3D modeling of heat transfer and gas flow in a grooved ring fuel element for nuclear thermal propulsion

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3D MODELING OF HEAT TRANSFER AND GAS FLOW
IN A GROOVED RING FUEL ELEMENT FOR NUCLEAR
THERMAL PROPULSION

by

LAURA ASHLEY BARKETT

A THESIS

Submitted in partial fulfillment of the requirements
for the degree of Master of Science in Engineering
in
The Department of Mechanical and Aerospace Engineering
to
The School of Graduate Studies
of
The University of Alabama in Huntsville

HUNTSVILLE, ALABAMA

2014
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Laura Ashley Barkett

(date)
THESIS APPROVAL FORM

Submitted by Laura Ashley Barkett in partial fulfillment of the requirements for the degree of Master of Science in Engineering in Aerospace Engineering and accepted on behalf of the Faculty of the School of Graduate Studies by the thesis committee.

We, the undersigned members of the Graduate Faculty of The University of Alabama in Huntsville, certify that we have advised and/or supervised the candidate of the work described in this thesis. We further certify that we have reviewed the thesis manuscript and approve it in partial fulfillment of the requirements for the degree of Master of Science in Engineering in Aerospace Engineering.

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ROCD JUN 26 '14
ABSTRACT

School of Graduate Studies
The University of Alabama in Huntsville

Degree Masters of Science College/Dept. Engineering/Mechanical and in Engineering Aerospace Engineering

Name of Candidate Laura Ashley Barkett


In the past, fuel elements with multiple axial coolant channels have been used in nuclear propulsion applications. A novel fuel element concept that reduces weight and increases efficiency uses a stack of grooved rings. Each fuel ring consists of a hole on the interior and grooves across the top face. Many grooved ring configurations have been modeled, and a single flow channel for each design has been analyzed. For increased efficiency, a fuel ring with a higher surface-area-to-volume ratio is ideal. When grooves are shallower and they have a lower surface area, the results show that the exit temperature is higher. By coupling the physics of fluid flow with those of heat transfer, the effects on the cooler gas flowing through the grooves of the hot, fissioning ring can be predicted. Models also show differences in velocities and temperatures after dense boundary nodes are applied. Parametric studies were done to show how a pressure drop across the length of the channels will affect the exit temperatures of the gas. Geometric optimization was done to show the temperature distributions and pressure drops that result from the manipulation of various parameters, and the effects of model scaling was also investigated. The inverse Graetz numbers are plotted
against Nusselt numbers, and the results of these values suggest that the gas quickly becomes fully developed, laminar flow, rather than constant turbulent conditions.

Abstract Approval: Committee Chair

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<tr>
<td>Latin</td>
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<tr>
<td>$A$</td>
<td>Area [mm]</td>
</tr>
<tr>
<td>$A_{cs}$</td>
<td>Cross-Sectional Area $mm^2$</td>
</tr>
<tr>
<td>$D_H$</td>
<td>Hydraulic Diameter [mm]</td>
</tr>
<tr>
<td>$C_p$</td>
<td>Specific Heat at Constant Pressure</td>
</tr>
<tr>
<td>$h_c$</td>
<td>Channel Height [mm]</td>
</tr>
<tr>
<td>$Isp$</td>
<td>Specific Impulse [s]</td>
</tr>
<tr>
<td>$L_c$</td>
<td>Channel Length [mm]</td>
</tr>
<tr>
<td>$LH2$</td>
<td>Liquid Hydrogen</td>
</tr>
<tr>
<td>$LOX$</td>
<td>Liquid Oxygen</td>
</tr>
<tr>
<td>$m$</td>
<td>Mass</td>
</tr>
<tr>
<td>$MW$</td>
<td>Molecular Weight [kg/mol]</td>
</tr>
<tr>
<td>$p$</td>
<td>Pressure [Pa]</td>
</tr>
<tr>
<td>$p_A$</td>
<td>Absolute Pressure [Pa]</td>
</tr>
<tr>
<td>$p_{ref}$</td>
<td>Reference Pressure [Pa]</td>
</tr>
<tr>
<td>$Pr$</td>
<td>Prandtl Number</td>
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</table>
\( Pr_T \) Turbulent Prandtl Number

\( r_i \) Inner Radius of Disc [mm]

\( r_o \) Outer Radius of Disc [mm]

\( R_s \) Specific Gas Constant [J/kg-K]

\( R_u \) Universal Gas Constant [J/(mol-k)]

\( t \) Time [s]

\( T \) Temperature [K]

\( T_c \) Solid Centerline Temperature [K]

\( T_{con} \) Most Constant Temperature of Solid Centerline[K]

\( T_{gmax} \) Maximum Gas Temperature [K]

\( T_{smax} \) Maximum Solid Temperature [K]

\( T_i \) Temperature at Channel Inlet [K]

\( T_e \) Temperature at Channel Exit [K]

\( T_m \) Mixing-cup Temperature [K]

\( v_e \) Exit Velocity Magnitude [m/s]

\( w_c \) Channel Width [mm]

Vectors/Tensors

\( \mathbf{E} \) Elastic Entropy [J/m\(^3\)K]

\( \mathbf{F} \) Body Force Vector [N/m\(^3\)]
I  Identity Matrix
k  Thermal Conductivity Tensor [W/(m-K)]
q  Heat Flux [W/m²]
S  Strain-Rate Tensor [1/s]
u  Velocity in the x-direction [m/s]
v  Velocity in the y-direction [m/s]
w  Velocity in the z-direction [m/s]

Greek
β  Thermal Expansivity [1/K]
δ  Distance Between Solid Wall and Computation Fluid Domain [mm]
κ  Thermal Conductivity [W/(m-K)]
κ_T  Thermal Turbulent Conductivity [W/(m-K)]
µ  Dynamic Viscosity [Pa·s]
µ_T  Turbulent Viscosity
π  Pi
γ  Specific Heat Ratio
ρ  Density [kg/m²]
τ  Viscous Stress Tensor [1/s]

Typography
xvii
**Bold**  Bold type is used to identify vectors — that is, quantities that have both magnitude and direction in Cartesian coordinates, consisting of x, y, and z components. Tensors, or components changing linearly with coordinate transformations, are also denoted by bold type.

**Italics**  Italics type is used to identify book titles.
For friends and family.
1.1 Motivation

In the past, manned space flight propulsion systems have utilized chemical and solid fuels. Although chemical and solid rockets have been efficient for lunar explorations, a more efficient method of transportation, such as nuclear thermal propulsion, is needed for manned interplanetary travel [1]. Missions to Mars will benefit from propulsion systems with performance levels exceeding that of today’s best chemical engines. Nuclear Thermal Rocket (NTR) technology has the greatest potential for the near-term success of increasing performance, reducing cost, and increasing safety margins by reducing total fuel required, thus reducing total launches for Mars missions [2]. Nuclear fuels are ideal for long-term applications, especially space applications with long durations [3].

Utilizing the most optimal design will ultimately result in a lower weight, low-cost propulsion system and fewer launches needed for manned exploration of Mars. Current chemical rockets would require around 12 launches for Mars missions. According to recent assessments, nuclear thermal propulsion systems could reduce the number of launches needed for a successful Mars mission by four or five [1]. As
technology and expectations progress, interest in manned missions to Mars is elevated, and therefore nuclear thermal propulsion development has become a top priority for NASA (National Aeronautics and Space Administration) [4].

Although there have been several nuclear fuels tested for spaceflight, these solutions are not without disadvantages. A grooved ring element is investigated herein to determine the feasibility of designing a corrosion resistant fuel element with a larger surface-area-to-volume ratio for a higher heat transfer to the propellant. Rather than using the traditional, hexagonal fuel rods with fewer channels, disc shaped elements with hundreds of propellant flow channels will be used. Computations are needed in order to determine the heat transfer and flow behaviors within the flow channels, so that designs can be optimized to maximize heat output with the least amount of fissile material used, while possibly minimizing thermal stress. These computations will aid in showing the advantages of the grooved ring element over existing technologies. Qualitative analyses can show trends involved with changing certain geometric parameters and geometrically scaling the entire element.

1.2 Nuclear Technologies for Space Applications

During the 1960s and 1970s, the United States embarked on a nuclear rocket program called Rover/NERVA (Nuclear Engine for Rocket Vehicle Applications), which was successful in developing high performance nuclear fuel forms [2]. Solid core NTR engines during the Rover/NERVA program demonstrated specific impulses around 850 seconds, which are significantly greater than those possible with maximally efficient chemical engine systems with around 450 seconds [1]. In spite of this
success, however, there surfaced a number of materials and configuration issues which limited the ultimate performance of these engines. In particular, the relatively heavy and difficult to fabricate prismatic fuel block, with its small surface-to-volume ratio ($5.6 \, \text{cm}^{-1}$), caused large core pressure drops which consequently limited the engine thrust-to-weight ratios to around 3 or 4 [5]. These pressure drops were due to corrosion that occurred in the long flow channels of the fuel elements [6]. This corrosion led to lower specific impulse, lower thrust-to-weight ratio, lower life-cycle duration, increased demand on control systems controlling the reactor, and higher cost and complexity of ground development testing [5].

![Figure 1.1: The long channels in the traditional hexagonal fuel rods have historically been subject to mid-band corrosion.](image)

To address the problem of low thrust-to-weight ratios in the Rover/NERVA engine design, a new configuration was proposed. This configuration, called the particle bed reactor, used fuel that had a much higher surface-to-volume ratio (40 cm$^{-1}$) and a lower pressure drop. This engine was projected to have a thrust to weight ratio of 20 or greater, although the design ultimately proved unsatisfactory because of
1.3 Grooved Ring Fuel Element Design Concept

The GRFE (Grooved Ring Fuel Element) is a concept that seeks to eliminate the undesirable features of the Rover/NERVA fuel element and the particle bed fuels, by correcting some of the known problems, including but not limited to, pressure drops, corrosion, thermal instabilities, and intricacies in fabrication methods. On the surface, the GRFE has a propellant flow configuration which is roughly similar to that envisioned for the particle bed fuel element; however, there are significant differences. A conceptual drawing of the fuel element is shown in Figure 1.2. As illustrated, cold hydrogen enters reactor and is diverted down along the outside edge of the grooved fuel ring stack. The hydrogen propellant enters the stack of rings and flows radially along the grooved faces of the individual fuel rings. The rings are held in place by a hexagonal structure which directs the hydrogen flow into the fuel ring stack. The hexagonal structure may or may not contain moderating material depending upon whether the reactor is designed to be a fast reactor or thermal reactor. Because cold hydrogen flows in the region between the outer edge of the rings and the inner region of the hexagonal support structure, the support structure remains fairly cool during operation and only the rings experience high temperatures.

Figure 1.2 illustrates an example of an individual grooved fuel ring where the flow area remains constant along the face of the ring from its outside edge to its inside edge. As the hydrogen flows along the face of the fuel ring, it picks up heat until it
Figure 1.2: The grooved ring fuel element (left) is a grooved disc, through which heated gas flows. Discs are placed in a reactor (right), to create a stack efficient for nuclear thermal propulsion applications. Gas enters the top, flows through the grooves, then flows out the bottom. Finally exits into the interior of the fuel ring. The hot hydrogen then flows axially down the center of the fuel ring stack until it finally exits the fuel element assembly at the bottom. Other groove patterns on the fuel ring faces could be designed to achieve variable cross-sectional flow areas which could be more optimal from a fluid dynamics standpoint. Additionally, more flow channels will result in a higher surface-area-to-volume ratio, which will create more reactive surface area to transfer heat to the hydrogen propellant. This will subtract the amount of fissile material in each element while lowering the solid temperatures. It should also be possible for a moderated fuel element to yield very favorable radial power profiles where the power density decreases exponentially radially inward toward the center channel. Such power density profiles
minimize thermal gradients within the fuel ring, while allowing the entire ring to operate near its maximum allowable temperature [8].

1.4 Advantages of the Grooved Ring Fuel

The Grooved Ring Fuel Element (GRFE) could enable the development of a new NTR system with specific impulse of around 900 seconds or higher. Increases in specific impulse from 450 seconds to 850 seconds will reduce the amount of propellant required in orbit to save 3 SLS (Space Launch System) launches for a Mars mission [1]. Given that the current mission models at NASA show that a 75s improvement in Isp (specific impulse) over the NERVA/Rover technologies will change the number of SLS launches need for Mars missions by 1 launch, taking advantage of this Isp sensitivity will result in 4 fewer launches than needed for chemical rockets [9]. The higher surface-area-to-volume ratio of the grooved ring element could have the potential to make this small difference.

Fabrication of more complex fuel geometries is possible using new carbide fuel materials and with newly available ceramic manufacturing technologies. The hexagonal fuel elements previously used for the NERVA/Rover program were hard to fabricate due to the corrosion problems in the channels. Since the channels were long, it was hard to properly coat the material along the middle of the flow path to avoid oxidation and prevent corrosion. Additionally, the fabrication processes were lengthy due to the excessive fabrication techniques required to attempt correction of the oxidation [5]. Since the 1970’s, newer technologies such as sintering, electron beam melting, pulsed electric current, and hot isostatic pressing processes exist, making
fabrication capabilities more versatile than in previous decades when the hexagonal rods were designed. NASA currently has ongoing research into perfecting fabrication processes for new fuel materials [10]. Solid geometries not previously explored can now be considered.

Because the grooved structure of the fuel rings does not require inaccessible passages for the propellant flow, difficult extrusions, as shown in Figure 1.3, or machining techniques used for NERVA type fuel elements will not be required. This ease of fabrication will allow fuel elements to be made of more ideal exotic materials such as uranium tricarbide that present difficulties under normal circumstances due to extreme hardness and brittleness material properties.

![Figure 1.3: The hexagonal elements are fabricated with a special extrusion machine. This technique does not favor the use of many carbide materials that can be used.](image)

The GRFE, with its high surface-area-to-volume ratio and potential for refractory carbide use, has the potential to provide higher power densities, yielding NTR engines with a higher thrust-to-weight ratio around 10 to 15. This is around 3 to 5
times greater than the NERVA engine design, which used hexagonal axial flow reactor fuel elements.

1.5 Multiphysics Modeling

As stated previously, using better fuels with higher melting points will create a more efficient engine. Having more heat increases thrust, specific impulse and efficiency. This translates to a smaller fuel volume, less weight, and lower costs. Designing a fuel element using the newer materials in a way that is structurally sound and thermally efficient is a complex task. One problem with using the recently developed carbides is the brittleness of the material which causes sensitivities to thermal stresses. The main goal of this project is to design a grooved ring fuel element that has constant centerline temperatures in the channel walls, which will reduce thermal stresses, while maximizing the gas exit temperature and minimizing the volume of solid material needed. The element should be designed to yield a maximum gas exit temperature, while maintaining a solid temperature below the material melting point. Additionally, pressure differentials should be studied to show how pressure drops affect the temperature distributions at the centerline.

Several different models were made, each with varying parameters such as channel height, outer radius, or groove spacing angle. Straight-edged slices are taken from several design configurations, and analyzed in COMSOL. No curved-channel rings were analyzed for this effort. COMSOL is used to model, analyze, and geometrically optimize structures. Heat transfer and turbulent flow physics are used. Fission heat is produced in the solid fuel, then transferred to the coolant traveling through
the fuel channels. Pressures and velocities are found for the gas, and temperature values are solved for both the solid and the gas. The finite element analysis aids in designing elements that maximize the gas exit temperature, yielding a constant centerline temperature within the channel wall, and showing that the fuel has not exceeded thermal limitations of the materials utilized.

1.6 Outline

The rest of the thesis is organized as follows: Chapter 2 discusses various efforts to create fuel elements and similar finite element applications, and also lists relevant theory, equations, and material properties. Chapter 3 begins with a detailed problem statement, followed by an overview of the finite element method, relevant software, description of the baseline design, the approach to the fuel element disc design, and solvers used. Chapter 4 gives an in-depth review of the data found from the analyses by providing pressure, temperature, and velocity results. Surface area calculations are also shown here. Results are mostly qualitative, and the final model shows quantitative results. Chapter 5 summarizes the most important results and provides recommendations for future work.
CHAPTER 2

BACKGROUND INFORMATION

2.1 The Earliest Efforts in Nuclear Propulsion

The concept of nuclear rocket propulsion gained traction in the 1940's, with many entities publishing research and ideas. By the mid-1950's, sufficient proof was found to show that nuclear, heat-exchanger rocket engines could out-perform chemical engines [11]. Project Rover, a program of The Los Alamos Scientific Laboratory in New Mexico, was heavily involved in the facilitation of the first well-developed nuclear propulsion concepts. According to "The LASL Nuclear Propulsion Program" report from 1956, they defined the critical program tasks as "research and development in the fields of high-temperature materials, basic reactor performance, fluid dynamics, heat transfer, fuel element characteristics, engine control, and engine control testing techniques." Research of the interaction between the fuel and the propellant was limited to theoretical studies backed by experimental data. Since nuclear heating was not convenient at the required level, experiments were conducted using electronically heated elements, similar to those being done presently at NASA. However, material procurement and fabrication can be extremely expensive, especially without having knowledge of the fluid environment.
2.2 Existing Research of Heat Transfer and Flow Analysis in Nuclear Reactors

As advancements in computers and numerical methods enable solutions to 3D Navier Stokes problems that have no closed form solutions, computers can now reveal more to aid in the design of fuels. Computational methods are ideal for predicting behaviors of thermo-hydraulic environments in reactors before element fabrication takes place and testing is done, which results in fewer dollars spent on materials and unnecessary testing. It is difficult to determine temperature and flow properties accurately without 3D analysis. Recent modeling has included turbulent flow, structural mechanics, and heat transfer physics, with cylindrical axial flow channels. Objectives in these models typically include showing temperature profiles, thermal stresses, gas temperatures, and etc. Several groups have made progress in performing such computational analyses for nuclear applications in the last four years. In discussing recent research herein, attention was given to the purpose of the research projects, software tools, assumptions, meshing techniques, boundary conditions, inputs, types of parameters found through analysis, equations used, and results.

In 2010, dynamicists at Marshall Space Flight Center chose to explore a CFD/heat transfer multiphysics procedure for modeling a solid-core NTP reactor [12]. They used an unstructured grid for meshing, constant inlet pressure, non-equilibrium gas conditions, and porous media assumptions. Rather than computing all channels separately, the porous media was used to represent all the channels so that the modeling was simplified. In developing the methods needed for the fluids
model, equations for continuity, species continuity, momentum, total enthalpy, turbulent kinetic energy, and turbulent kinetic energy dissipation rate were identified. Similarly, the heat transfer conduction equation with a heat flux into gas boundary condition was also identified. Navier Stokes and energy equations were used for fluid flow and heat transfer in porous media, and a two-species, double reaction model was found for the dissociation and recombination of the hydrogen, since the expansion chamber were hydrogen quickly returns back to molecular form, was also part of the model.

![Figure 2.1: Results for ”Multiphysics Computational Analysis of a Solid-Core Nuclear Thermal Engine Thrust Chamber” published in 2010 [12].](image)

In 2011, Idaho National Laboratory and the University of Mexico participated in a design concept of a CERMIT NTR fission core [13]. Modeling was accomplished
via multiphysics modeling, using SolidWorks for solid modeling, MCNP (Monte Carlo Neutronics Program) for heat output, GAMBIT for meshing, and STAR-CCM+ for the CFD. This allowed for the computations of neutronics, stress, heat transfer, and fluid flow. The surface-area-to-volume ratios had to be around 15.0 for solid centerline temperatures to remain under 3000K. The peak temperatures of the fuel were 3414K for 61 channels, and 3211K for 91 channels. It was estimated that an analysis for a 127-channel configuration would place the peak temperature below 3000K because the increased surface-area-to-volume ratio decreased the fissile material temperature. Specific impulse calculations showed ∼950s. Both reactors analyzed could reach ∼25,000 lbf of thrust.

Figure 2.2: Results for ”Conceptual Design of a CERMET NTR Fission Core Using Multiphysics Modeling Techniques” published in 2011 [13].
In 2012, two scientists from China modeled a sub-channel of an AP1000 nuclear reactor core to study the 3D turbulent flow and convective heat transfer [14]. The FLUENT software was used for the single-phase, steady state problem and the k-\(\epsilon\) model was employed for turbulent enclosure of mixing vein cross-flows. Meshes were predominantly hexahedral and non-structured. Adiabatic walls governed the boundary conditions between the solid and gas along the length of the fuel. Uniform flow was specified at the inlet, and there was a constant pressure at the exit. A heat flux was applied to the fuel rod surface. The RANS (Reynolds Averaged Navier Stokes) equations for fluid flow were used. Their research showed that the k-\(\epsilon\) model is efficient for prediction of axial flow of a thermal hydraulic environment.

![Mesh for "Numerical Analysis of Turbulent Heat Transfer and Flow through Mixing Split Vane in a Sub-channel of AP1000 Nuclear Reactor" published in 2012 [14].](image)

**Figure 2.3:** Mesh for "Numerical Analysis of Turbulent Heat Transfer and Flow through Mixing Split Vane in a Sub-channel of AP1000 Nuclear Reactor" published in 2012 [14].

The same year, NASA Glenn Research Center and Idaho National Laboratories participated in a multiphysics simulation of a nuclear fuel element [15]. In addition to the heat transfer and gas flow predictions, the material thermal stresses
were found to address concerns about the non-elastic creep effects. In addition to finding maximum material temperatures and exit flow temperature variations, this modeling was also done to study the sources of stress and coating stress. This project was performed utilizing a finite element analysis on a small, 30 degree wedge of the hexagonal fuel element. Power density calculations were done via MCNP and used for input. FLOTRAN was used for steady-state compressible flow, and was solved with the RANS equations. The k-\(\epsilon\) turbulence model was also used. The outlet pressure of each channel is specified, and the inlets are at constant temperature with axial velocity. Boundary conditions included the fuel adiabatic exterior, and no-slip solid walls. Mass flows were taken as a reactor average for each channel. They found a maximum solid temperature of 3168 K, a coolant exit temperature of 2650, an inlet and outlet Reynold’s numbers of 85,000 and 15,000 respectively, and a pressure drop of 0.81 MPa. The gas centerline velocity range was from 31.3 to 820.0 m/s.

![Figure 2.4: Mesh for "Thermal, Fluid, and Structural Analysis of a Cermet Fuel Element" published in 2012 [15].](image-url)
Another recent effort performed by scientists from Indonesia’s Institut Teknologi Bandan, used a turbulent model to analyze one flow channel of the fuel in a power plant reactor [16]. Unlike the finite element methods, a genetic algorithm was used to obtain mass flow rates and acceptable element temperatures. Vanderbilt University did a study on nuclear airplanes that used ANSYS FLUENT to find temperatures and velocity vectors of reactor configuration at different altitudes [17].

These research efforts indicate that there are established methods of solving problems involving heated gases. Theory for fluids, heat transfer, boundary layers, viscous flow, wall functions, ideal gases, and turbulence are needed to analyze the grooved ring fuel element designs. Recognizing the need for these models, we utilized the multiphysics tool COMSOL. Below, numerical models are discussed in detail.

2.3 CFD Governing Equations

In the case that a temperature field is not homogeneous, the fluid density varies. This warrants the fully compressible forms of the continuity and momentum, given by:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{2.1}
\]

\[
\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot \left[ \mu \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right] + \mathbf{F} \tag{2.2}
\]
2.4 Heat Transfer Equations

The heat equation for fluid is shown in equation 2.3. Q is the sources of heat other than viscous heating, such as power density, and \( \tau \) is the viscous stress tensor. \( \mathbf{S} \) is the strain-rate tensor, given by:

\[
\rho C_p \left( \frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T \right) = - (\nabla \cdot \mathbf{q}) + \tau : \mathbf{S} - \frac{T}{\rho} \frac{\partial p}{\partial T} \left( \frac{\partial p}{\partial t} + (\mathbf{u} \cdot \nabla) p \right) + Q \quad (2.3)
\]

\[
\mathbf{S} = \frac{1}{2} \left( \delta \mathbf{u} + (\delta \mathbf{u})^T \right) \quad (2.4)
\]

For modeling heat transfer in solids, the formula is:

\[
\rho C_p \frac{\partial T}{\partial t} = - (\nabla \cdot \mathbf{q}) - T \frac{\partial E}{\partial t} + Q \quad (2.5)
\]

where \( E \) is the elastic component of entropy [18]. This elastic increase is very nearly reversible, and is given by [19]:

\[
\delta E = Q \delta \left( \frac{1}{T} \right) \quad (2.6)
\]

Thermal conduction describes the relationship between heat flux \( \mathbf{q} \) and \( \delta T \). For flows with high Reynold’s numbers, the equation used for turbulent thermal conductivity is:

\[
\kappa_T = \frac{C_p \mu_T}{Pr_T} \quad (2.7)
\]
where $C_p$ is the constant pressure coefficient, $\mu_T$ is the turbulent viscosity, and $Pr_T$ is the turbulent Prandtl number [18]. The Kays-Crawford model can be used for the turbulent Prandtl number, given by:

$$Pr_T = \left[ \frac{1}{2Pr_{T\infty}} + \frac{0.3}{\sqrt{Pr_{T\infty}}} \frac{C_p\mu_T}{\lambda} - \left( \frac{0.3C_p\mu_T}{\lambda} \right)^2 \left( 1 - e^{-\lambda(0.3C_p\mu_T\sqrt{Pr_{T\infty}})} \right) \right]^{-1} \tag{2.8}$$

where $Pr_{T\infty} = 0.85$ and $\lambda$ is conductivity.

2.5 Boundary Layers and Viscous Flow

The boundary layer region is important because it is the area in which heat is transferred to the gas from the solid material [20]. Behaviors of the boundary layers are a result of fluid-surface interaction. Roughness and shear stress caused from heat near the fluid wall can cause turbulence. It is important to accurately model temperature in the thermal boundary layer in order to compute a predictive heat conduction and convection between the fluid and the solid channel walls. A viscous heating term, which dominates this layer is:

$$\tau : \mathbf{S} \tag{2.9}$$

2.6 Wall Functions

In the temperature field, wall functions are necessary to define the theoretical displacement of the computational domain between the solid wall and the fluid. This displacement describes the distance between the wall and the first mesh node away
from the wall. The heat flux within this distance is given by:

\[ q_{w f} = \frac{\rho C_p C \mu^{1/4} \kappa_{TE}^{1/2} (T_w - T_f)}{T^+} \]  \hspace{1cm} \text{(2.10)}

where \( T_w \) and \( T_f \) are the temperatures of the wall and fluid, respectively. \( T^+ \) is a dimensionless temperature given by:

\[ T^+ = Pr \delta_w^+ \text{ for } \delta_w^+ < \delta_w^+ \]  \hspace{1cm} \text{(2.11)}

\[ T^+ = \left( 15 Pr^2 - \frac{500}{\delta_w^2} \right) \text{ for } \delta_w^+ \leq \delta_w^+ < \delta_w^+ \]  \hspace{1cm} \text{(2.12)}

\[ T^+ = \frac{Pr}{\kappa} \ln \delta_w^+ \text{ for } \delta_w^+ \leq \delta_w^+ \]  \hspace{1cm} \text{(2.13)}

Equations 2.11, 2.12, and 2.13 are dependent upon the point of measurement, as the nodes progress away from the wall. Displacement values can be found by:

\[ \delta_w^+ = \frac{\delta_w \rho \sqrt{C_\mu^{1/2} k}}{\mu} \]  \hspace{1cm} \text{(2.14)}

\[ \delta_{w1}^+ = \frac{10}{Pr^{1/4}} \]  \hspace{1cm} \text{(2.15)}

\[ \delta_{w2}^+ = 10 \sqrt{10 \frac{\kappa}{Pr_T}} \]  \hspace{1cm} \text{(2.16)}

For calculating these distances, the Prandtl number and thermal expansivity, \( \beta \), are found using the following:

\[ Pr = \frac{C_p \mu}{\lambda} \]  \hspace{1cm} \text{(2.17)}
\[ \beta = 15Pr^2 - \frac{PrT}{2\kappa} \left[ 1 + \ln \left( 1000 \frac{\kappa}{PrT} \right) \right] \]  

(2.18)

where \( \lambda \) is thermal conductivity and \( \kappa \) is the von Karman constant, given at 0.41.

### 2.7 Dimensionless Parameters

Reynolds and Eckert numbers are used to characterize flow [21]. The Reynolds numbers can be found by the following equation:

\[ Re = \frac{\rho u L}{\mu} \]  

(2.19)

The Eckert number, which characterizes dissipation, is given by:

\[ Ec = \frac{V^2}{C_p \delta T} \]  

(2.20)

The Nusselt and Graetz numbers are found with the mixing-cup temperature, conductivity, mean velocity, and hydraulic diameter [21]. The mixed mean fluid temperature, or mixing-cup temperature, according to Kays and Crawford’s *Convective Heat Transfer*, is ”the temperature which characterizes the average thermal energy state of the fluid,” and is given by:

\[ T_m = \frac{1}{A_{ch}} \int uT \, dA \]  

(2.21)

The heat transfer coefficient, \( h_{con} \), is found by:
\[ h_{\text{con}} = \frac{\dot{q}}{T_w - T_m} \]  

(2.22)

The Nusselt number is given by the following:

\[ Nu = \frac{h_{\text{con}}D_H}{\kappa} \]  

(2.23)

For a long and skinny channel, geometry for parallel plates can be used. The hydraulic diameter for parallel plates is simply twice the plate spacing. The Graetz equation can be given by:

\[ \frac{1}{Gr} = x^+ = \frac{2x/D_H}{RePr} \]  

(2.24)

2.8 Ideal Gas Relations

Pressure, temperature, and density of the gas are related via the ideal gas law, given by

\[ p = \rho RT \rightarrow \rho = \frac{p_A}{R_sT} = \frac{M_n p_A}{RT} \]  

(2.25)

where \( p_A \) is the absolute pressure, \( R_s \) is the specific gas constant, \( M_n \) is the mean molar mass, and \( R \) is the universal gas constant.

2.9 Turbulence Models

Turbulence occurs when there are high velocity gradients in a flow field due to wall contact, different velocities in adjacent flow regions, high Reynold’s numbers, and
unstable flows resulting in flow rotations and variable size eddies \[22\]. DNS (direct numerical simulation) can be used to resolve all of the eddies, but is computationally expensive. However, the mesh refinements required by these deterministic solutions are not needed for RANS modeling, which makes RANS more feasible and suitable for industrial problems.

For turbulence computer modeling, the k-ε model is the most common \[20\] \[23\].

The specific turbulence energy \( k \), is given by

\[
k = \frac{1}{2} \left[ (u')^2 + (v')^2 + (w')^2 \right]
\]  \hspace{1cm} (2.26)

The key equation to this model lists \( \epsilon \), which is given by:

\[
\epsilon = C_D \frac{k^{3/2}}{L}
\]  \hspace{1cm} (2.27)

where \( \epsilon \) is the dissipation rate of the turbulent energy. The Eddy Viscosity is given by:

\[
\mu_T = \frac{pC_\mu k^2}{\epsilon}
\]  \hspace{1cm} (2.28)

The Reynold’s stress tensor is given by:

\[
\tau_{ij} = 2\mu_T - S_{ij} - \frac{2}{3} \rho k \delta_{ij}
\]  \hspace{1cm} (2.29)
Equations 2.26, 2.27, 2.28, and 2.29 can be used with the equation for turbulence kinetic energy, given by:

\[
\frac{\rho k}{t} + \rho U_j \frac{\partial \epsilon}{\partial x_j} = \tau_{ij} \frac{\partial u_i}{\partial x_j} - \rho \epsilon + \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_T}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right]
\]  

(2.30)

Terms on the left-hand side of Equation 2.30 are the unsteady term and the convection, and the sum of the two results in the rate of the change of turbulence energy following a fluid particle. The first term on the right-hand side represents production, which is the rate that kinetic energy is transferred from the mean fluid flow to the turbulent flow. The second term in the right-hand side is the dissipation rate of turbulence energy, or the rate that the turbulence energy is converted into thermal energy. This dissipation rate is also equal to the amount of work being done by the strain rate on the viscous stresses. Molecular diffusion is represented by the \( \frac{\mu \partial k}{\partial x_j} \) term. The last term, \( \frac{\mu_T}{\sigma_k} \frac{\partial k}{\partial x_j} \) is the coupled form of turbulent transport and pressure diffusion, where \( \sigma_k \) is a closure coefficient discussed later. This is the energy equation used for all turbulence models. The turbulence dissipation rate is found by:

\[
\frac{\partial k}{\partial t} + \rho u_i \frac{\partial k}{\partial x_j} = C_1 \frac{\epsilon}{k} \tau_{ij} \frac{\partial U_i}{\partial x_j} - C_2 \rho \frac{\epsilon^2}{k} + \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_T}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right]
\]  

(2.31)

The sum of the two terms on the left-hand side represent the rate of change of dissipation. The first two terms on the right-hand side represent the production of dissipation and the dissipation of dissipation. The last two terms show the molecular
diffusion of dissipation and turbulent transport of dissipation [23]. Acceptable values for the constants shown will be discussed later.

2.10 Material Properties

Many different coolants have been used in nuclear reactors, including carbon dioxide, helium, and dinitrogen tetroxide [16]. Because of its low molecular weight, hydrogen yields twice the specific impulse as a chemical engine utilizing LOX and LH2. The equation for specific impulse is given by the following:

$$I_{sp} = \frac{1}{g} \sqrt{\frac{2\gamma}{\gamma - 1} \frac{R_u}{MW} T}$$  \hspace{1cm} \text{(2.32)}$$

Equation 2.32 reveals how using hydrogen doubles the efficiency [15]. However, the temperature limit of hydrogen in this application is limited to the maximum allowed solid temperature [2]. Since one of the primary motivations for nuclear thermal propulsion is obtaining a high specific impulse as can be enabled by pure hydrogen, we limited the study to modeling hydrogen as the working fluid. Material properties for hydrogen gas were input into COMSOL, and properties for uranium zirconium carbide were used for the solid, since there are current efforts to recapture technologies pertaining to UZrC materials, and because it was previously found to be effective for similar applications [24]. Because not all properties were known for the fissile material, some were extrapolated from data taken by Los Alamos Laboratories [25]. The temperature limit for carbide materials was 3000 K, which limits the hydrogen coolant to the same temperature.
CHAPTER 3

PROBLEM STATEMENT AND METHODOLOGY

3.1 Problem Statement

Several facts were taken into account when developing the requirements for the design. The maximum temperature of the carbides could not exceed thermal limitations. However, it was assumed that there would be temperature changes throughout the solid portion of the model as fluid traveled along the channels. High temperature gradients within the fissile material would cause more thermal stress, so minimizing temperature gradients was preferable. By attempting to create a model with a constant solid centerline temperature, thermal stresses could be minimized. A maximum amount of heat transfer to the gas was desired, and the possibility that this could be implemented by creating more flow channels was considered. Along the channels, a very small pressure drop would result in a low exit velocity, so there was an arbitrary minimum limit given to the exit pressure. In summary, the objective of the project is to design a fuel element disc structure that maximizes the temperature, minimizes temperature gradients, maintains a pressure drop to generate a significant exit velocity, and attempt to create a solid centerline temperature that is almost constant from the exterior to the interior portion of the disc.
3.1.1 Summary of Given Parameters

As mentioned in Chapter 2, uranium zirconium carbide has been found to be a great material for nuclear thermal propulsion applications [24]. Hydrogen was chosen for its low molecular weight, and ability to enable a high specific impulse. The maximum temperature of the carbide is 3000 K [24]. Other material properties, such as conductivity, were found by Los Alamos National Laboratories in the 1990’s [25], and were also noted.

3.1.2 Summary of NASA Requirements

The structure was required to be a disc with grooves along the top face [26]. Another requirement was to investigate ability to control the solid centerline temperature along the middle of the solid adjacent to the flow channels, such that from the exterior to the interior of the disc, it must not differ by more that 50K. It was also required to investigate the heat transfer from the solid to the gas. A pressure drop of at least 50.0 kPa (10psi) was required from the gas inlet to the gas exit [26]. Additionally, NASA designated the inlet pressure to be 6.89 MPa (1000 psi), which meant that the exit pressure had to be at least 6.84 MPa to accommodate the 50.0 kPa minimum difference.

3.1.3 Summary of Assumptions

Turbulence was assumed due to a tremendous amount of heat transfer to the gas [20]. Also, the coolant is an ideal gas [27], and the model was assumed to be
steady-state. Because the hydrogen could not exceed 3000 K, equilibrium conditions were assumed.

3.2 Overview of the Finite Element Method

It is often appropriate to compute approximate numerical solutions for complex problems, in which exact closed-form solutions are difficult to obtain [28]. FEA (finite element analysis) is accomplished by discretizing, or dividing the materials under analysis into many sub-regions, or elements, that interconnect at multiple nodes. Before these elements are established, there are an infinite number of solutions, but by discretizing, the number of solutions are finite, and equal to the number of nodes. These nodes are solved by reducing partial differential equations into either linear or non-linear simultaneous equations, which are then used to solve variables of interest at those nodes. As mentioned previously in Chapter 2, finite element methods have been used successfully for turbulent flow and heat transfer problems.

3.3 COMSOL Multiphysics

COMSOL is a multiphysics program, designed to couple many different types of physics using finite element analysis to solve partial differential equations [29]. The packages available for COMSOL solve several physics-based models, including, but not limited to, those for electrostatics, structures, fluids, heat transfer, chemical species transport, and acoustics. COMSOL has the ability to perform parametric studies, so that many computations can be done and compared against parameter changes. It can interface directly with SolidWorks so that changes are immediately reflected
in the model. It interfaces with MATLAB, so that models can be ran according to scripted specifications. COMSOL can be used for 3D modeling, meshing, and graphing results [29].

COMSOL contains a CFD module that can solve 2D or 3D fluid flow problems with stationary or time-dependent solutions [30] [18]. The laws of conservation for momentum, mass, and energy are used for flow interfaces. The module solves the conservation laws with differential equations to generate results. For this project, the Non-Isothermal and Turbulent Flow portions of the Computation Fluid Dynamics module was used to do heat transfer from the solid to the gas in turbulent conditions, computing fluid flow as the default model. Materials properties for hydrogen and uranium zirconium carbide were use as inputs. All meshes were done in COMSOL, and most of the model results were plotted in COMSOL.

3.4 Baseline Designs and Geometry

Several examples of the GRFE (grooved ring fuel element) have been designed to maximize the surface-area-to-volume ratio of reactive surfaces in nuclear propulsion fuel elements. For comparison, the NERVA design (dimensions given by NASA) was used to show significant improvements in the ratios of reactive area to volume using a verified wxMaxima code. Most baseline designs yielded surface area improvements of at least 100 percent over the surface area values for a hexagonal fuel element with the same volume. As more grooves were added, surface area increased significantly. Several designs were created so that different geometries could be considered. Many discs with both curved and straight grooves were modeled.
The baseline design, shown in Figure 3.1 had an outer radius of 20.0 mm, an inner radius of 6.3 mm and a thickness of 1.0 mm. This baseline was given by NASA, and was modified throughout optimization efforts [26]. To simplify initial finite element computations, the straight groove design was used for initial analysis.

![Image of baseline design](image)

**Figure 3.1:** After finding acceptable geometries, straight grooves in Cartesian coordinates can be converted to radial coordinates, forming a disc with curved grooves. It is possible for flow channels and grooves to have constant and equal widths.

### 3.5 Model Development

A heat transfer analysis was done for several models in an attempt to obtain the temperatures of the hydrogen and the fuel element. Lower temperature gradients should result in a reduction of thermal stress, improving the structural integrity of the fuel ring; therefore, the goal was to create a structure with geometry such that the heat flux gradients are minimized. Rather than modeling the flow through an entire disc, a small portion of each disc was analyzed. Heat transfer physics coupled with those of fluid flow show how the element cools during use.
The \( \kappa-\epsilon \) model is solved with the Reynolds Averaged Navier Stokes model type, and the Kays Crawford heat transport turbulent model is used. The RANS model was used to reduce the computational expense otherwise endured by the deterministic method [22]. The Kays-Crawford model is good for most wall-bounded turbulent flows [18]. Turbulent flow was used due to the high Reynold’s numbers that are inherent to nuclear reactor flows [14]. Not only have similar models assumed high Reynold’s numbers in the past, but also, the shear stress caused from the heat and the roughness of the material can also cause turbulence [20].

The MUMPS (MUltifrontal Massively Parallel sparse direct Solver) application was used across 6 hyper-threaded processors for computations. This solver utilizes Gaussian elimination for large systems of linear algebraic equations. Each solution was completed with 2 segregated solvers. Segregated Solver 1 was used to find \( \kappa \) and \( \epsilon \). Segregated Solver 2 was used to find temperature, pressure, and velocity. Each solver was set so that both had to converge to an error of \( 10^{-3} \) for termination, or were set to a certain number of iterations, as seen in Figure 3.2. The computational setup included a water-cooled Intel Core i7-3630k processor with hyper-threading technologies, an Asus Rampage IV Extreme motherboard with a water-cooled chipset and water-cooled VRM (voltage regulator module), 32 Gb of RAM (random access memory) running at 1600 MHz, and an NVidia Geforce GTX 560-TI graphics card with a gigabyte of VRAM (video random access memory), 380 CUDA cores, and the PhysX physics engine.
Figure 3.2: Here a convergence plot shows that 80 iterations were specified to terminate the computations.

3.5.1 Single Channel Modeling

Discs with straight and constant-area flow channels were analyzed. When temperature, velocity and pressure profiles are acceptable, the straight grooves can then be converted to curved grooves. Any straight and constant-area grooved design can be converted to a curved-grooved design by:

$$x_1 = \sqrt{r_o^2 - r_i^2} - \cos^{-1} \left( \frac{r_i}{r_o} \right)$$

which should be done at a later date. This equation uses inner and outer radius values to find the angle value at which the groove terminates on the disc interior.
For simplification, initial multiphysics models were performed only on one channel and one groove. This approach was further simplified by reducing the structure being analyzed to 1/2 of one channel and 1/2 of one groove. Additionally, only 1/2 of the disc base, which is the lower portion without grooves, was analyzed. Since the discs were assumed to be stacked, the flows through any disc were assumed to be affected by the transfer of heat from the disc stacked directly above. The area of interest in Figure 3.3 shows an example of a disc portion to be analyzed, reflected in Figure 3.4.

Figure 3.3: Four discs are shown in part of a stack. The solid portion, shown in red, represents an example of 1/2 of the disc base being modeled, and 1/2 of the disc base that would be stacked above it. Additionally, only 1/2 of the flow channel and solid groove were analyzed. In this case, symmetrical boundary conditions can be used on domains that are halved.
Figure 3.4: Illustrated is an example of 1/2 of a single channel with 1/2 of a groove. 1/2 of a disc base is shown with 1/2 of the disc base of the ring theoretically stacked above.

3.5.2 Boundary Conditions and Inputs

The hydrogen inlet had a given pressure of $6.89 \times 10^6$ Pa, and no viscous stress. For heat transfer purposes, the temperature specified for this boundary was 293.15K. A general heat transfer outflow was given for the hydrogen exit. The reference velocity scale was 1m/s, turbulent intensity was 0.05, and the turbulence length scale was 0.01m. The hydrogen exit pressure was usually specified at around $6.83 \times 10^6$ Pa, but was varied during parametric studies to find a suitable range for the computations.

Many symmetrical boundaries were applied due to the halving of geometries, as illustrated in Figure 3.4. Symmetrical geometries and volumes exist normal to these boundaries. It should be noted that any time a geometrical feature was halved,
boundary conditions on these features can be assumed symmetrical, which speeds computations. For heat transfer computations, only two boundaries on the gas-facing side that could be designated symmetrical were not. These were instead given as adiabatic. Only one boundary condition could be given as symmetrical for the turbulent flow calculations. Figure 3.5 shows the heat transfer symmetrical boundaries, and gas symmetry boundary is shown in Fig 3.6.

![Diagram](image)

**Figure 3.5:** The highlighted portions indicate boundary conditions designated as symmetrical for heat transfer computations.

A general heat source was applied at a constant $10^{10}$W/m$^3$. Power density was varied occasionally during studies to observe the differences in behavior of the temperature profiles. Because power density was not expected to be exactly constant across the entire geometry, all final designs should undergo analysis using a neutronics
Figure 3.6: Turbulent Flow Symmetrical Boundary: The highlighted portion indicates the only boundary conditions designated as symmetrical for turbulent flow computations.

code to show power variations to replace the constant power density definition initially used for the models.

As part of the $\kappa$-$\epsilon$ model, the turbulence parameters in table 3.1 are recommended values for channel flows [31]. Reasonable values for the logarithmic constant $B$ are given between 5.0 and 5.5.
### Table 3.1: Turbulent Flow Parameters

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Parameter</th>
<th>Accepted Value [Unitless]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_\mu$</td>
<td>Viscosity Constant</td>
<td>0.09</td>
</tr>
<tr>
<td>$\kappa_v$</td>
<td>Von Karman Constant</td>
<td>0.41</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Logarithmic Law Constant</td>
<td>5.20</td>
</tr>
<tr>
<td>$C_1$</td>
<td>Generation Constant</td>
<td>1.44</td>
</tr>
<tr>
<td>$C_2$</td>
<td>Destruction Constant</td>
<td>1.92</td>
</tr>
<tr>
<td>$\sigma_\epsilon$</td>
<td>Effective Prandtl Number for Dissipation</td>
<td>1.30</td>
</tr>
<tr>
<td>$\sigma_\kappa$</td>
<td>Effective Prandtl Number for Energy</td>
<td>1.00</td>
</tr>
</tbody>
</table>

#### 3.5.3 Meshing

In the models, meshes interconnect at the discretized nodes. Interfaces between the carbide fuel and the hydrogen were meshed using triangular distributions, and shown in Figure 3.7. For Models 1-4, both the hydrogen and the carbide element were meshed using free tetrahedral grids. Since COMSOL allows the user to input the maximum and minimum element sizes, the grid used for the hydrogen was made finer for accuracy. The free tetrahedral meshes are superimposed and shown in Figure 3.8. For Models 5-10, a boundary mesh was used instead of a tetrahedral mesh for accuracy.
Figure 3.7: The interfaces between the gas and solid are meshed with triangular distributions.

Figure 3.8: The gas and solid portions of all models are meshed with tetrahedral distributions.
4.1 Initial Flow Channel Geometry: Models 1-4

The first four models were quantitative trend studies, and showed the effects of geometry changes. These models did not contain any boundary layers and had coarse meshes. Models 1-4 were analyzed in order to find the appropriate angle spacing and number of flow channels that would allow the gas to maintain a higher velocity while cooling the solid temperature and also to show effects of flow channel geometry changes. The angle spacing used was the angular degree separation of the center of each flow channel, to the center of the next flow channel around the disc. The first model had channel angle spacing of two degrees, resulting in 180 channels around the entire disc. In order to increase the heat transfer to the gas and decrease the temperature of the fuel, more flow channels were added. Models 2, 3, and 4 had 1 or 2 degrees of angle spacing, resulting in 180 or 360 channels, equidistant around the disc. To increase the amount of heat transfer to the gas and further decrease the fuel temperature, the channels were made deeper and longer. The main goal of the first four models was to make sure that the maximum solid material temperature was around 3000K, while observing the fluid temperatures and velocities. Pressure results
for these models are not shown, as the pressure differences from the inlet to the exit $(6.89 \times 10^4 Pa)$ are the same for each model.

Table 4.1: Models 1-4: Summary of Disc Dimensions

<table>
<thead>
<tr>
<th>Model</th>
<th>Flow Channels</th>
<th>$r_o$ [mm]</th>
<th>$w_c$ [mm]</th>
<th>$h_c$ [mm]</th>
<th>$L_c$ [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>180</td>
<td>20</td>
<td>0.01</td>
<td>0.20</td>
<td>13.7</td>
</tr>
<tr>
<td>2</td>
<td>360</td>
<td>20</td>
<td>0.08</td>
<td>0.20</td>
<td>13.7</td>
</tr>
<tr>
<td>3</td>
<td>360</td>
<td>20</td>
<td>0.08</td>
<td>0.25</td>
<td>13.7</td>
</tr>
<tr>
<td>4</td>
<td>360</td>
<td>22</td>
<td>0.08</td>
<td>0.25</td>
<td>15.7</td>
</tr>
</tbody>
</table>

4.1.1 Heat Transfer Results: Models 1-4

Heat transfer analyses were done on the solid and gas domains of the model. Conduction was an input and temperature the output of importance, plotted in 3D and 2D. Plots were made for temperature changes along the length. As mentioned in Chapter 3, NASA required small temperature changes along the length to minimize any thermal stresses. It was found that adding more flow channels decreased the temperature in the solid. Figures 4.1 and 4.2 compare the steady-state solid temperatures of a disc with 2 degree separation angles to one with 1 degree of separation between channels. More gas was available to take away more heat with more flow channels. Temperatures were also controlled with deeper flow channels and elongation of the channels by a larger outer radius.
To prove the effectiveness of cooling the solid with more flow channels, four models were analyzed and compared. Figure 4.1 shows a disc with 2 degrees of separation and 180 flow channels. Models with 1 degree separation angles were found to yield lower and more acceptable temperatures, as shown in Figure 4.2. With more channels, maximum temperatures for the solid decreased by around 3000K and the gas centerline temperatures decreased by only 600-900 K. However, the flow channel widths had to be decreased in order to accommodate the extra grooves. Model 3 had a deeper flow channel, which yielded lower temperatures for both the solid and gas. All models except for model 4 had the same inner and outer radius values for the disc. To show the effects of longer gas flow channels, Model 4, shown in Figure 4.4, was constructed with a larger outer radius. By increasing the outer radius by 2 mm and maintaining the deeper groove used in Model 3, the maximum solid temperature at steady-state was around 3062K, and the gas exit temperature was 975K.

Model 4 shows an example of groove temperatures decreasing rapidly at the exterior portions and decreasing more slowly when approaching the ring interior. The exterior-most areas of the ring cooled much faster as the channels become thinner and longer. This was significant because a more constant temperature is preferred to mitigate the risk of thermal stresses. Ideally, the entire groove should have small temperature changes.

The fluid temperatures are shown in Figures 4.9, 4.10, 4.11, and 4.12. The solid temperature affects the gas temperature, becoming lower with lower temperatures. However, the gas can become warmer by moving through elongated flow channels.
**Figure 4.1:** 3D Heat Transfer for Model 1: High temperatures, given in Kelvin, are expected with larger flow channel angles of separation.

**Figure 4.2:** 3D Heat Transfer for Model 2: The temperatures, given in Kelvin, begins to drop with more flow channels across the top of each disc.
Figure 4.3: 3D Heat Transfer for Model 3: The temperatures, given in Kelvin, drops more as the channels become less shallow.

Figure 4.4: 3D Heat Transfer for Model 4: With deeper, elongated flow channels and smaller angles of separation, the fissile material cools, as shown by the Kelvin temperature scale. The outer radius was increased by 2.0mm.
Figure 4.5: Solid temperatures cool along the length of the grooves slowly when there is a larger volume of solid.

Figure 4.6: Solid temperatures cool along the length of the grooves more quickly when many more flow channels are added and there is a decreased volume of solid.
Figure 4.7: Solid temperatures cool along the length of the grooves more quickly when flow channels are deeper.

Figure 4.8: When there are more channels, the grooves must be thinner, so that the solid cools faster.
**Figure 4.9:** Gas Temperatures for Model 1: Gas temperatures rise as they travel through the channel.

**Figure 4.10:** Gas Temperatures for Model 2: Gas temperatures decrease with lower solid temperatures.
Figure 4.11: Gas Temperatures for Model 3: Gas temperatures decrease further when the solid temperatures fall.

Figure 4.12: Gas Temperatures for Model 4: Gas temperatures can get higher when the flow channels are longer.
Table 4.2 shows a summary of heat transfer results for all four models. By extending the flow channel a few millimeters, the exit temperature of the gas increases significantly. More flow channels decrease the volume of the solid and cause the material to cool faster.

<table>
<thead>
<tr>
<th>Model</th>
<th>Flow Channels</th>
<th>( r_o ) [mm]</th>
<th>( h_c ) [mm]</th>
<th>( T_{\text{smax}} ) [K]</th>
<th>( T_e ) [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
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<td>1642.50</td>
</tr>
<tr>
<td>2</td>
<td>360</td>
<td>20</td>
<td>0.20</td>
<td>3224.1</td>
<td>960.10</td>
</tr>
<tr>
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<td>360</td>
<td>20</td>
<td>0.25</td>
<td>2784.9</td>
<td>786.80</td>
</tr>
<tr>
<td>4</td>
<td>360</td>
<td>22</td>
<td>0.25</td>
<td>3062.6</td>
<td>975.00</td>
</tr>
</tbody>
</table>

4.1.2 Flow Results for Models 1-4

Figures 4.13, 4.14, 4.15, and 4.16 show the velocity magnitude. Model 1 had 180 flow channels and an exit velocity of 155 m/s. The high velocity was related to the higher temperatures caused by the higher fuel volume. The fuel volume of the disc was drastically reduced in Model 2, Model 3, and Model 4, since there were 360 flow channels per disc. Model 2 had an exit velocity reduction of around 37 m/s. The exit velocity was further reduced by 11 m/s in Model 3, which had a larger cross-sectional flow channel area due to taller channel heights. The flow channel in Model 4 was longer by decreasing the inner radius value by 2 mm, so that more heat transfer was allowed before the gas exit, and this resulted in a slight velocity increase.
Table 4.3: Models 1-4: Summary of Flow Channel Parameters

<table>
<thead>
<tr>
<th>Model</th>
<th>Flow Channels</th>
<th>$v_e$ [m/s]</th>
<th>$w_c$ [mm]</th>
<th>$h_c$ [mm]</th>
<th>$L_c$ [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>180</td>
<td>155</td>
<td>0.01</td>
<td>0.20</td>
<td>13.7</td>
</tr>
<tr>
<td>2</td>
<td>360</td>
<td>118</td>
<td>0.08</td>
<td>0.20</td>
<td>13.7</td>
</tr>
<tr>
<td>3</td>
<td>360</td>
<td>107</td>
<td>0.08</td>
<td>0.25</td>
<td>13.7</td>
</tr>
<tr>
<td>4</td>
<td>360</td>
<td>111</td>
<td>0.08</td>
<td>0.25</td>
<td>15.7</td>
</tr>
</tbody>
</table>

Figure 4.13: Model 1: The velocity magnitude is higher with higher temperatures
Figure 4.14: Model 2: The velocity magnitudes decreased with lower gas temperatures. Lower temperatures resulted from doubling the amount of flow channels.

Figure 4.15: Model 3: The velocity magnitude of this model is only slightly lower than the velocity magnitude of Model 2. This was caused by using deeper flow channels at the same pressure.
Figure 4.16: Model 4: Although this model has deep flow channels like Model 3, the channels were longer and the velocity profile almost matches that of Model 2. Recall that the temperature of the gas along the length of the channel for this model almost exactly matches the channel temperature profile of Model 2, except the channels for this model are longer. Additionally, there is a higher volume of solid material on this model, due to the smaller disc inner radius created to elongate the channel.

4.2 Addition of Dense Boundary Nodes - Model 5

Models 1-4 showed a low amount of heat being transferred to the gas (this is discussed more below), which should be remedied by adding finer meshing about the boundaries. Pressure results are not given for Model 5, as the pressure values are the same as for Models 1-4. These results are quantitative, and are to reveal how additional boundary nodes change the heat transfer to the gas.
4.2.1 Heat Transfer Results - Model 5

In order to satisfy the expectation that most of the heat transfer occurs in the boundary layer, a different mesh and viscous heating was used in Model 5. Rather than only using a tetrahedral mesh for the gas domain, a boundary mesh was added. This mesh produced expected results, and the solid material was further cooled, as shown in Figures 4.17 and 4.18. The gas temperatures are shown in Figure 4.19. Although the geometry for Model 5 was the same as Model 4, the gas temperatures were cooler due to effective heat transfer from the solid. At steady state, the gas has absorbed more thermal energy. This caused more heat to flow through the channel exit, which in turn made the solid cooler.

However, without the additional heat transfer physics and the denser meshing, the gas temperatures for Models 1-4 ranged from 2000K to 8000K less than those of their corresponding solid domains. The dense meshing around the boundary caused the gas and solid temperatures to differ by only around 200K. It is also noteworthy that the temperature differences between the highest and lowest in the centerline of Model 4 were around 1800K, but the centerline differences of Model 5 are around 130K. The maximum temperature of the solid and gas of Model 5 were 990K and 860K respectively, but the maximum temperatures of the solid and gas of Model 4 were similarly 960K and 3000K. This means that the gas maximum temperature of Model 5 was approximately 86% of the maximum solid temperature, but the maximum gas temperature for model 4 was only about 32% of its highest solid temperature.
Figure 4.17: 3D Heat Transfer for Model 5: The temperature drops with the addition of a boundary mesh.

4.2.2 Flow Results - Model 5

Figure 4.20 shows the gas velocity magnitude profile for Model 5. In comparison with Model 4, which has the same geometry and input parameters, Model 5 has a slightly higher velocity, but there is only a 7m/s difference. The x and y-components of the velocity were relatively small, and close to those same parameters for Model 4.
Figure 4.18: Centerline Temperatures for Model 5: The temperature difference throughout the solid becomes lower when considering with finer meshing.

Figure 4.19: Gas Temperatures for Model 5: Gas temperatures are still cooler because the solid is cooler due to effective heat transfer computations
Figure 4.20: Velocity Profile for Model 5: Model 5 has approximately the same velocity as Model 4, despite great temperature differences.

4.3 Scaling Effects with Parametric Pressure Studies - Models 6-8

Since the denser boundary nodes caused the temperatures to drop in Model 5, the models were scaled geometrically in an effort to achieve desired results without complex geometrical changes. Results for these models are quantitative and show how scaling effects model parameters solved. Model 6 was scaled by a factor of 2, and Model 7 by a factor of 3, and Model 8 by a factor of 5. Parametric studies were performed to reveal the effects of pressure drops on the temperatures of the gas and solid. Large pressure differences resulted in higher velocities through the channels causing the gas to be cooler as it exited. Pressure drops are caused by friction factor, and the frictional effects of contraction and expansion of gases, otherwise known as the inlet/outlet factor [16]. Ranges for which the studies were done were
in given increments, and each model had a different pressure range with which it could complete computation. The figures below shows how greater pressure drops yield higher velocities which results in lower exit temperatures. When the pressure drop was lower, the gas had more time to acquire heat, thus resulting in higher exit temperatures. A minimum pressure drop of \((6.89 \times 10^4 Pa)\), or 10.0 psi was assumed for each model.

4.3.1 Heat Transfer Results - Model 6

The parametric study done on model 6 contained pressure differences between the inlet and exit varying in increments of \((6.89 \times 10^4 Pa)\). A starting exit pressure of \(6.48 \times 10^6 Pa\) was increased with each run by the increment given until the it reached \(6.83 \times 10^6 Pa\). As shown by Figure 4.21, the highest solid temperature was well under 3000K, indicating that more scaling needed to be done. However, the centerline temperatures are almost constant, which was the preferable condition to minimize thermal stresses through the fuel element. 3D plots showing temperature profiles, display a lingering effect of heat towards the exterior portion of the disc, as shown in Figure 4.22. When the pressure drop was lower, the gas moved slower through the channels, increasing the temperature as it moved towards the exit, while a larger pressure drop induces a higher velocity, and cools the exterior portion, as shown in Figure 4.23. The behaviour of the solid material becoming more heated towards the end of the flow, as shown in Figure 4.24 has been proven in the NTREES lab at NASA Marshall Space Flight Center [32]. The gas enters through flow channels in the rod on the left and exits them to the right. The solid temperature is much higher
Figure 4.21: Centerline Temperatures for Model 6: Each line represents a run computed with a different exit pressure. 

Towards the exiting area of the rod, the gas heats along the channel, it absorbs less of the heat from the rod as it approaches the exit. Figure 4.25 shows the hydrogen gas temperature profiles for Model 6.
**Figure 4.22**: Solid Temperature for Model 6 at 6.83MPa: This temperature profile shows heat lingering toward the exterior of the disc. The exterior portion of the slice is the portion that is thickest.

**Figure 4.23**: Solid Temperature for Model 6 at 6.76MPa: This temperature profile shows heat prevalent toward the interior of the disc, while the exterior is cooled. This is a result of a higher velocity due to greater pressure drop.
Figure 4.24: Heating Behavior of a Fuel Rod Testing at the NTREES Facility: As the gas enters through the rod on the left and exits on the right, the solid temperature is much higher towards the exiting area of the rod.

Figure 4.25: Gas Profiles for Model 6: Exit Temperatures of the Hydrogen can be seen using several exit pressures.
4.3.2 Heat Transfer Results - Model 7

Model 7 is scaled by a factor of 3, causing temperatures to be higher than those of Model 6, with lower velocities. By observing the results shown in Figure 4.26, it can be assumed that for the maximum solid temperature to be around 3000K, the model with a pressure exit pressure 6.75 MPa should be used. Figure 4.27 shows the temperature profile for this pressure profile. Since, the exit pressure is relatively high, the lower velocity results in a warmer disc exterior. However, the interior portion is visibly heating slowly toward the interior.
**Figure 4.26**: Centerline Temperatures for Model 7: Each line represents a run computed with a different exit pressure.

**Figure 4.27**: Solid Temperature for Model 7 at 6.75 MPa: The maximum temperature for this model is acceptable.
4.3.3 Heat Transfer Results - Model 8

Model 8 was scaled by a factor of 5. At 6.55-6.61 MPa, the maximum temperatures were too high, but the centerline temperatures were constant at around 3000K [33]. Because maximum temperatures were too high, the outer radius was decreased, but this only made the centerline temperatures too low. Several efforts were made to bring down the maximum temperatures. When the flow channels were made deeper, the change of temperature along the centerline was more than 400K. Using the original flow channel depth with a shorter disc height created similar problems, with a maximum temperature of around 3800K. Decreasing the disc height while simultaneously increasing the flow channel depth lowered the maximum temperature to around 2480K, while making the temperature change along the centerline rise to
Figure 4.29: Centerline Temperatures for Model 8: Each line represents a run computed with a different exit pressure.

600K. These solutions are conducive to thermal stress and lower centerline temperatures. Greater temperature gradients should be avoided for structural integrity. Also, larger pressure drops resulted in shorter temperature spikes along the exterior portions of the disc, which become constant more quickly, which result in lower overall temperature changes throughout the solid. It is also noteworthy that this model yields temperatures in the non-equilibrium range, although no chemical reactions are accounted for.
Figure 4.30: Solid Temperature for Model 8 at 6.55 MPa: The maximum temperature for this model is high, but most of the centerline is right at 3000K.

Figure 4.31: Gas Profiles for Model 8: Exit Temperatures of the Hydrogen can be seen using several exit pressures.
4.3.4 Flow Results - Models 6-8

Figures 4.32, 4.33, and 4.34 shows the velocity profile down the center of the flow channel on Model 6-8. As the scale factors increase, the exit velocities increase significantly. These velocities occur as a result of pressure profiles that behave the same on each model. Table 4.4 shows a summary of results for heat transfer and flow of these models.

Table 4.4: Models 6-8: Summary of Results

<table>
<thead>
<tr>
<th>Model</th>
<th>Scale</th>
<th>$P_e$ [MPa]</th>
<th>$T_{max}$ [K]</th>
<th>$T_{con}$ [K]</th>
<th>$T_{ge}$ [K]</th>
<th>$\Delta T_{cent}$</th>
<th>$v_e$ [m/s]</th>
</tr>
</thead>
<tbody>
<tr>
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<td>2</td>
<td>6.82</td>
<td>2592.9</td>
<td>2300.0</td>
<td>2100.0</td>
<td>190</td>
<td>180</td>
</tr>
<tr>
<td>7</td>
<td>3</td>
<td>6.75</td>
<td>3282.1</td>
<td>3000.0</td>
<td>2125.00</td>
<td>600</td>
<td>280</td>
</tr>
<tr>
<td>8</td>
<td>5</td>
<td>6.58</td>
<td>6134.1</td>
<td>2700.0</td>
<td>2700.0</td>
<td>2000</td>
<td>420</td>
</tr>
</tbody>
</table>
Figure 4.32: Parametric Velocity Profiles for Model 6

Figure 4.33: Parametric Velocity Profiles for Model 7
4.4 Optimization of Exposed Surface Area

One of the main project goals is to investigate the possibility of a higher surface area exposed to coolant than that the hexagonal fuel rods. A code developed in the maxima language was used to input the volume of the disc model, and output the flow channel surface area for a hexagonal fuel rod with the equivalent volume. The maxima code can be found in Appendix A. This code also, gave a specific height that was used as input into a SolidWorks model, so that the Maxima code could be verified by measuring the volume in the CAD program. The cross sectional area of the fuel rod would remain the same, at 0.57, and the height would be varied to match the volume of the fuel disc. The surface-area-to-volume ratio of the hexagonal fuel rod stayed the same regardless of the height given to match the volume of the fuel disc.
However, the exposed surface area changed in both the disc and hexagonal fuel rod as the sizes were changed. Additionally, scaling of the model significantly lowered the ratio for the disc. Table 4.5 shows the surface-area-to-volume ratio calculations for each model.

To correct low surface-area-to-volume ratio, Model 9 was created to duplicate the features of Model 8, except with a disc height of 0.4 mm, rather than 1.0 mm. This model was analyzed in SolidWorks, and it was discovered that although the volume decreased, the ratio difference relative to the hexagonal fuel rod, -70.11%, was still unacceptable. No analysis was done on Model 9, since the ratio was known to be undesirable.
Table 4.5: Surface Area and Volume Ratios

<table>
<thead>
<tr>
<th>Model</th>
<th>Scale</th>
<th>Channel Area $[mm^2]$</th>
<th>$V_{disc} [mm^3]$</th>
<th>Rod Channel Area $[mm^2]$</th>
<th>Ratio $[1/mm]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1479.60</td>
<td>1082.63</td>
<td>626.75</td>
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</tr>
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</tr>
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<td>1</td>
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<td>1282.80</td>
<td>742.62</td>
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<tr>
<td>10</td>
<td>1.4</td>
<td>2434.32</td>
<td>2980.52</td>
<td>1725.46</td>
<td>0.82</td>
</tr>
</tbody>
</table>

When finer grids were added, the temperatures dropped, so the model was geometrically scaled, but surface-area-to-volume calculations showed poor ratios in scaled models. Recall that the scaling of Models 6-8 was done to increase the volume of the disc, so that the total power output would increase, and also raise temperatures. Model 1 had a desired ratio and was not scaled, but the temperatures were unacceptably high. These high temperatures were taken advantage of so that desired results could be obtained. Adding dense boundary meshing to Model 1 caused the temperatures to fall, yielding a max solid temp of around $1800K$. In addition
to the added physics, sacrificing ratio values by very slightly scaling Model 1 by a factor of 1.4 increased the temperature and nearly satisfied all conditions, leaving a slightly higher than desired temperature gradient along the centerline. This model was called Model 10, and was the accepted solution for this project. A small increase of one-tenth of a scale factor from 1.4 to 1.5, decreased the ratio improvement by 10%. Efforts to scale further and reduce disc height to control volume decreased ratios as expected. Because this model only has 180 flow channels, increasing the scale caused temperature gradients to be much higher than the models scaled with 360 flow channels.

Table 4.6 shows the differences between the surface-area-to-volume ratios of the disc and the fuel rods. All fuel rods ratios were 0.57.
Table 4.6: Surface Area and Volume Ratio Differences

<table>
<thead>
<tr>
<th>Model</th>
<th>Ratio</th>
<th>Ratio Improvement over Fuel Rod</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.37</td>
<td>58.29%</td>
</tr>
<tr>
<td>2</td>
<td>2.62</td>
<td>78.27%</td>
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<tr>
<td>3</td>
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<td>81.91%</td>
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<td>4</td>
<td>2.91</td>
<td>80.40%</td>
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<tr>
<td>5</td>
<td>2.91</td>
<td>80.40%</td>
</tr>
<tr>
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<td>0.73</td>
<td>21.59%</td>
</tr>
<tr>
<td>7</td>
<td>0.32</td>
<td>-76.41%</td>
</tr>
<tr>
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<td>0.12</td>
<td>-390.04%</td>
</tr>
<tr>
<td>9</td>
<td>0.34</td>
<td>-70.11%</td>
</tr>
<tr>
<td>10</td>
<td>0.82</td>
<td>30.21%</td>
</tr>
</tbody>
</table>

4.5 Model 10: Final Design

The final design, Model 10, was chosen based on conditions satisfied. It has an acceptable maximum temperature, a relatively low temperature gradient along the centerline, a desirable heat transfer to the gas, and has a large surface-area-to-volume ratio improvement over the hexagonal fuel rod with an equivalent volume.
4.5.1 Model 10 Heat Transfer Results

Figure 4.35 shows the parametric centerline temperatures of the solid portion of Model 10 for pressures from 6.75 MPa (980 psi) to 6.82 MPa (990 psi). Figure 4.36 shows the 3D fuel temperature profile at 6.81 MPa (989 psi) and Figure 4.35 shows that the temperature difference along the centerline at that pressure is 250K. The maximum temperature at this pressure is just under 3000K. The exit temperature of the gas at this pressure was around 2250 K as shown in Figure 4.37.
Figure 4.36: Solid Temperature of Model 10

Figure 4.37: Gas Temperature of Model 10
4.5.2 Model 10 Flow Results

Figure 4.38 shows the inlet and exit pressures used for the parametric studies, and Figure 4.39 shows the parametric values for velocity along the center of the flow channel. The exit velocities ranged from 210 m/s to 240 m/s, and this figure shows the exit velocity for the chosen optimal exit pressure was around 215 m/s. The mass flow rate is given by:

\[ m = \rho v \cdot A \]  \hspace{1cm} (4.1)

The density and velocity were found by placing a virtual probe at the end of the flow channel and at the center of the cross sectional area in the COMSOL model. Probe density was found to be 0.64 kg/m\(^3\) and velocity magnitude was 204.37 m/s.
Figure 4.38: Pressure Profiles of Model 10

Figure 4.39: Velocity Magnitude of Model 10
4.5.3 Model 10: Dimensionless Parameters

To find the importance of turbulence, the Reynolds Number was calculated close to the inlet, at 0.005 mm. The corrected hydraulic parameter, $D_H$, was found by using the width and height of Model 1 scaled by factor of 1.4. At this point, the velocity was 35 m/s, the density was 5.25 kg/m$^3$, the hydraulic diameter modified for a rectangular duct was 0.0000095, and the dynamic viscosity was 9.7x10$^{-6}$ Pa/s. The resulting Reynolds number was 180, which indicates that the turbulent model was not needed. This was confirmed by observing the y-component and the z-component plots of velocity, where those parameters were very close to zero.

The Eckert number was found at another point, farther into the channel. The characteristic velocity was 147 m/s, the change of temperature was 100 K, and the specific heat was 15500 J/(kg-K). Using Equation 2.20, an Eckert number of 0.01 was found, proving that viscous heating could have been neglected.

Graetz numbers and Nusselt numbers were found by using post-processing techniques and with Equations 2.21- 2.24. Values for velocity and temperature were found at cut planes made at 0.1mm, 0.5mm, 1.0mm, 2.1mm, and 4.2mm along the channel. The mean velocity was found by summing all values taken on the plane, and dividing by the number of elements on that plane. The integral values were found by calculating $\sum T u A$ at each node, with the $A$ value being approximated as the average area around each node. The cross-sectional area was calculated to be 0.01$mm^2$. The mixing cup temperature at each cut plane along the channel was then found by the following equation:
\[ T_m = \frac{1}{VA_{cs}} \sum uTA_{average} \] (4.2)

The temperature at the wall was assumed to be the maximum temperature values found on the corresponding cut plane, and the heat flux on the wall was given by COMSOL. The heat transfer coefficient was then found by Equation 2.22. These values were used to find the Graetz and Nusselt numbers, given by Equations 2.24 and 2.23.

Results for the Graetz and Nusselt numbers were close to the theoretical values found in *Convective Heat Transfer* by Kays and Crawford [21], suggesting that the flow quickly becomes laminar, as shown in Table 4.7. At the channel entrance, the Nusselt numbers will tend towards infinity, and then begin to decrease, and finally converge when the flow is fully developed. Computed values for the Nusselt numbers could be higher than theoretical values due to the gas expansion and corresponding velocity increase, which results in a constant mass flow rate. The higher Nusselt values could also be explained by the heat flux magnitude, given in range of MW/(m² − K).

Table 4.7 and Figure 4.40 show the departure of the COMSOL model from theory. Departures at lower values of the Graetz number indicate that there could be some error due to grid resolution. As the flow reaches the developed region, any errors in grid resolution decrease in significance as the thin boundary layers vanish and a coarser mesh becomes more efficient, making the computation more correct. In spite of the departures in the development region which are likely due to element
size limitations, the agreement in the fully developed region suggests that the heat transfer within the microchannel is well predicted by standard laminar flow theory.

**Table 4.7: Graetz and Nusselt Numbers**

<table>
<thead>
<tr>
<th>$x^+$</th>
<th>Theoretical Nu</th>
<th>Computed Nu</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$\infty$</td>
<td>$\infty$</td>
</tr>
<tr>
<td>0.005</td>
<td>None</td>
<td>12.65</td>
</tr>
<tr>
<td>0.01</td>
<td>7.46</td>
<td>None</td>
</tr>
<tr>
<td>0.02</td>
<td>6.05</td>
<td>9.20</td>
</tr>
<tr>
<td>0.04</td>
<td>None</td>
<td>8.28</td>
</tr>
<tr>
<td>0.05</td>
<td>4.45</td>
<td>None</td>
</tr>
<tr>
<td>0.10</td>
<td>4.38</td>
<td>4.64</td>
</tr>
<tr>
<td>0.20</td>
<td>4.22</td>
<td>4.56</td>
</tr>
</tbody>
</table>
4.5.4 Model 10 Grid Resolution

The gas domain was meshed with densely distributed boundary nodes against the wall, and a tetrahedral grid for the rest of the domain, as shown in Figure 4.41. Figure 4.42 shows the grid resolution error for the tetrahedral mesh of the gas domain, and Figure 4.43 shows the grid resolution error for the nodes distributed along the boundaries of the gas domain.
Figure 4.41: Model 10 Mesh
Figure 4.42: Percent Error Vs. Minimum Tetrahedral Element Size

Figure 4.43: Percent Error Vs. Minimum Boundary Element Size
4.5.5 Model 10 Final Design Summary

Table 4.8 shows a summary of parameters for the final design. The maximum fuel temperature and exit velocity are for the accepted exit pressure value.

Table 4.8: Final Design Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outer Radius</td>
<td>20 mm</td>
</tr>
<tr>
<td>Inner Radius</td>
<td>6.2 mm</td>
</tr>
<tr>
<td>Flow Channel Length</td>
<td>13.8 mm</td>
</tr>
<tr>
<td>Number of Flow Channels</td>
<td>180</td>
</tr>
<tr>
<td>Maximum Fuel Temperature</td>
<td>2987 K</td>
</tr>
<tr>
<td>Constant Centerline Temperature</td>
<td>2750 K</td>
</tr>
<tr>
<td>Temperature Gradient Along Centerline</td>
<td>250K</td>
</tr>
<tr>
<td>Exit Hydrogen Density</td>
<td>0.64 kg/m³</td>
</tr>
<tr>
<td>Exit Cross Sectional Area</td>
<td>0.02 mm²</td>
</tr>
<tr>
<td>Exit Pressure</td>
<td>6.81 MPa</td>
</tr>
<tr>
<td>Exit Velocity</td>
<td>215 m/s</td>
</tr>
<tr>
<td>Mass Flow Rate at Exit</td>
<td>2.62 kg/s</td>
</tr>
<tr>
<td>Reynold’s Number</td>
<td>100 &lt; Re &lt; 550</td>
</tr>
<tr>
<td>Surface Area to Volume Ratio</td>
<td>0.82/mm</td>
</tr>
<tr>
<td>Ratio Improvement over Fuel Rod</td>
<td>30.21 %</td>
</tr>
</tbody>
</table>
CHAPTER 5

CONCLUSION AND RECOMMENDATIONS

5.1 Summary of Results

Processes for 3D modeling, discretization, meshing, identifying boundary conditions, and post processing were defined, and models that coupled flow physics with those of heat transfer have been used to generate profiles for pressure, temperature, velocity, and other important parameters. Results showed expected behaviors of these parameters, which must be considered when designing elements using brittle carbide materials. Failures resulting from thermal stress can be prevented by observing the temperatures found from analysis.

The first four models revealed how adding more channels to the fuel element would reduce element temperatures, and how elongating the channels would increase the gas exit temperatures. Model 5 showed the effects of adding finely distributed boundary node. This greatly cooled the element and increased heat transfer to the gas. Models 6, 7, and 8 were scaled by variable factors, and showed parametric pressure studies that yielded different temperature profiles for the propellant and the fuel. Scaling effects for these models revealed that larger models produce higher temperatures, due to the total power produced by the fuel. Units of power density are
Watts per cubic meter, so more cubic meters produced more power. By observing the results of parametric studies, a correlation between pressure drop and velocity can be found. Lower pressures at the exit resulted in higher pressure drops, and higher exit velocities. Model 9 was a theoretical model created to reduce the fuel volume, to correct the problem of unreasonable surface-area-to-volume ratios caused by scaling in Models 6, 7, and 8. Because the ratio for this model was still unacceptable after a volume decrease, analysis was never done. Because Model 1 had an excessively high temperatures that could be reduced by the addition of boundary layer nodes, as evident by observation of the Model 5 results, Model 1 was chosen to be the basis for the final design. With the physical events at the fuel wall under consideration and a very slight scaling of a factor of 1.4, Model 10 was created. The centerline temperature was almost constant, the thermal limitations of the fuel were not exceeded, and the surface-area-to-volume ratio exceeded that of the NERVA/Rover fuel rod.

By observing the graphs of the centerline temperatures, a smaller temperature change along the flow channel length was It was evident by observation of the centerline temperature graphs, that generally lower temperature profiles generated the lower temperature changes. When the boundary nodes were added to Model 5, the solid temperature was lowered such that the maximum was 1029 K, and $\Delta T$ was only 100 K.

Charts for Nusselt and Graetz numbers show that dimensionless parameters could be calculated in lieu of complex computer modeling. Since the results for this model follow the results for theory for a channel with the same aspect ratio, turbulent flow terms can be neglected and laminar flow can be assumed.
5.2 Comments on Methodology

Several projects mentioned in the earlier literature review performed CFD analysis with coupled heat transfer physics by selecting a small portion of their fuel element, while others assumed all channels could be simulated via porous media assumptions. Similarly, the grooved ring fuel element computations were done on a small portion of the element. Other similarities between the projects were $k$-$\epsilon$ models and the RANS model types. This study was done using well-established methods on a novel fuel element geometry.

5.3 Plan to Move Forward

Future analysis will advance to incorporate the entire fuel element stack. The porous media assumptions listed in section 5.2 could be used to simplify the computations, or the model could be analyzed by meshing and solving the entire configuration. The modeling will look at additional GRFE configurations for a more optimal system. Computations thus far have been performed on a single-node desktop, but a multi-node setup should be considered for entire disc stack models.

Neutronics calculations using Monte Carlo N-particle (MCNP) code will be performed on the final fuel element design or future designs to determine expected power profiles resulting from fuel and moderator density variations. These power profiles will be incorporated into CFD calculations to optimize existing fuel ring heating profiles.
With a design of a working GRFE model, a representative GRFE will be fabricated using various fabrication techniques (cold isostatic press, hot isostatic press, and/or rapid prototyping) to demonstrate producibility. Long-term plans include test article design and test planning in the Nuclear Thermal Rocket Element Environmental Simulator (NTREES), which uses induction heating to simulate the expected high-temperature environment [32]. Validation needs to be done on the designs to investigate inconsistencies in the models. The NTREES setup could be used for model validation.

A thermal stress analysis should be done, to show the limits of the structure. In doing this analysis, the researcher could also use several different types of carbides for comparison of structural integrity. The finite element model for the final design could be expanded to include the stress analysis, which could then be confirmed in the NTREES facility. Evidence of undue stress, such as fracture and deformation, could be investigated via many means of metrology, such as profilometry, scanning electron microscopy, or optical microscopy.
APPENDICES
APPENDIX A

WXMAXIMA CODE FOR SURFACE AREA AND RATIO CALCULATIONS

/* [wxMaxima batch file version 1] [ DO NOT EDIT BY HAND! ]*/

/* [ Created with wxMaxima version 12.04.0 ] */

/* [wxMaxima: input start ] */

kill(all)$

v1: 1082.63$

v2: 1053.04$

v3: 1033.31$

v4: 1282.80$

v5: 1282.80$

v6: 10262.41$

v7: 34635.62$

v8: 160350.10$

v9: 55662.02$

87
v10: 96183.98
v11: 3665.9
v12: 16724

/* v=Ah */
/* Volume of disk must equal volume of hexagonal rod */
V[spiral] : matrix([v1],[v2],[v3],[v4],[v5],[v6],[v7],[v8],[v9],[v10],[v11],[v12])*mm^3
print('V[spiral], " = ", V[spiral])

/* Find Area of Triangles */
/* base is 1/2 the length from side to side */
/* height is one side of the hexagon */
b : 9.550*mm
h[t] : 11.027*mm
print("Base is ", b, " and height is ", h[t])
A[tr] : 1/2*b*h[t]
print("Area of triangle is: ", A[tr])
print("Area of all triangles is: ", A[Alltr])

/* Find Area of Rectangle */
l : 19.1*mm
w : 5.5137*mm
\[A_{\text{rec}} : l \times w\]\n
\begin{verbatim}
print("Length is ", l, ", \"and width is \", w)\n
print("Area of rectangle is \", A[rec])\n
/* Find Area of Holes */

n : 19 /* number of holes */

r : 1/2*2.3*mm

\(\pi : 3.14\)

\(A_{\text{cir}} : \pi \times r^{-2}\)

\(A_{\text{Tcir}} : A_{\text{cir}} \times n\)

print("For \", n, "holes with a radius of \", r, ", \")\n
print("The cylindrical surface area is \", A[Tcir])\n
/* Find Total Area of Hexagon */

\(A_{t} : A_{\text{Alltr}}+A_{\text{rec}}-A_{\text{Tcir}}\)

print("The total area of the hexagonal face is \", A[t])\n
/* Equate Volumes of Hexagonal and Disc Structures */

\(V_{h} : V_{\text{spiral}}\)

/* Solve for height needed */

\(h_{\text{hex}} : V[h]/A[t]\)
\end{verbatim}
print("Height needed is ", h[hex])$

/* Cylindrical Area Calculations for Holes */
A[cyl] : 2*pi*r*h[hex]$  
print("Reactive surface area of 1 hole is ", A[cyl])$
print("Reactive surface area of all holes is ", A[cyln])$

/* Get reactive surface area of hexagonal rod */
print("For Hexagonal Rod...")$
SV: A[cyln]/V[h]$
print("Surface Area/Volume Ratio: ", SV)$
/* [wxMaxima: input end ] */

/* Maxima can’t load/batch files which end with a comment! */
"Created with wxMaxima"$
REFERENCES


