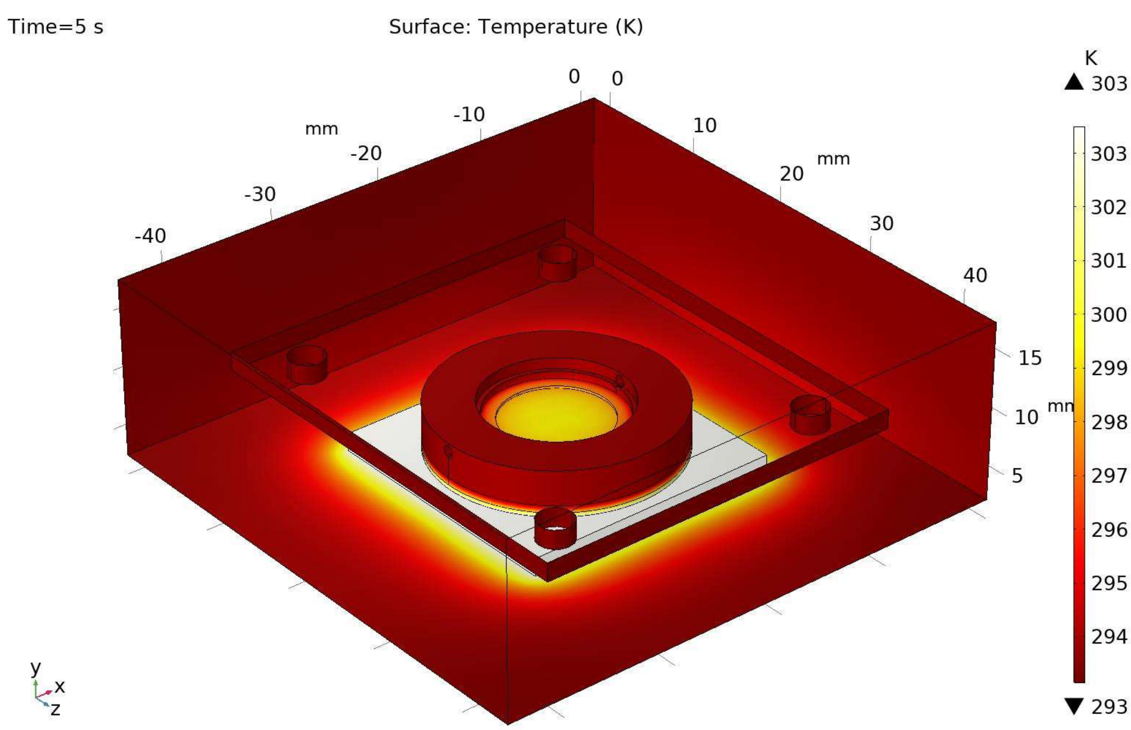


Figure X-G Line Plots of Rate of Temperature Change at the Top Surface of the PEC and Copper Sheet



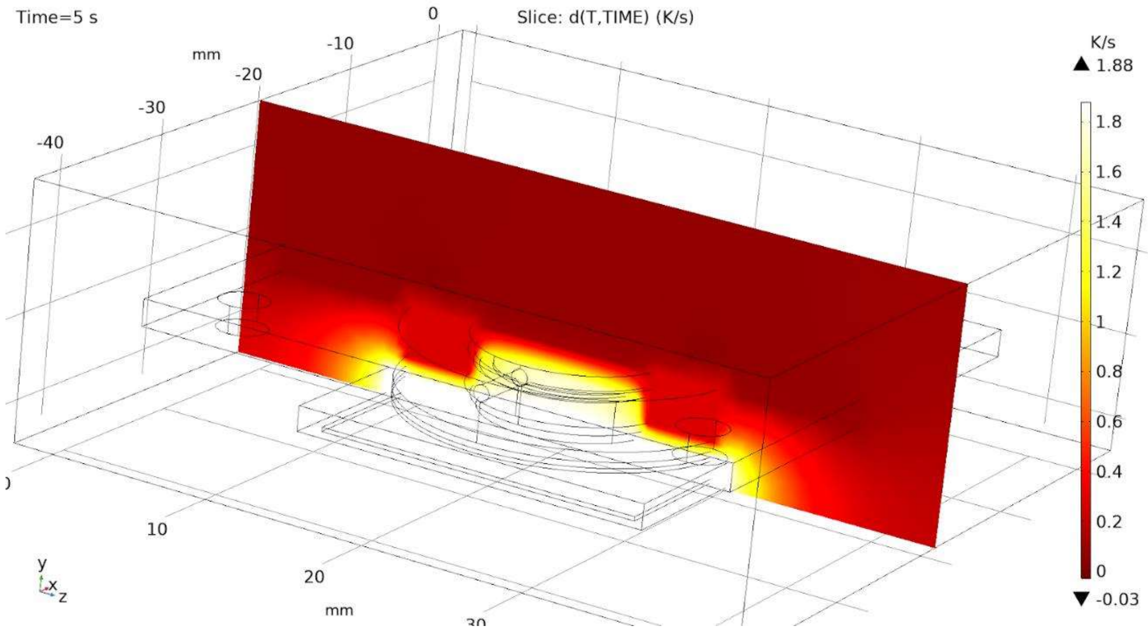


Figure X-H. Surface Plot of Temperature and Slice Plot of Rate of Temperature Change at 5s