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Transient Heating and Thermomechanical Stress Modeling of Ceramic HEPA Filters

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Abstract

The purpose of this report is to showcase an initial finite-element analysis model of a ceramic High-Efficiency Particulate (HEPA) Air filter design. Next generation HEPA filter assemblies are being developed at LLNL to withstand high-temperature fire scenarios by use of ceramics and advanced materials. The filters are meant for use in radiological and nuclear facilities, and are required to survive 500 ℃ fires over an hour duration. During such conditions, however, collecting data under varying parameters can be challenging; therefore, a Finite Element Analysis model of the filter was conducted using COMSOL ® Multiphysics to analyze the effects of fire. Finite Element Analysis (FEA) modelling offers several opportunities: researchers can quickly and easily consider impacts of potential design changes, material selection, and flow characterization on filter performance. Specifically, this model provides stress references for the sealant at high temperatures. Modeling of full filter assemblies was deemed inefficient given the computational requirements, so a section of three tubes from the assembly was modeled. The model looked at the transient heating and thermomechanical stress development during a 500 ℃ air flow at 6 CFM. Significant stresses were found at the ceramic-metal interfaces of the filter, and conservative temperature profiles at locations of interest were plotted. The model can be used for the development of sealants that minimize stresses at the ceramic-metal interface. Further work on the model would include the full filter assembly and consider heat losses to make more accurate predictions.

1. Purpose

The purpose of this report is to showcase an initial finite-element analysis model of a ceramic High-Efficiency Particulate (HEPA) Air filter design. HEPA filters are used in the capture of biological, chemical, and radiological aerosols, but current filter designs have been historically proven vulnerable to structural and operational failure caused by accident scenarios that exposed the filter to fire, water, and corrosive gas. To overcome these challenges, a new filter design utilizing a fused alumina ceramic was developed at Lawrence Livermore National Laboratory. The new filter design is expected to survive extreme operational conditions, such as a fire, but there is insufficient experimental data to fully characterize the behavior of the filter in fire scenarios. The intermediary solution to this is a model that possesses the material properties of the filter and utilizes worst-case fire conditions to extrapolate design performance. Specifically, the model looks at the thermomechanical stress and transient heating of the filter design under conditions that are beyond what a filter in a facility would encounter even in ultra-fast growth fire conditions (500 °C, 6 cubic-feet-per-minute (CFM)), and is simulated in the finite element analysis (FEA) software COMSOL® Multiphysics version 5.3.

2. Background

The use of HEPA filters became common place in radiological and nuclear facilities starting at the onset of the Manhattan Project to prevent radiation exposure to facilities and personnel via radiological aerosols. While multiple designs for HEPA filters have been created over time, the primary operational requirement for all designs, as stated by the Department of Energy, is that the filter shall maintain a minimum efficiency of 99.97% at a test aerosol diameter of 0.3 micrometers [2]. This standard has traditionally been achieved with a glass fiber medium that captures particulates, as illustrated in Figure 1.

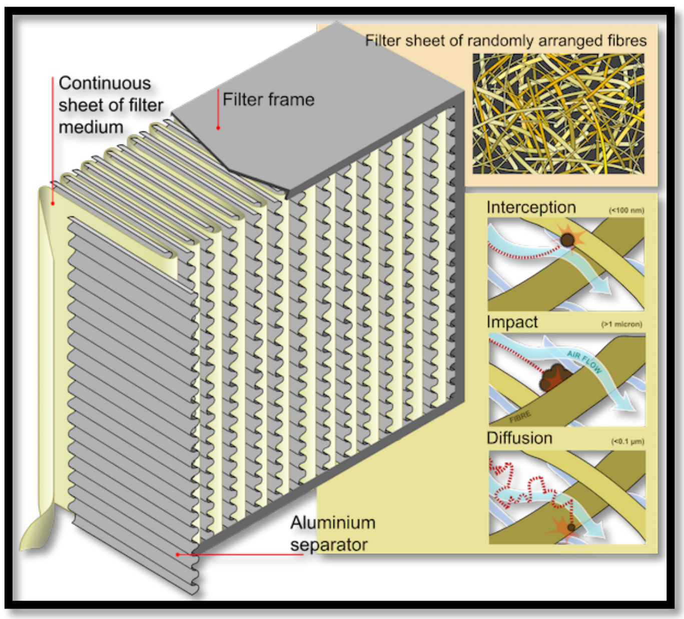

Figure 1 Traditional Fibrous Filter with modes of particulate capture

The fibers in the traditional filters are a weakness because they are prone to damage from fire, water, and corrosives that would compromise the filter's efficiency. A catastrophic failure occurred at Rocky Flats Plant in 1957, where a fire spread through the facility and destroyed its HEPA filters. The destruction of the filters, as seen in Figure 2 [2].

Figure 2 Rocky Flats radiological filter bank after catastrophic fire (Source: Department of Energy)

This incident created the precedent for LLNL to design the ceramic filter pictured in Figure 3. The filter consists of a cylindrical ceramic media attached to a stainless-steel base plate and held in place with a stainless-steel cap attached. The ceramic is connected to the stainless steel via a flame-resistant sealant material. This filter is expected to operate under intermittent high-temperature (below 500℃) air flow conditions, but if it can operate at 500 ℃ flow then it would be reasonable to assume it would operate at intermittent conditions.

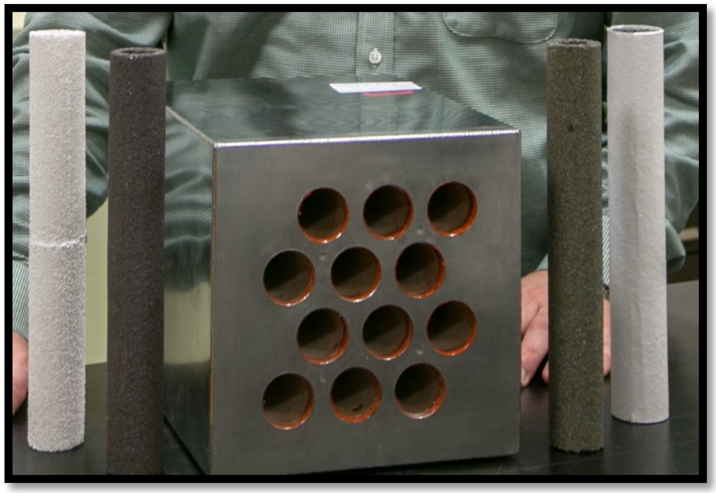

Figure 3 Full filter assembly with ceramic tubes to the side

3. Methodology

The finite element analysis (FEA) work was conducted on COMSOL® Multiphysics 5.3 using computational fluid dynamics (CFD), heat transfer, and structural mechanics modules. The scenario simulated was beyond a worst-case ultra-fast growth fire in which the fire heated the air entering the filter to 500 °C. [1] The filter was set to run at a standard operation flow of 6 CFM. The air, acting as the fluid, was heated and transferred heat via convection to the steel and ceramic media. The steel and ceramic were also transferred heat via conduction, which caused expansion and stress development. The purpose of the model was to simulate the transient heating of the ceramic media, steel cap, and steel baseplate when exposed to the elevated air, and to measure the magnitude of thermomechanical stresses. The process of constructing the model coincided with a systematic approach recommended by COMSOL®. The approach included defining the filter's geometries, assigning material properties, including the physics nodes, setting initial and boundary conditions, applying a mesh for computation, and running an appropriate study.

a) Geometries

Initially, it was desired to fully import a 3-D Computer-Aided Design (CAD) into the model, as seen in Figure 4, and run the simulation. However, this became impractical due to computation time constraints. A simplified 2-D geometry was created, then the model was move into 3-D modeling space after verifying successful implementation of physical conditions. The simplified 2-D geometry in Figure 5 shows the filter defined in an asymmetric plane. Figure 6 was created to demonstrate the stress development between the ceramic and steel base plate of the filter. Once the 2-D models were completed, 3-D simplified models, such as in Figure 7, were also made. However, to reduce computational time, planes of symmetry were applied to the cylindrical geometry. Finally, 3-D imported CAD designs shown in Figure 8, were created to apply physical conditions to the complex geometry. Figures 4 through 8 can been seen on the following pages.

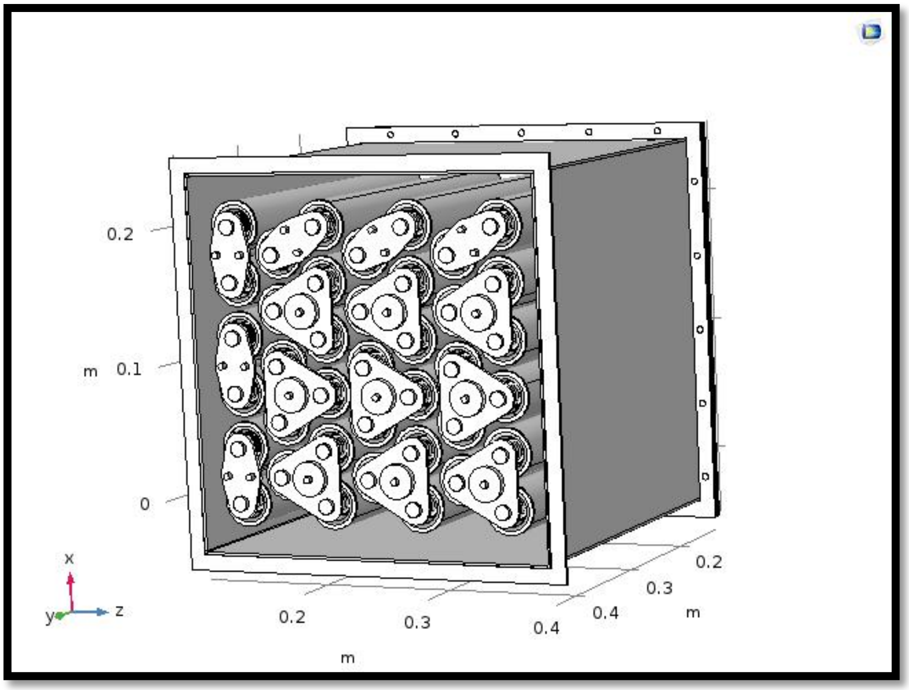

Figure 4 Full filter assembly CAD import

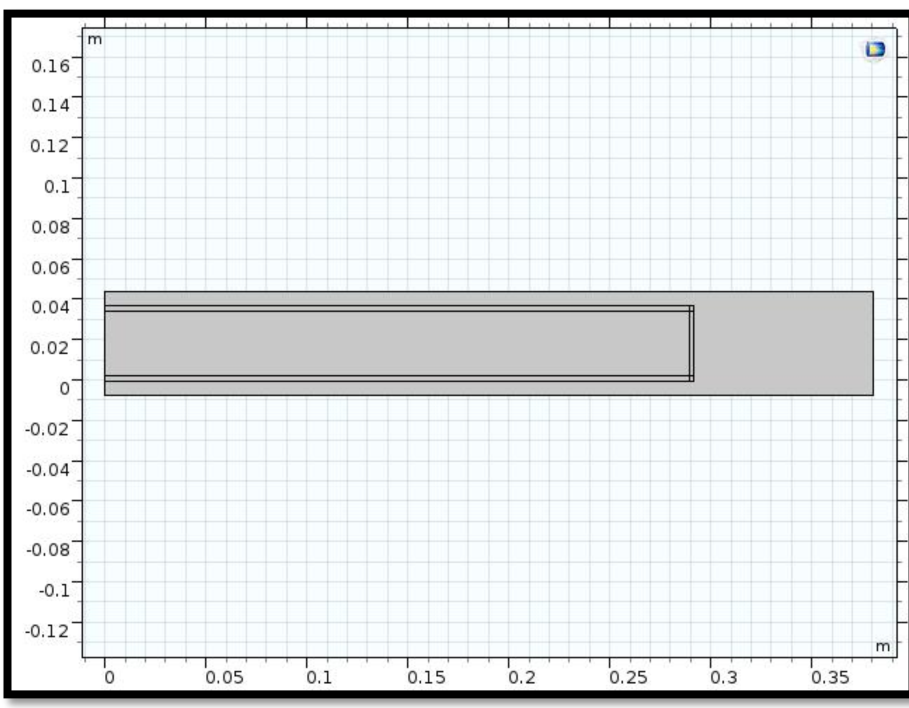

Figure 5 Simplified 2D filter geometry

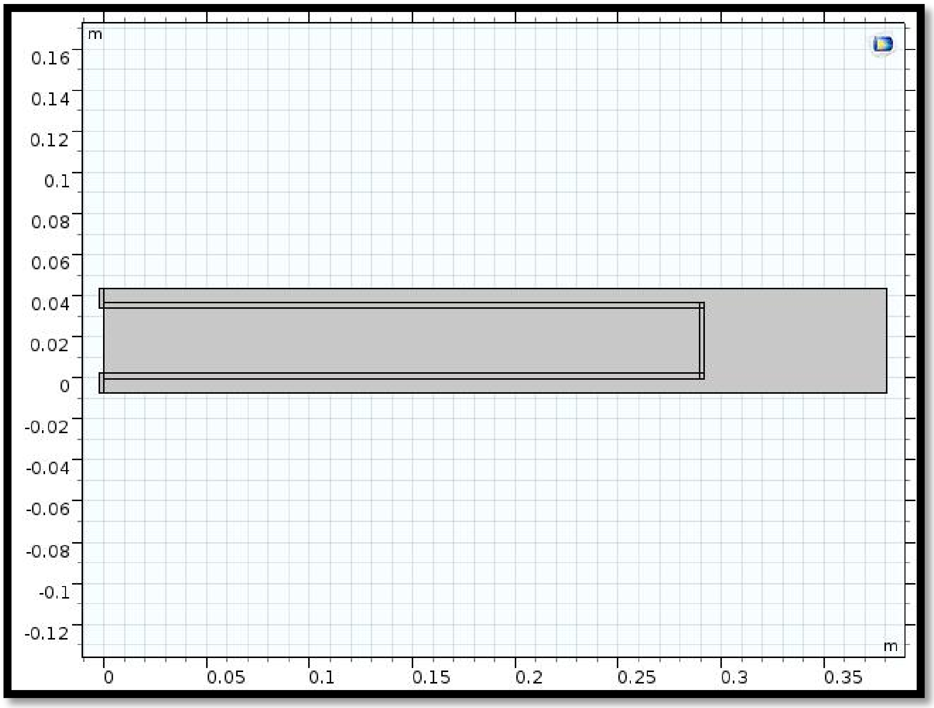

Figure 6 Simplified 2D filter with steel baseplate attached

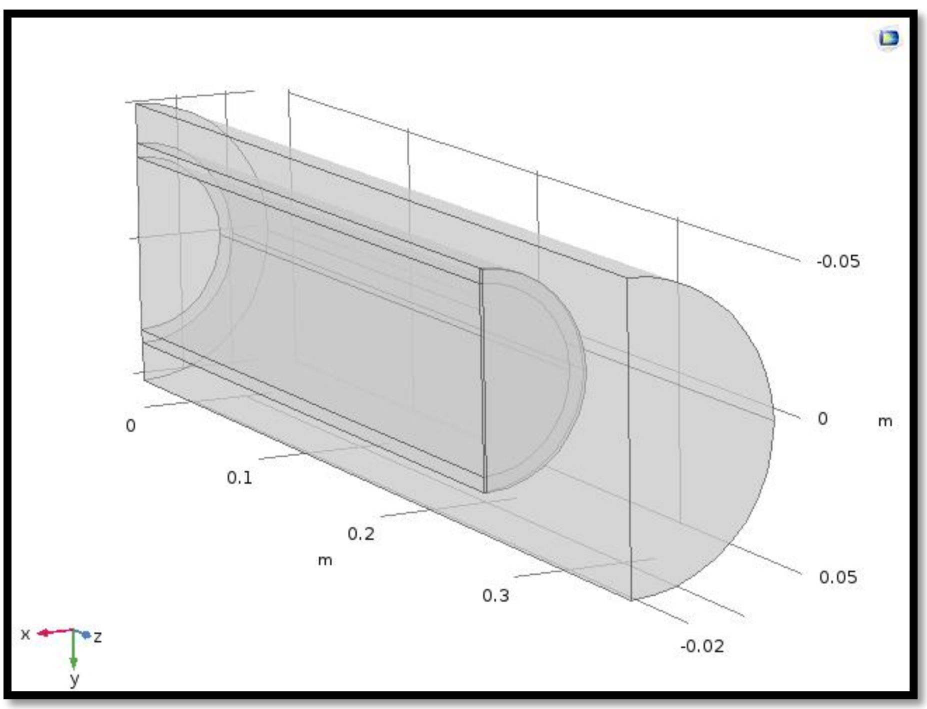

Figure 7 Simplified 3D filter with symmetry plane applied

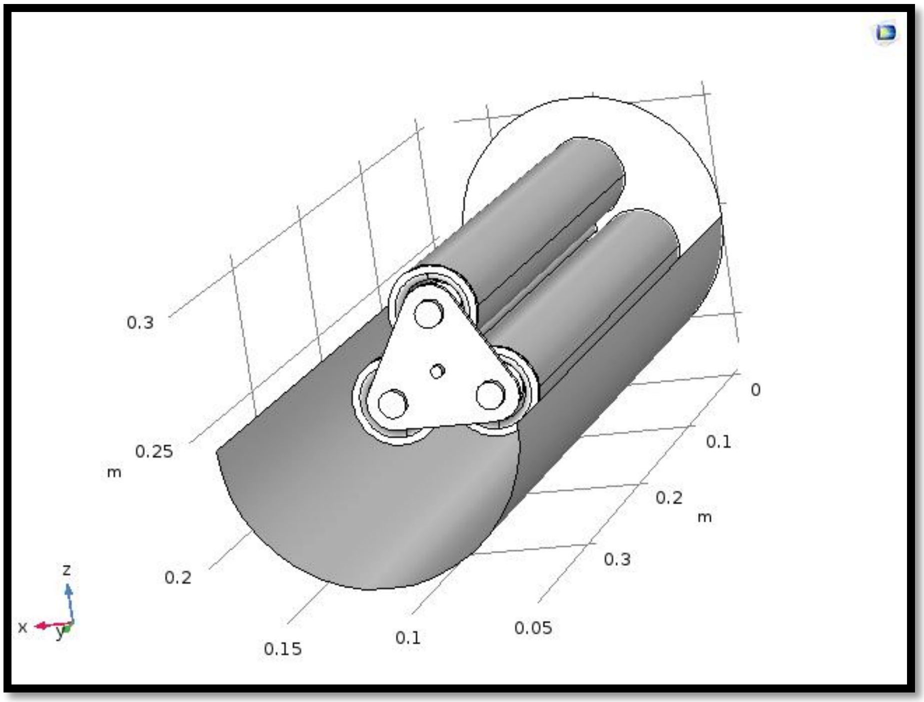

Figure 8 Three tube filter assembly 3D CAD import

b) Material Properties

An important component of the modeling process was the designation of material properties for the FEA computations. For this model, properties needed to be defined for a 410-stainless steel cap and base plate, the designated ceramic media filter, the air flow, and epoxy. COMSOL® included a variety of materials to select, but the materials for the ceramic media and epoxy were not readily available on this software; thus, the ceramic and epoxy were designated "Blank Materials" and had their properties added based upon the requirements of the physic nodes used for modeling. Table 1 includes the complete property values at the end of this report.

c) Physics

The scenario the model was simulating involves heating the air flow and viewing the resulting thermomechanical stresses that develop; therefore, the physical phenomena that occurred were fluid flow, heat transfer, and structural mechanics. These were labeled as “physics nodes” in COMSOL®. Each physics node in COMSOL® required initial condition “sub nodes,” to be assigned. This included tasks like classifying the air in the model as a fluid. The sub nodes also included the designation of boundary conditions for the FEA software and relations, such as defining the inlet air temperature as a function of time. Once the initial conditions and relationships were designated, the FEA software could deliver a solution. The physical conditions for each physics node are listed below.

i) Turbulent Flow

The flow node selected from COMSOL was the ‘Turbulent Flow yPlus’ node based on experimental determination using flow data for a single ceramic tube. The optimal flow of 6 CFM was determined by the filter design and requirements. Solving for the Reynold’s number of 6 CFM, it was discovered the flow was in the turbulent flow regime. The ‘Turbulent Flow yPlus’ node also had an option to solve the flow equation through a porous media that was then used during modeling.

For the initial conditions, an ‘inlet’ was designated as the space where air entered the filter at 6 CFM, and an ‘outlet’ was designated as the only exit for the air. The ceramic was designated as the ‘porous media’ so that the air could flow through it. This left all the other surfaces as impermeable boundaries.

ii) Heat Transfer

The heat transfer node selected was the 'Conjugate Heat Transfer' node. This node has a built-in physics coupling function for the heat transfer and turbulent flow. The coupling function automatically designated the air as a fluid and the ceramic as a conductive porous media. The steel in the filter was designated a conducting material, and all other surfaces were considered perfectly insulated surfaces. The beauty of this coupling function was that the FEA could solve the heat transfer caused by thermal conduction and convection in this scenario.

The initial conditions specific to the heat transfer node included setting the inlet temperature and designating the outlet for heat flow for transient heating. The inlet was defined in two separate methods: a ramp-up function and through tabulated values. The ramp-up function was defined as the raising of air temperature from ambient (20℃) to 500℃ in four seconds. Tabulated values were the temperature values for a fire over a length of time for a specific fire scenario. The outlet was an exit designation for heat for the FEA calculations to ensure heat would only flow through the system.

iii) Structural Mechanics

The structural mechanics node was a general physics node that had a coupling function between the heat transfer and mechanics node. This allowed the FEA to know that the stress experienced by the filter was due to the occurring heat transfer. The mechanics node required only the designation of parts that would experience stress, such as the steel, epoxy, and ceramic filter components. The air only acted as a medium and was therefore not the subject of stress. For initial conditions, the steel baseplate was designated a ‘fixed rigid body,’ to ensure no deformation of the baseplate would cause the other parts to deform around it.

d) Mesh

The mesh of the FEA was generated from polygons that defined the geometric domain that allowed for stress and heat calculations to occur within the model. The mesh acted as the basis for the solver in determining the spatial values for flow, heat transfer, and structural mechanics. The mesh created by COMSOL® was based upon the input physics nodes. Defining the mesh by the physical constraints allowed COMSOL® to increase the concentration of polygons around areas such as corners and surfaces. This is seen in Figure 9. This process gave more accurate results from the solver.

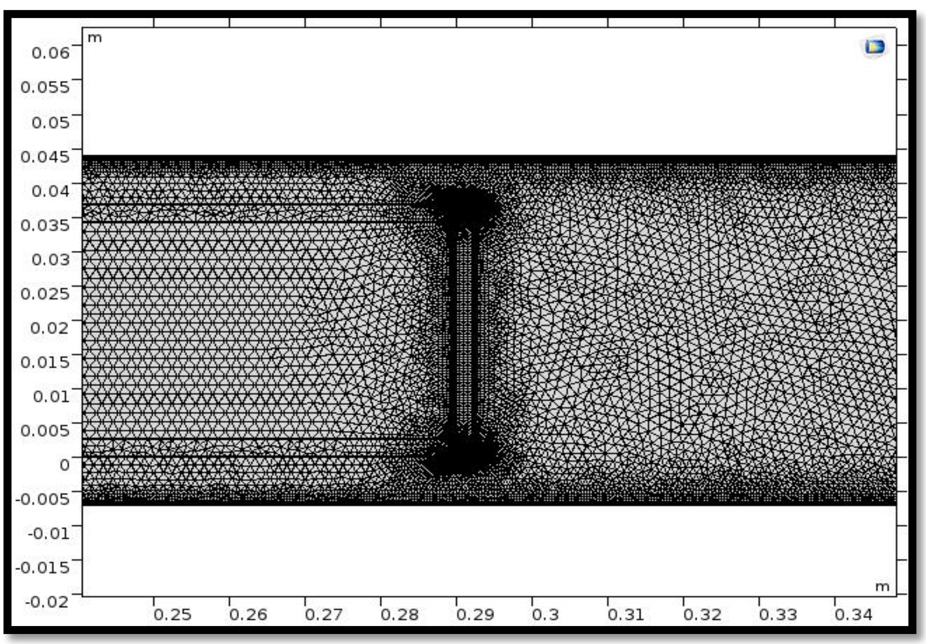

Figure 9' Fine' mesh applied to simplified 2D geometry

e) Study

The thermomechanical stress and transient heating nature were the desired results from the model. However, a limiting factor in modeling was the computation time given the nature of the study. COMSOL® can solve for a time-dependent or a stationary study, but a time-dependent study requires a longer computation time to converge to a solution. Thus, it became mandatory to split the model into one time dependent and one stationary scenario for the model to converge. For transient heating, heating went from a start to an end time, so a time-dependent solver was used to find the flow and heat transfer over the prescribed time without considering stress also changing over time. This study involved a ramp-up heating function for 4 seconds then maintaining 500 ℃ for 60 seconds and tabulated temperature values for 6000 seconds. The stationary study told the model that the filter experienced a maximum temperature of 500 ℃, and it solved for the maximum and minimum stress the filter experienced at this temperature.

4. Results

a) Thermomechanical Plots

2-D Thermomechanical stress plots provided von Mises stress and first principal strain under the steady state 500 ℃ air flow. From Figure 11, stresses of ~2 GPa were seen at the stainless steel-ceramic filter interface, and it was assumed the components were bonded and would not fracture. Strain was found primarily in the steel cap.

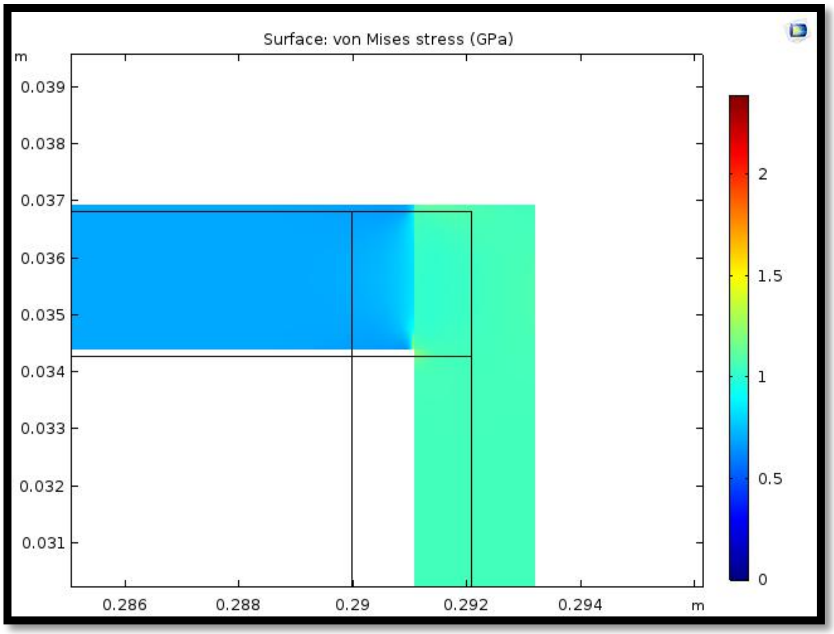

Figure 10 Spatial stress plot of 2D geometry at ceramic-steel cap interface

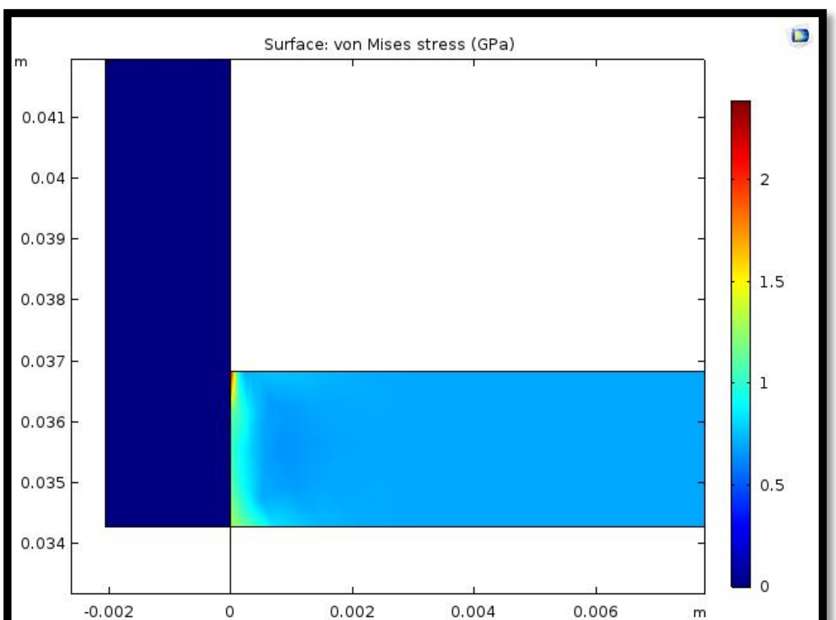

Figure 11 Spatial stress plot of 2D geometry at ceramic-steel baseplate interface

Figure 12 is the 3-D plot of the von Mises stress with ~2 GPa stress at the steel-ceramic interface. 3-D simulations were conducted at a steady state 500 ℃ air flow. The 3-D exaggerated deformation plot showed the ceramic tube expanding radially outward and displacing the steel rod and cap.

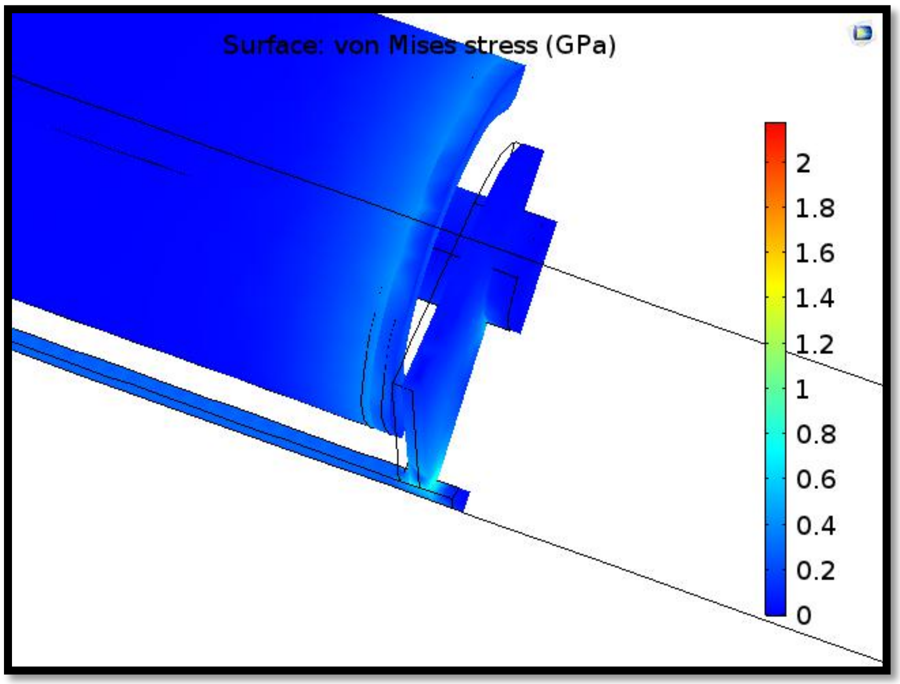

Figure 12 Spatial stress plot of 3D 3 Tube assembly with exaggerated deformation in radial direction

The 3-D plots with the sealant layer between the bottom of the ceramic tube and steel base plate, such as in Figure 13, changed the distribution of the stress at the interfaces. Specifically, the sealant layer experienced ~3 GPa of stress, but the ceramic-sealant interface experienced upwards of ~2 GPa.

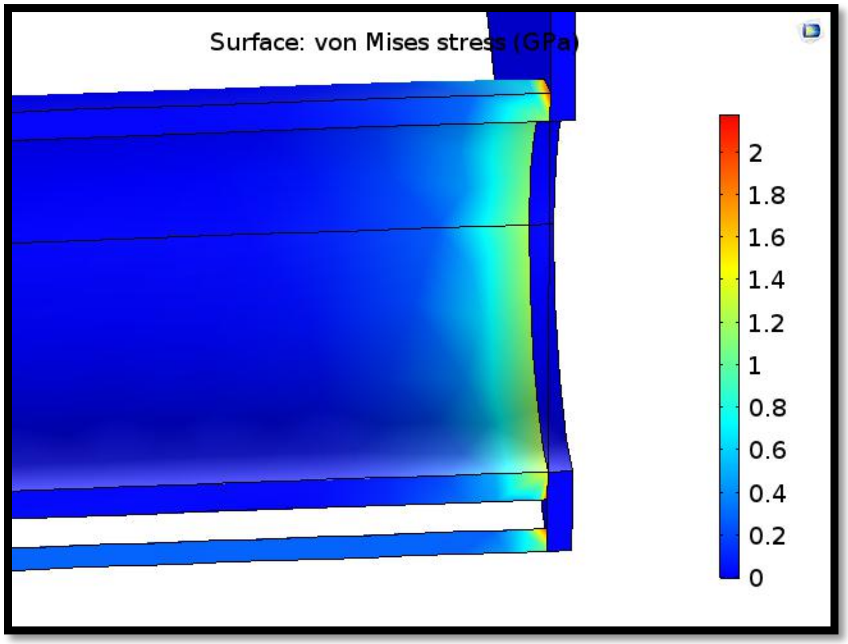

Figure 13 Spatial stress plot of 3D 3 tube assembly at ceramic-steel baseplate interface and connecting rod

a) Transient Heating Plots

The 2-D plots run at a constant 500 °C, 6 CFM air flow, shown in Figure 14, display the temperature gradient forming in the ceramic tube. Figure 15 also shows the heat flux direction arrows along the length of the filter. Additionally, Figure 16 shows the temperature at the spatial locations in the filter at 14 sec.

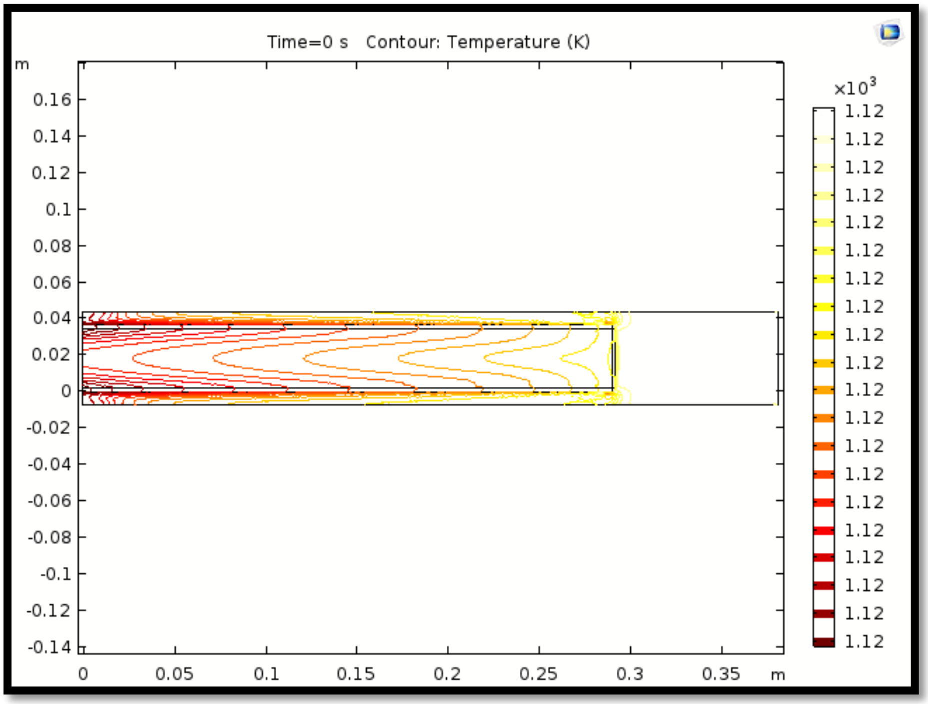

Figure 14 Temperature gradient contours of 2D geometry at 0 second

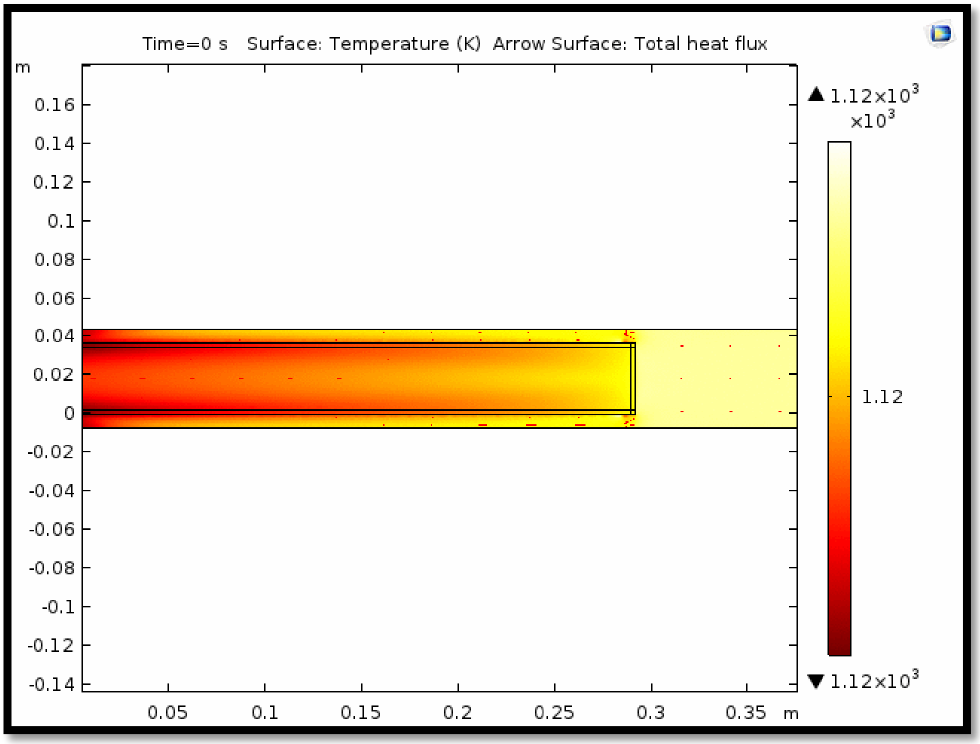

Figure 15 Spatial Temperature and heat flux direction arrows of 2D geometry at 0 seconds

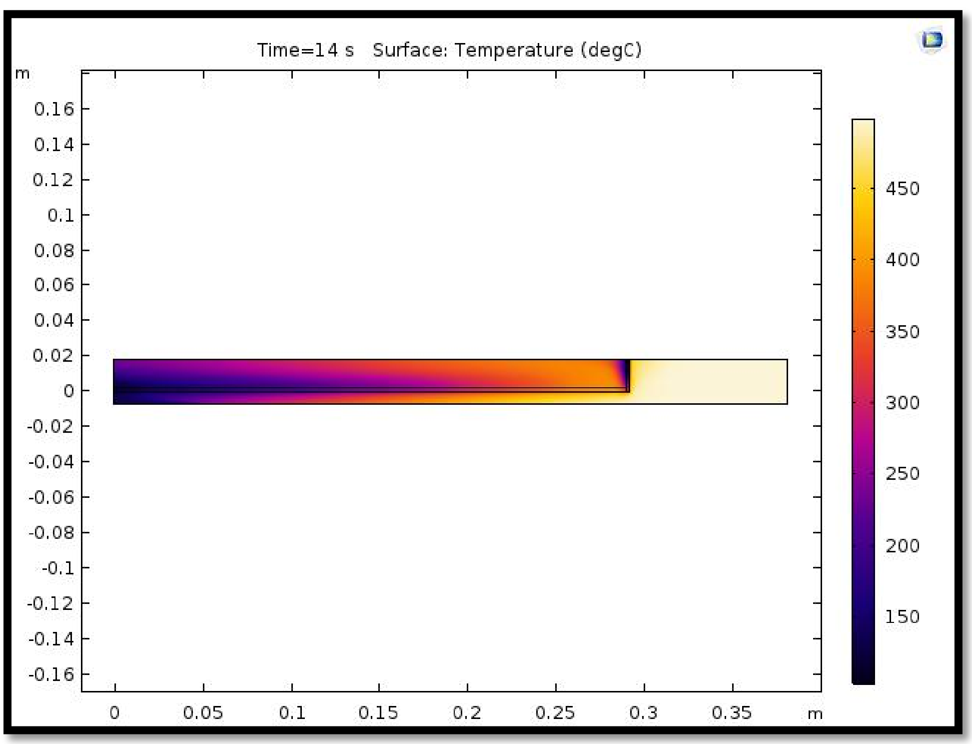

Figure 16 Spatial temperature plot of 2D geometry at 14 seconds

Figure 17 is the average temperature of the inlet, stainless steel cap, and ceramic-steel interface for the 2-D model. This model had the incoming air initially at ambient temperature and increased it to 500 °C within four seconds. It then maintained the air at 500 °C for the remainder of the run time. The plot below shows how the steel and ceramic heated up to 90% of the inlet temperature within 60 seconds.

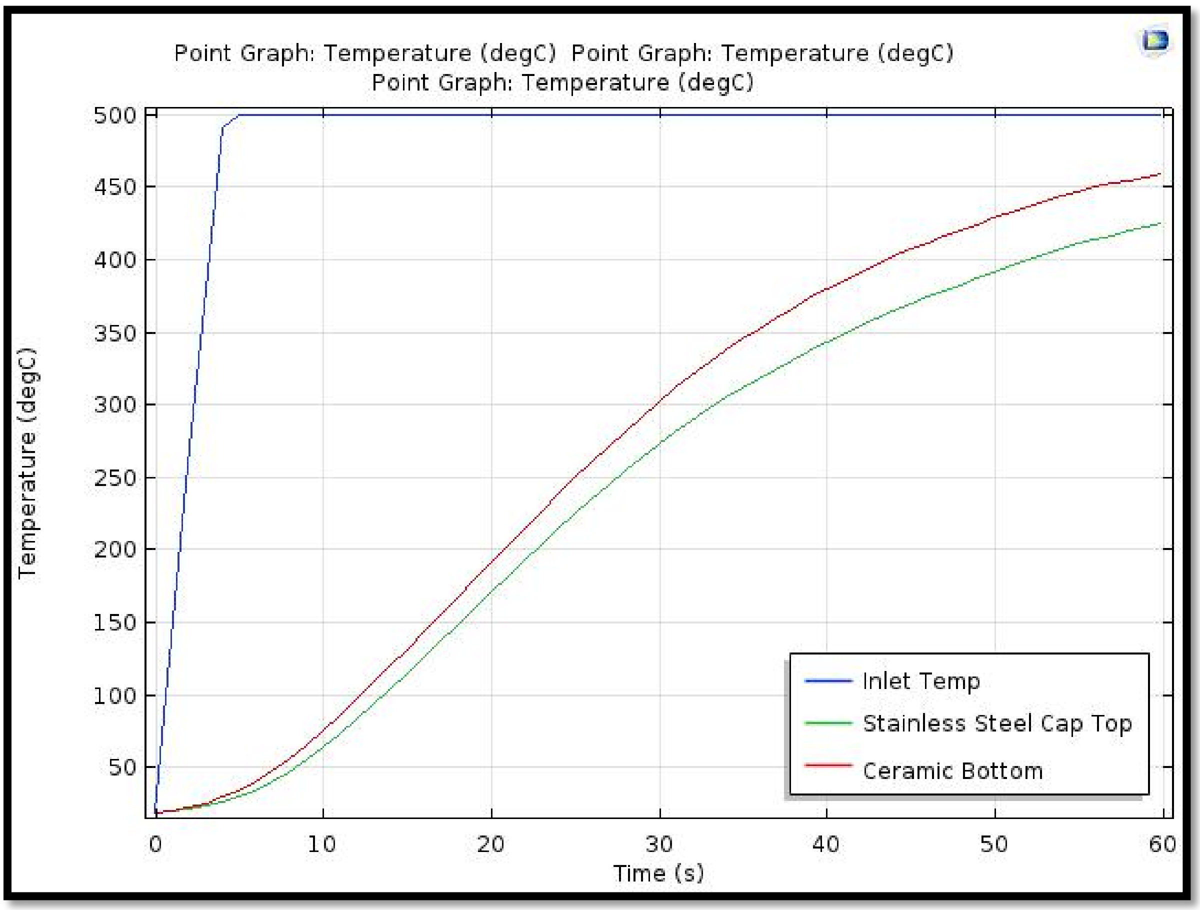

Figure 17 Temperature-Time plot of specified boundaries for the 2D geometry using ramp-up function

Figure 18 shows the spatial distribution of temperature on the 3-D model at 220s of heating.

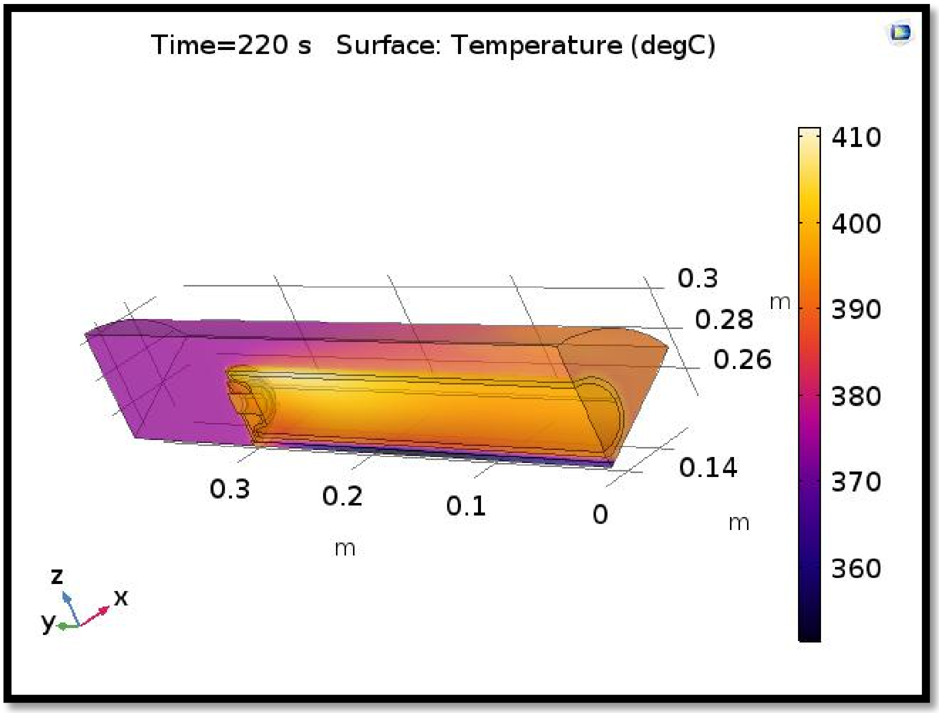

Figure 18 Spatial temperature plot of 3D 3 Tube assembly at 220 seconds

Figure 19 is a plot of the average temperature of the inlet, steel cap, and ceramic-steel interface over time, but for a 3-D model. The temperature of the cap and ceramic increased linearly in the first 10 seconds, then experienced a logarithmic increase. Once again, the cap and ceramic heated up to within 90% of the inlet temperature in 60 seconds.

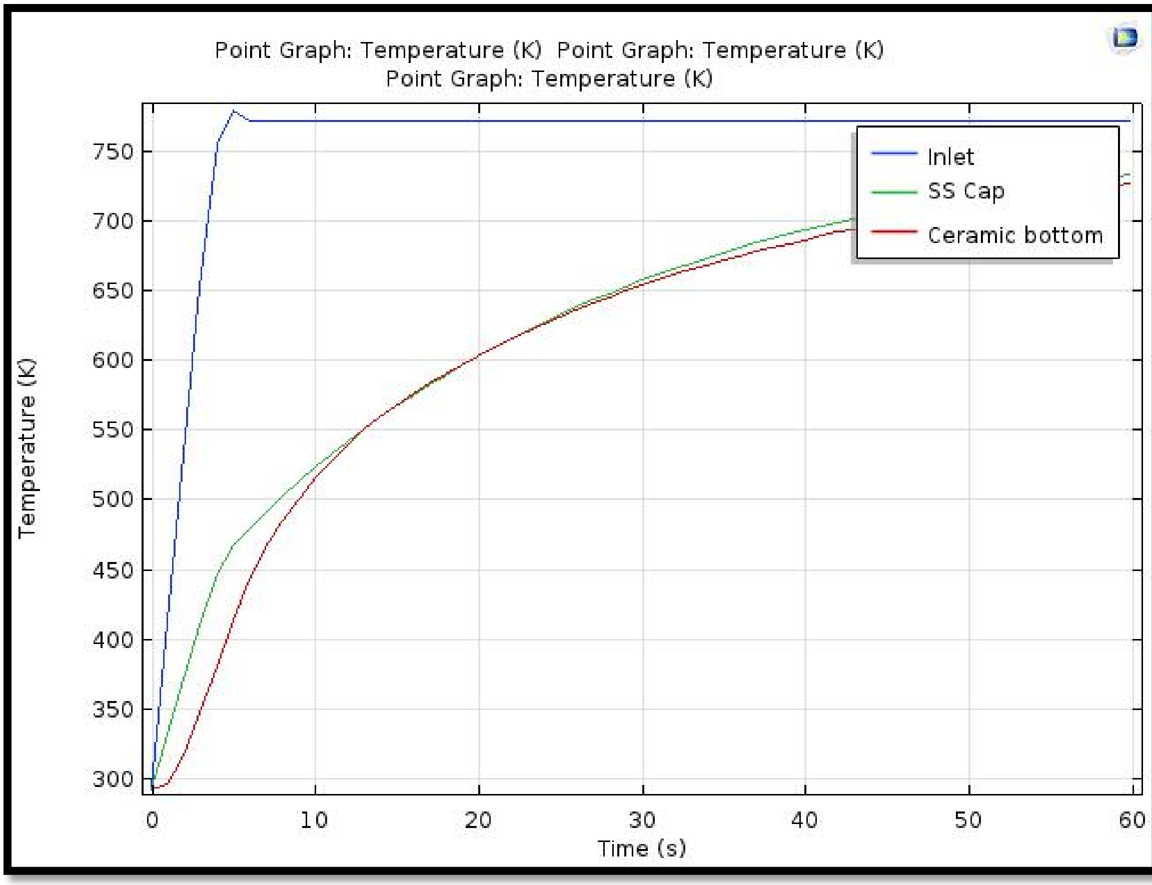

Figure 19 Temperature-Time plot of specified boundaries for the 3D geometry using ramp-up function

Figure 20 is a plot of the 3-D model using the fire model temperature data over time via tabulated values.

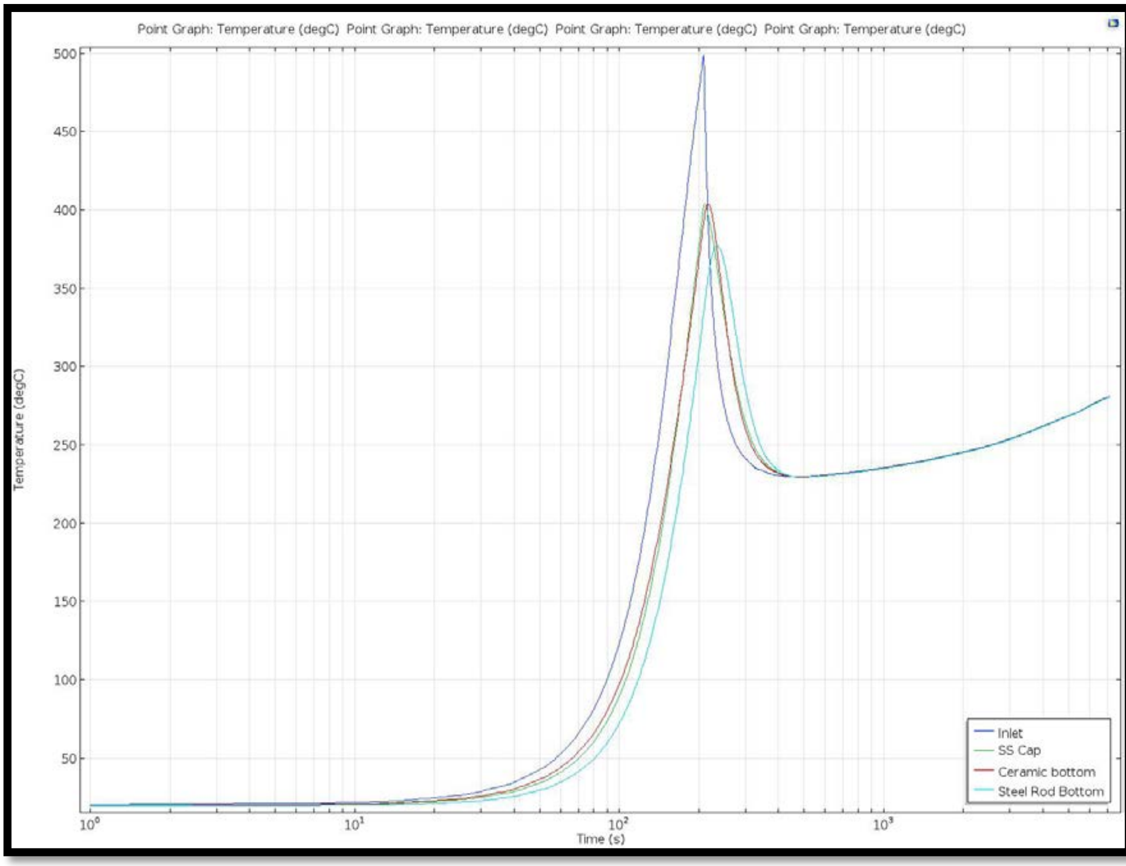

Figure 20 Temperature-Time plot of select boundaries for 3D 3 Tube assembly using tabulated values

5. Conclusions

The resulting plots of the thermomechanical stress and transient heating have provided a start in characterizing the filter performance under fire scenarios, and allow researchers to evaluate potential design changes and impact of materials selection. The thermomechanical stress plot provided a thermal strain characterization of the ceramic tube-stainless steel interface for sealant design. From the current model, the sealant experienced 3 GPa of stress, but it would be productive to use the model to determine sealant properties and characteristics that minimize stress. It was also observed from Figures 18 and 19 that the filter would heat up to

90% of the inlet temperature within 60 seconds. Figure 20 also showed for the short interval the fire was at 500 ℃, that none of the filter components reached 500 ℃. This means that the filter will more likely withstand and survive this high temperature fire scenario.

This report shows the potential for FEA modeling of filter performance, and it is only an initial investigation for modeling a 500 ℃ fire scenario near a ceramic HEPA filter. Future work on the model could include scaling up models to include the complete filter assembly, including the housing to calculate the heat loss via the steel housing around the filters. Additional investigations of unique fire scenarios with set distances away from the filter would be beneficial, along with a model of the fire heating the air in the ductwork that leads to the filter. This scenario would allow for modeling of the heat transfer to the filter as a function of distance and would also benefit from experimental data comparisons to check model validity. Finally, future work could be validating filter components with experiments to improve the models. In conclusion, the models in this report are an initial step towards understanding the ceramic filter's performance under a fire scenario.

6. Acknowledgement

I would like to thank Dr. Jeffrey Haslam, Dr. James Kelly, and Mark Mitchell first and foremost for their guidance in this project. I would also like to thank the Office of Science, specifically the Science Undergraduate Laboratory Internship (SULI) Program, NNSA NSR&D, and Lawrence Livermore National Laboratory for providing this opportunity.

7. References

1. Mohammdai, K. (2016). LLNL-CONF-698278, Temperature-Time Curves for Real Compartment-Fire Conditions. *EFCOG Nuclear & Facility Safety, Safety Analysis Workshop.* Argonne, IL.

2. *DOE-STD-3020-2015*. June 2015. *Specification for HEPA Filters Used by DOE.* Washington D.C.: United States Department of Energy.

8. Tables

Sealant	Value	Units
Density	5000	kg/m^3
Young's Modulus	1.50E+11	Pa
CTE	1.10E-05	1/K
Poisson's Ratio	0.27	1
Thermal Conductivity	9	W/(m*k)
Heat Capacity	800	J/(kg*K)
Porous Ceramic		
CTE	6.31E-06	1/K
Heat Capacity	730	J/(kg*K)
Density	514	kg/m^3
Thermal Conductivity	35	W/(m*K)
Young's Modulus	2.30E+11	Pa
Poisson Ratio	0.25	1
Porosity	0.3	1
Permeabitlity	3.31E-10	m^2
Volume Fraction	0.65	1
SS 409		
Thermal Conductivity	25	W/(m*K)
Density	760	kg/m^3
Heat Capacity	477	J/(kg*K)
Young's Modulus	2.00E+11	Pa
Poisson's Ratio	0.28	1
CTE	1.10E-05	1/K

Table 1 Material Property values used in COMSOL