Thermal model of a centrifugal nuclear thermal propulsion system

Jacob T. Keese

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THERMAL MODEL OF A CENTRIFUGAL NUCLEAR THERMAL PROPULSION SYSTEM

by

JACOB T. KEESE

A THESIS

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

HUNTSVILLE, ALABAMA

2022
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(student signature)  (date)

________________
9/12/2022

(Jacob Keese)
THESIS APPROVAL FORM

Submitted by Jacob Keese in partial fulfillment of the requirements for the degree of Master of Science with an option in Aerospace Systems 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 on 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 with an option in Aerospace Systems Engineering.

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Committee Chair
9/14/2022

Dr. L. Dale Thomas
September 13, 2022

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ABSTRACT

The School of Graduate Studies
The University of Alabama in Huntsville

Degree Master of Science College/Dept. Engineering/Mechanical and Aerospace Engineering

Name of Candidate Jacob T. Keese

Title Thermal Model of a Centrifugal Nuclear Thermal Propulsion System

A numerical model was developed to study the heat transfer within the reactor of a Centrifugal Nuclear Thermal Propulsion system wherein liquid uranium heats hydrogen gas via direct-contact heat transfer. This one-dimensional, steady-state model treats the liquid uranium annulus of the centrifugal reactor as a conducting solid with internal energy generation and includes models of convection on the outside of the reactor, nonuniform energy generation from a detailed neutronics calculation, and models of bubble velocity and heat transfer. Results for three annulus geometries were compared for a variety of run conditions with the goal of maximizing the propellant output temperature within constraints on wall temperature and void fraction. Temperatures of approximately 3800 K can be achieved with wall temperatures of roughly 1500 K, while wall temperatures of roughly 2500 K are required to achieve core temperatures on the order of 5000 K.

Abstract Approval: Committee Chair

Department Chair

Graduate Dean
DEDICATION

To my mother and father.
ACKNOWLEDGEMENTS

First, I would like to express my gratitude to my thesis advisor, Dr. Keith Hollingsworth. His guidance and insight was invaluable to this research; without it, this work would not have been possible. I would also like to thank Dr. Dale Thomas for overseeing the CNTP work at UAH and his continual support of this research, as well as Dr. George Nelson for serving on this committee and helping to refine this work. Finally, thanks must be given to Dr. Michael Houts for funding this research effort.
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<td>( c_v )</td>
<td>Constant-volume specific heat</td>
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<td>( \bar{c}_{p,g} )</td>
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<td>Diameter</td>
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<td>$g$</td>
<td>Gravitational or centrifugal acceleration</td>
<td>$\frac{m}{s^2}$</td>
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<td>$g_c$</td>
<td>Gravitational acceleration on Earth at sea level</td>
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<td>Thermal conductivity</td>
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<td>Mass inside of single bubble</td>
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<td>Mass of molten uranium of equivalent volume to a bubble at injection</td>
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<td>Mass of a bubble with a uranium shell</td>
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<td>Mass flow rate through a CFE</td>
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<td>Mass flow rate through a given cell</td>
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<td>Pressure</td>
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<td>Pressure in central core of CFE</td>
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<td>$r$</td>
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<td>$r_B$</td>
<td>Radius of curvature of a spherical cap bubble</td>
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<td>$r_s$</td>
<td>Outer radius of fuel annulus</td>
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<tr>
<td>$t$</td>
<td>Time</td>
<td>s</td>
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<td>$t_d$</td>
<td>Time that a bubble is in the detachment stage of bubble formation</td>
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<td>$t_s$</td>
<td>Thickness of a hypothetical uranium shell surrounding a bubble</td>
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<td>Propellant radial velocity</td>
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<td>$v$</td>
<td>Velocity vector</td>
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<td>$x^+$</td>
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<td>$z$</td>
<td>Pressure integration term</td>
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<td>Definition</td>
<td>Unit</td>
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<td>$A$</td>
<td>Coefficient matrix for system of temperature equations</td>
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<td>$A_B$</td>
<td>Surface area of a bubble</td>
<td>$m^2$</td>
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<tr>
<td>$A_c$</td>
<td>Surface area of a channel segment</td>
<td>$m^2$</td>
</tr>
<tr>
<td>$A_{tot}$</td>
<td>Total surface area in contact with propellant in cell</td>
<td>$m^2$</td>
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<tr>
<td>$C_Q$</td>
<td>Empirical constant for void fraction-centrifugal acceleration equation</td>
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<td>$C_T \equiv u \frac{dT_l}{dr}$</td>
<td>Lagrangian temperature constant</td>
<td>$\frac{\kappa}{s}$</td>
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<td>$\vec{c}$</td>
<td>Solution vector for system of temperature equations</td>
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<td>$Eo \equiv \frac{g(\rho_l-\rho_g)d_B^2}{\sigma}$</td>
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<td>$\dot{E}_{gen}$</td>
<td>Heat generated in a computational cell</td>
<td>$W$</td>
</tr>
<tr>
<td>$\dot{E}_{in}$</td>
<td>Heat transferred into a computational cell</td>
<td>$W$</td>
</tr>
<tr>
<td>$F$</td>
<td>Rocket engine thrust</td>
<td>$lbf$</td>
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<tr>
<td>$F_N$</td>
<td>Neutronics scaling term</td>
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\[ I_{sp} \quad \text{Specific Impulse} \quad s \]

\[ L \quad \text{Length of CFE} \quad m \]

\[ M \quad \text{Total number of computational cells, Morton number} \quad - \]

\[ \mathcal{M} \quad \text{Molecular weight} \quad \frac{kg}{kmol} \]

\[ N \quad \text{Total number of computational cells in liquid annulus} \quad - \]

\[ Nu \quad \text{Nusselt number} \quad - \]

\[ Pe \equiv RePr \quad \text{Peclet number} \quad - \]

\[ Pr \equiv \frac{v}{a} \quad \text{Prandtl number} \quad - \]

\[ Q \quad \text{Volumetric flow rate} \quad \frac{m^3}{s} \]

\[ \dot{Q}_{bubbles} \quad \text{Total power imparted to bubbles in annulus} \quad W \]

\[ \dot{Q}_{channels} \quad \text{Total power imparted to propellant in channels} \quad W \]

\[ \dot{Q}_{cond} \quad \text{Heat conducted between computational cells} \quad W \]
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<th>Definition</th>
<th>Unit</th>
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<td>( \dot{Q}_{gap} )</td>
<td>Total power imparted to propellant in clearance gap</td>
<td>( W )</td>
</tr>
<tr>
<td>( \dot{Q}_{gen} )</td>
<td>Total power generated in a CFE</td>
<td>( W )</td>
</tr>
<tr>
<td>( \dot{Q}_{net\ in} )</td>
<td>Net heat into the local system</td>
<td>( W )</td>
</tr>
<tr>
<td>( R )</td>
<td>Radial location of a computational cell node</td>
<td>( m )</td>
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<tr>
<td>( R_{\text{gap}} )</td>
<td>Outer radius of clearance gap</td>
<td>( m )</td>
</tr>
<tr>
<td>( R_i )</td>
<td>Radius of internal surface of fuel annulus</td>
<td>( m )</td>
</tr>
<tr>
<td>( R_o )</td>
<td>Radius of the outer surface of the CFE</td>
<td>( m )</td>
</tr>
<tr>
<td>( R_u )</td>
<td>Universal gas constant</td>
<td>( \frac{J}{kmoi\cdot K} )</td>
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<td>( R_{eB} )</td>
<td>Reynolds number for a bubble</td>
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<tr>
<td>( R_{eD} )</td>
<td>Reynolds number for frit channels</td>
<td>–</td>
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<tr>
<td>( T )</td>
<td>Temperature</td>
<td>( K )</td>
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<tr>
<td>( T_{\text{entry}} )</td>
<td>Temperature of propellant entering the frit</td>
<td>( K )</td>
</tr>
<tr>
<td>( T_l )</td>
<td>Temperature of bubble-liquid interface</td>
<td>( K )</td>
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</table>
\[ Ta = \frac{a^2R_{\text{in}} (\alpha_h)}{v^2} \]\(^3\)  

Taylor number

\[ Ta_c \]  

Critical Taylor number

\[ \dot{T} \]  

Temperature rate of change \( \frac{K}{s} \)

\[ V \]  

Volume \( m^3 \)

\[ V_{\text{fuel}} \]  

Total volume of the uranium fuel in the annular fuel region \( m^3 \)

\[ V_e \]  

Total volume of the uranium fuel in the annular fuel region \( m^3 \)

\[ V_{\text{H}2} \]  

Total volume of hydrogen in the annular fuel region \( m^3 \)

\[ V_{\text{total}} \]  

Total volume of the annular fuel region \( m^3 \)

\[ \overline{V}_{\text{rel}} \]  

Velocity across control surface \( \frac{m}{s} \)

\[ \dot{W}_{\text{net in shaft}} \]  

Shaft work \( W \)

\[ X \]  

Void fraction

\[ \alpha \]  

Matrix coefficient term, thermal diffusivity \( \frac{m^2}{s} \)

**Lowercase Greek**

\[ \alpha \]  

Matrix coefficient term, thermal diffusivity \( \frac{m^2}{s} \)
\( \beta \)  
Matrix coefficient term  

\( \gamma \)  
Hydrogen specific heat ratio, matrix coefficient term  

\( \theta \equiv T_i - T_g \)  
Temperature difference  

\( \theta_H \)  
Homogeneous solution  

\( \theta_P \)  
Particular solution  

\( \dot{\theta} \)  
Temperature difference rate of change  

\( \kappa \equiv \frac{\mu_g}{\mu_l} \)  
Viscosity ratio  

\( \mu \)  
Dynamic viscosity  

\( \nu \)  
Kinematic viscosity  

\( \rho \)  
Density  

\( \sigma \)  
Surface Tension  

\( \tau \)  
Lagrangian analysis time constant  

\( \omega \)  
Angular velocity of CFE
### Uppercase Greek

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<td>Radial thickness of a computational cell</td>
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<td>$\Delta R$</td>
<td>Distance between cell nodes</td>
<td>$m$</td>
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<tr>
<td>$\Delta V$</td>
<td>Velocity change</td>
<td>$\frac{m}{s}$</td>
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<tr>
<td>$\Delta \theta$</td>
<td>Angle subtending differential elements of a CFE</td>
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### Subscript

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CHAPTER 1. INTRODUCTION

Nuclear Thermal Propulsion (NTP) is a form of advanced rocket propulsion which has been proposed by NASA and is under development for future advanced missions. It has gathered particular attention for manned missions to Mars [1,2], but also shows potential for robotic missions to Jupiter and Saturn [3] as well as even further destinations including the ice giants and Pluto and Europa [4,5]. The concept was successfully demonstrated in the ROVER/NERVA program which began in 1953 as a joint effort between the Atomic Energy Commission and NASA and performed 23 reactor tests in Nevada before its termination in 1973 [6,7]. A flight test was planned but cancelled before it was performed [7,8].

The operating principle of an NTP engine involves heating a single propellant species, usually hydrogen, inside of a nuclear reactor and then expelling the propellant through a converging-diverging nozzle. Thus, the primary difference between an NTP engine and a chemical liquid rocket engine is that the enthalpy imparted to the propellant comes from the nuclear fission process inside of the reactor instead of a chemical combustion as in most bipropellant liquid rocket engines. A cutaway schematic of an NTP engine is shown in Figure 1.1.
The attractiveness of NTP comes from its increased performance; in particular, NTP promises dramatically increased specific impulse values compared to chemical rocket engines [6]. The specific impulse, or $I_{sp}$, of a rocket engine is defined as:

$$I_{sp} \equiv \frac{F}{g_c \dot{m}}$$  \hspace{1cm} (1.1)

where $F$ is the thrust of the engine, $\dot{m}$ is the mass flow rate of propellant, and $g_c$ is the gravitational acceleration on Earth at sea level ($9.81 \text{ m/s}^2$ or $32.17 \text{ ft/s}^2$). Physically, $I_{sp}$ represents the amount of time that one pound of propellant can produce one pound of thrust and is reported in seconds. It is analogous to fuel economy or “miles-per-gallon” in a car, since a higher specific impulse represents a more efficient use of propellant per unit mass to generate thrust.

The $I_{sp}$ can be predicted based on the thermodynamic properties of the propellant in the rocket chamber before being exhausted through the nozzle. An idealized equation for the specific impulse in a vacuum with an infinitely expanded nozzle flow is given as:
Where $\gamma$ is the specific heat ratio of the propellant being expelled through the nozzle, $R_u$ is the universal gas constant, $T_c$ is the chamber propellant temperature, and $\mathcal{M}$ is the molecular weight of the hydrogen propellant. While this equation will slightly overpredict the specific impulse for a finite-sized nozzle, it is nonetheless useful for getting an upper bound on $I_{sp}$ with only a handful of thermodynamic properties and it also shows the influence of these different properties on the $I_{sp}$. Since $I_{sp}$ is proportional to the square root of the chamber temperature, it is clearly desirable to maximize the temperature of the propellant. However, the $I_{sp}$ is inversely proportional to the square root of the molecular weight of the propellant. This is actually the reason that NTP offers increased specific impulse. While the chamber temperatures of bipropellant liquid rocket engines can be in the neighborhood of 3500 K, the chamber temperatures of NTP engines using a solid-core reactor are in the range of 2500 to 3000 K due to material limitations of the nuclear fuel. However, since an NTP engine can use pure hydrogen as a propellant, with its low molecular weight, the overall specific impulse is greatly increased compared to that of the best chemical rocket engines. NTP is believed to be capable of producing specific impulses of 900 s or more, while the highest-performing chemical rocket engines are only capable of producing specific impulses of around 450 s.

Although 900 s is a significant improvement over chemical rocket engines, NTP does have some drawbacks. One is that due to the low density of liquid hydrogen, to use NTP for a mission requiring a large $\Delta V$ would necessitate large propellant tanks; leading to mission architectures for missions such as a round-trip manned mission to Mars that call
for a large transfer vehicle to be assembled in Earth orbit with several hydrogen propellant
tanks launched separately [9]. Therefore, it is desirable to increase the specific impulse
even more beyond the 900 s mark.

The main limitation of specific impulse for “traditional” NTP which uses a solid-
fuel reactor is that beyond about 3000 \( K \), even the most advanced fuel materials which
have been developed would begin to melt. Therefore, it has recently been proposed to
investigate the possibility of using a reactor which operates with fuel in the molten phase
to achieve higher temperatures, and therefore higher \( I_{sp} \). This introduces the difficulty of
containing the molten fuel, since very few structural materials can exist in solid form above
3000 \( K \) anyways. However, it has been proposed that the fuel could be held within a
rotating centrifuge. By rotating the centrifuge fast enough, an annulus of fuel would form
in contact with the cylinder walls and leave a hollow central region. Gaseous propellant
could then be injected into the fuel at the cylinder walls, after which it would bubble
through the fuel annulus before collecting in the hollow cavity. The propellant would then
be exhausted axially from the hollow core region, passing through a converging-diverging
nozzle to generate thrust.

An early schematic of such an engine is seen in Figure 1.2, although current
investigations call for an engine using multiple centrifugal drums (referred to as centrifugal
fuel elements, or CFEs). Due to the centrifugal drums, this high-performance NTP concept
is referred to as Centrifugal Nuclear Thermal Propulsion, or CNTP. It has recently been
suggested that such a CNTP system could achieve propellant temperatures of roughly 5000
to 5500 \( K \) [10,11], providing a significant increase to specific impulse to as high as 1800
s [10,11]. Further details about the current CNTP concept will be given in Chapter 2.
Despite the potential for vastly improved performance, there are a number of serious engineering challenges which exist and must be overcome before such a system can be realized. Several of these challenges have been identified previously [13] and are listed here:

1. The heat transfer between the molten fissile fuel and the propellant bubbles must be sufficient to both heat the propellant to the desired level and to cool the molten annulus so that the temperature of the outer annulus is below the maximum safe operating temperature of the SiC/ZrC cylindrical retaining wall.

2. A porous retaining wall must be designed for the CFEs which will allow propellant to enter and bubble through the molten fuel while preventing the fuel from back flowing through the retaining wall.

3. A coating for the interior CFE walls must be designed to withstand the high temperatures of the molten fissile fuel.
4. The drive system and bearings for the CFEs must be designed for operation at thousands of \( rpm \).

5. Contingencies must be developed for failure of individual cylinders.

6. Methods must be developed to minimize uranium fuel loss and vibrational instabilities during transient startup and shutdown.

7. The reactor and cylinder exits must be designed to minimize the uranium loss rate.

8. Methods must be developed to replenish uranium fuel that is burned up or lost in entrainment in propellant flow.

9. The neutronic design must be optimized using lessons from past liquid nuclear reactor development.

10. Methods must be developed to incorporate a CNTP reactor into a traditional NTP engine design.

While all of these considerations are important and must be addressed, the current study focuses on developing a conduction-based numerical thermal model of the heat transfer processes within a CFE. It is intended that this model will help to predict key performance parameters such as

- the maximum propellant temperatures attainable at the core of the annulus,
- the resulting temperature of the containing wall for a given maximum propellant temperature, and
- the propellant mass flow rate and void fraction distribution for a realizable set of operating conditions.
This study will also investigate the influence of various design parameters on the performance metrics; namely, different CFE geometries, core pressures, rotation speeds, and power distributions within the annulus.

Chapter 2 of this document will review the relevant literature surrounding CNTP, as well as physical models relevant to the current investigation. Chapter 3 will discuss the formulation of the numerical model and how various physical phenomena were treated in the model. Chapter 4 will present the key results from the numerical model runs for various parameters. Finally, Chapter 5 presents conclusions and recommendations for future work.
CHAPTER 2. LITERATURE OVERVIEW

The concept of a centrifugal nuclear thermal propulsion system (CNTP) was first proposed in 1954 by McCarthy [14]. Over the following two decades, a handful of studies were performed investigating the feasibility of a CNTP or similar design. Interest in the CNTP concept seemed to end abruptly after the early 1970’s, coinciding with the termination of Project ROVER. Although some similar concepts, such as the Liquid Annular Reactor System [15], received attention in the intervening years, little work has been performed towards a CNTP system until the past few years. This chapter will review some of the original studies of a liquid-fueled nuclear rocket, and also review some of the key studies of various physical phenomena present in a CNTP system that were necessary in constructing the present model. However, recent studies have also been performed to investigate system-level behavior in a CNTP system such as the neutronic performance and $I_{sp}$ given the anticipated reactor temperatures.

2.1. Conceptual Studies of CNTP Systems

A centrifugal nuclear thermal rocket, or CNTR, is a rocket driven by CNTP. Both acronyms are popular in the literature; furthermore, the basic concept of what is currently referred to as a centrifugal nuclear thermal rocket has gone by different names such as the liquid-fuel nuclear rocket or liquid-core nuclear rocket. Here they will all be referred to retroactively as a CNTR. The first proposal of a CNTR from McCarthy in 1954 [14] was brief and highly conceptual. It proposed operating a single centrifuge with molten fissile fuel, such as uranium, thorium, or plutonium, operating as a fast neutron reactor. No suggestion of control drums was included, and instead control could be accomplished with
a small amount of solid fissile fuel outside of the main reactor with control rods used to control the reactor. Although little analysis was performed, the concept would be further developed by other authors.

2.2. Study Performed by Boeing

The next significant study published was performed by Barrett [12,16] for the Boeing company in 1963–1964. This was a more detailed system-level design than the original proposal by McCarthy but assumed the same basic configuration. It included preliminary neutronic analysis, treating the reactor as a fast-neutron reactor. This study primarily looked at estimating the specific impulse using various alternative nuclear fuels, the heat transfer in the system, and possible mass flow rates of propellant.

The specific impulse was evaluated for various pressures, and it was determined that the maximum specific impulse of such a system in the range of 1200 to 1400 seconds [12]. However, this analysis does not consider the effect of H₂ dissociation, treating the molecular weight and specific heat ratio of the hydrogen as constants. Dissociation would reduce the average molecular weight of the mixture, thus increasing the specific impulse perhaps by a significant amount over what was estimated by Barrett.

Barrett’s study also looked at vaporization of the nuclear fuel into the propellant in the core. He assumed the partial pressure of the vaporized fuel in the mixture of H₂ and fuel vapor in the core would be equal to the vapor pressure of the fuel at the core temperature. The fuel vapor would be exhausted with the propellant. The concentration of the fuel vapor in the propellant would then increase with temperature, increasing the average molecular weight of the gas flow out of the rocket and reducing the specific impulse as the core temperature climbs and the fuel vapor pressure increases. Figure 2.1
shows Barrett’s computations regarding the effect of increasing the core temperature (and by extension the fuel vapor pressure) on specific impulse. Figure 2.2 shows that increasing the core pressure increased this maximum specific impulse slightly for the fuels considered. Because of this effect, Barrett predicted a specific impulse in the range of 1200 to 1400 seconds [16].

Figure 2.1 Specific Impulse Versus Core Temperature for Alternative Fuels [16]
2.3. Studies Performed at Princeton

Perhaps the most in-depth study thus far was conducted by a group at Princeton University and is reported by Nelson et al. [17] in 1963–1965. This system design called for having several smaller centrifugal fuel elements instead of a single large centrifuge. This is the preferred arrangement in subsequent designs as well. The advantage of this design is that it increases the neutronic efficiency, provides a larger total flow area, and allows for the implementation of moderator materials in the interstitial spaces between cylinders; this means that the critical mass of the reactor can be reduced, and it can operate in the thermal neutron spectrum instead of the fast. This system configuration is shown in Figure 2.3. This configuration shows 19 rotating fuel elements, with the interstitial space being occupied by zirconium hydride moderator material and surrounded by a beryllium reflector. The hot propellant from all fuel elements would be collected and exhausted through a single large nozzle. Before being injected into the fuel elements, the propellant
is routed through coolant passages in the nozzle, moderator block, and reflector to keep these components at acceptable temperatures.

The Princeton design also specified that the primary fuel in each element would be UC₂, which would be heavily diluted with ZrC. Because of the high melting point of both UC₂ and ZrC, this design would be operated such that a large portion of the UC₂/ZrC mixture would be solid, with only a relatively thin and isothermal liquid “topping layer” adjacent to the core which would raise the propellant temperature to the desired value. Figure 2.4 shows a cross-section of such a fuel element, along with the flow passages for cooling the moderator block.

For the neutronics analysis, a three-group two-region diffusion code was used and the critical mass of U-235 for the reactor was determined for different ZrC dilution ratios and volume fractions of ZrH₂ moderator. This analysis indicated a sharp increase in critical
mass when the ZrH$_2$ volume fraction was below 0.15 and little reduction in critical mass when the ZrH$_2$ fraction was increased beyond this point.

![Figure 2.4 Fuel element cross-section from the Princeton design [17]](image)

When analyzing the bubble flow through the liquid layer, the bubble regime was assumed to be in the spherical cap regime. Bubbles in this regime are at their largest size. Based on this assumption, Nelson et al. used the terminal velocity of a spherical cap bubble given in the classic work by Davies and Taylor [18]. This approach will be adopted for the present study in Chapter 3 as it allows for a simple analysis approach without having to perform complex simulations of bubble dynamics.

This study also reports a maximum feasible void fraction of 0.3 to 0.4. The authors are concerned that beyond this value the gas bubbles will merge and the liquid will effectively become liquid droplets suspended in the gas [19]. If this occurs, it could be much easier for the fuel to be blown out of the reactor by the gas flow.
Nelson et al. also point out the same limitation on specific impulse from the Barrett study by assuming a vapor phase of the fuel mixed with the propellant being exhausted from the core. Again, it is assumed that the partial pressure of that vapor phase is the tabulated vapor pressure of the fuel. Therefore, a similar limit on specific impulse was found based on the core pressure and dilution ratio of ZrC to UC₂ in the fuel as shown in Figure 2.5. It can be seen that the specific impulse of pure hydrogen exhaust would rise dramatically, while the presence of uranium from vapor pressure losses would significantly degrade specific impulse beyond a certain point. From the analysis in Nelson et al., having a large dilution ratio and increasing the core pressure serve to mitigate the specific impulse degradation with increasing temperature.

Nelson et al. also performed a simplified heat transfer analysis of the heating of the bubbles, examining both the heat transfer in the liquid boundary layer on the outside of the bubble and the heating of the gas contained within the bubble itself. This analysis predicted that the bubbles would come into a local equilibrium with the surrounding fuel very rapidly, meaning that the rate of heat transfer to the bubbles would not be a limiting factor in this reactor design.
2.4. Bussard and DeLauer

In *Fundamentals of Nuclear Flight* published in 1965, Bussard and DeLauer make brief mention of various advanced NTP concepts, among them a liquid-fuel nuclear rocket [20]. The authors seem to refer to a configuration similar to that proposed by Nelson *et al.* which would use uranium carbide fuel diluted with zirconium carbide and have a maximum operating temperature of roughly 4400 °C, albeit no mention is made of a reactor with multiple cylindrical fuel elements. The authors point out that the specific impulse with hydrogen at temperatures of roughly this value and pressures of a few atmospheres could be roughly 1600 seconds, a dramatic improvement over solid-fuel NTP. Further summaries of historical work on CNTP-like designs can be found in Refs. [21,22].
2.5. Recent CNTP Investigations

NASA’s recent interest in CNTP has resulted in revised conceptual designs and a number of publications investigating their feasibility [10,11,13,23–27]. The configurations proposed in most of these works draw heavily from the Princeton study in that they call for a CNTR which uses multiple CFE’s in a cluster, as shown in Figure 2.6. However, there are a few key differences. To begin with, the fuel selected is currently metallic uranium, as opposed to the uranium carbide proposed in the Princeton study [17]. This choice arises from the concern that the high fuel temperatures proposed would cause a compound such as uranium carbide to dissociate into uranium and carbon. This could leave only the elemental uranium in the reactor and could expel carbon in the propellant exhaust which would reduce the specific impulse. Furthermore, it has been proposed to operate the fuel at even higher temperatures, with a target goal of heating the propellant to 5500 $K$ [11]. The various materials and their respective temperatures for the given CFE are shown in Figure 2.7.

The analysis of Leer [26] modeled the heat transfer between the uranium fuel and a single bubble passing through it. Leer divided the uranium fuel into three regions: a solid region, a liquid region, and a vapor region. Both the solid and liquid regions were modeled as solids for the purpose of energy analysis. He modeled heat transfer to the hydrogen gas as it passed through all three of these regions, focusing on a single bubble of hydrogen in the liquid region. The energy balance equation was solved for both the bubble and the uranium fuel. A number of simplifying assumptions were used in this analysis. Of note is that Leer assumed that the heat generation from the uranium fuel was assumed to be constant throughout the uranium layer, neglecting any radial variation in power production.
It will be seen later, however, that the heat generation monotonically decreases from a peak power production near the outer radius of the fuel annulus to a much lower value near the core.

The bubble motion within the liquid uranium layer was analyzed by summing the forces on the bubble in the radial direction. This was taken to be the sum of the pressure force acting on the bubble, the drag from pressure, and the buoyancy on the bubble.

Figure 2.6 CNTP Reactor with 19 CFE’s [11]
2.6. Alternative Advanced Concepts

In order to overcome various limitations of the “bubble-through” Liquid-Core Nuclear Rocket as envisioned by authors in the 1960s such as Nelson et al. [17] and Bussard and DeLauer [20], a few alternative concepts were proposed which deserve mention. One of the most notable of these is the radiation-transfer liquid-core nuclear rocket, proposed by Ragsdale et al. [28]. Ragsdale et al. note the possible limitation on $I_{sp}$ due to vaporization of the nuclear fuel into the propellant stream, as pointed out by Barrett [12,16] and by Nelson et al. [17]. It has been suggested that the “bubble-through” concept would result in equilibrium concentrations of heavy vapor in the propellant exhaust, from mass diffusion into the propellant bubbles while they are also receiving heat from the liquid fuel. The radiation liquid core nuclear rocket seeks to alleviate this problem by injecting the propellant axially down the central channel of the fuel annulus instead of first bubbling it through the liquid fuel. The primary mode of heat addition to the propellant would be
through radiation, and therefore the hydrogen propellant must be seeded with solid particles opaque to radiation [28]. A schematic of this design is shown in Figure 2.8.

![Figure 2.8 Radiation Heat Transfer Liquid Core Nuclear Rocket Concept [28]](image)

Additional analysis of this concept has been performed by Ragsdale [29] and by Putre and Kascak [30]. Although predicted specific impulse values were high, the main drawback of this design in comparison to the bubble-through design is related to the thermal gradients. In order for heat to be transferred to the propellant in the central cavity of the reactor, the inner surface of the fuel annulus must be at a very high temperature. However, because heat is being lost at this surface, the peak temperature of the fuel itself must be somewhere in the middle of the fuel annulus with a temperature possibly as high as several thousand Kelvin. This will also cause significant temperatures to exist at the containment wall. Putre and Kascak reported that even when designed for a reduced specific impulse of 1250 seconds, the required wall temperature would be roughly 4000 K.
By contrast, for a design with a specific impulse of 1430 seconds, the required wall temperature could be as high as 4720 K. These numbers are significantly higher than the melting points of almost all structural materials and could cause a serious problem for the radiation heat transfer concept.

Additionally, researchers at Brookhaven National Laboratory proposed a Liquid Annular Reactor System propulsion system that appears to have been primarily based on the radiation heat transfer liquid core nuclear rocket concept, and further details can be found in Refs. [15,31].

Another similar concept which has been proposed previously is the colloidal core nuclear reactor. This would involve a collection of solid or molten fuel particles suspended in a gas vortex contained within a rotating drum. Though it will not be discussed in depth here, further information can be found in Refs. [32–34].

2.7. Experimental Investigations for CNTP Systems

Barrett [12] also reports an experiment conducted by Boeing to measure the heat transfer coefficient of bubbles in liquid metal. The liquid metals used were mercury and a low melting temperature metal similar to Woods’ metal (an alloy of bismuth, lead, cadmium, and tin with a melting point of roughly 70 °C). The apparatus is shown below in Figure 2.9. The apparatus consisted of a vat of liquid metal at rest on a porous distributor (in this case filter paper). Gas is injected through the bottom of the apparatus and bubbles through the sitting liquid metal. The approach was to follow a method for fluidized beds developed by Wamsley and Johanson [35]. However, this method proved unsuccessful for measuring large heat transfer coefficients and was only able to measure a lower value for the heat transfer coefficient. Their results with mercury indicated that the heat transfer
coefficient should be greater than approximately $100 \text{Btu}^\circ R \cdot ft \cdot hour \ (\sim 568 W/m^2K)$. Another noteworthy result from this experiment occurred when tests were performed with the alloy comparable to Woods’ metal. Measurements of the heat transfer coefficient were unsuccessful because some of the constituent elements of the alloy evaporated and raised the melting point which caused the metal to solidify. However, it was observed that the metal solidified such that air channels were formed around the bubble streams, instead of blocking off the gas flow. This indicates that for an actual CNTP system, propellant channels may form upon shutdown of the engine. This would greatly aid in the restart process of such an engine.

![Figure 2.9 Liquid Metal Heat Transfer Coefficient Experimental Apparatus [12]](image)

In order to accurately predict the performance of a CNTP reactor, it is clear that the motion of the bubbles must be predicted. A number of bubble motion studies have been
performed to understand bubble motion in CNTR systems or in other applications. Lieberherr [36] studied the motion of bubbles at 1-g in water. While the actual conditions of the experiments were far removed from those which would be found in a CNTP system, it was noted that in experiments dealing with bubble columns, the bubbles did not seem to have a significant impact on each other’s motion. This may suggest that even in a CNTP reactor with dense bubble concentrations and high void fractions, the bubble behavior may not significantly deviate from that of low void fractions.

A significant experimental study was conducted by Schrage and Perkins [37,38] at the University of Arizona in the late 1960s. This study sought to characterize isothermal bubble motion in a rotating liquid annulus at various levels of centrifugal acceleration. The apparatus consisted of a rotating drum with a gas orifice serving as a bubble injector located at the outer radius of the drum. The overall system can be seen in Figure 2.10, where it is shown that the axis of rotation of the drum is horizontal. Bubbles were injected one at a time into the drum, which was transparent on one end. Water and a glycerin-water mixture were chosen as the molten uranium simulants for various runs. Controlled parameters included the rotation speed of the drum, diameter of the gas orifice, and the radial location of the injection point. The latter was controlled by using an extended tube protruding from the gas orifice to accomplish injection at different radial positions in the drum.

Still images were taken with a camera parallel to the axis of rotation as a bubble travelled toward the center of the drum. From these images, the position of the bubbles was measured as well as their traversal time and velocity at various points. These were plotted and used to validate predictions developed by the authors describing the bubble motion in the drum. A typical plot of this data using water can be seen in Figure 2.11,
where the squares represent measured data points and the continuous curve represents the results from the theoretically derived solution.

Figure 2.10 Experimental Apparatus for Isothermal Bubble Motion Experiment [37]
McGuirk and Park [39] performed an experimental investigation to determine the rotation speed necessary for a CFE. They reported an equation relating, approximately, the relationship between mass flow rate and centrifugal acceleration based on the work of Zuber and Findlay [40]. This is shown below in Eq. 2.1 where \( Q \) is the volumetric flow rate, \( X \) is the void fraction, \( A_l \) is the area at the inner surface of the liquid annulus, \( \sigma \) is the liquid surface tension, \( g \) is the centrifugal acceleration, \( \rho_l \) is the liquid density, and \( C_Q \) is an empirical constant varying from 1.1 to 1.6.

\[
Q = 1.53A_l \left( \frac{\sigma g}{\rho_l} \right)^{0.25} X / (1 - C_Q X)
\]  

(2.1)
The McGuirk and Park experiment attempted to verify this equation for the flow scenario envisioned in a CNTR. The schematic of this apparatus is shown in Figure 2.12. The experimental apparatus consists of two coaxial cylindrical drums. The inner drum rotates and has a porous nickel wall, and the outer shell is pressurized with air. The inner drum is filled with water, and as it rotates the water will collect at the outer surface of the inner drum in an annulus. During operation, air will pass through the porous chamber wall and bubble through the liquid annulus before collecting in the central cavity and exiting axially through an outlet. One end of both drums contains viewing windows which will allow observation of the liquid profile. Based on the thickness of the liquid layer, the void fraction could be calculated experimentally. The schematic of this apparatus is shown in Figure 2.12. It is reported that there was a relatively large uncertainty in the measurement of the liquid layer thickness, and therefore void fraction; however, the results did agree reasonably well with the prediction. The experimental apparatus is also interesting from the perspective that it simulated the distributed porous orifices in the rotating cylinder, and a similar design may be useful in future CNTP investigations.
While most of the experimental studies examined were performed at temperatures much lower than that anticipated for a CNTP reactor, at least one experimental program was operated to study liquid metals at high temperatures at Temple University by A. V. Grosse [41,42]. In order to study metals at high temperature, Grosse developed a centrifugal chemical reactor capable of containing liquid metal, in particular molten aluminum and aluminum oxide, at temperatures of roughly 3800 K. A schematic of this apparatus is shown in Figure 2.13. In this design, a steel cylinder with aluminum oxide bricks is rotated at a few hundred rpm. Meanwhile, an aluminum rod is fed into the cylinder from the right and burns in oxygen within the center of the centrifugal drum. While it does not seem that these particular experiments were done for the application of
CNTP (although passing reference is made to it in [42]), similar arrangements could be utilized for future experiments to investigate the behavior of liquid metals at high temperatures.

![Figure 2.13 Centrifugal Chemical Reactor [15] (Original Figure from [42])](image)

2.8. Bubble Behavior

Since the propellant bubbling through the reactor is a key component of this concept, the behavior of the propellant bubbles must be well understood. Interestingly, bubbles can typically be divided up into certain regimes based on their morphology. These, generally, are bubble spheres, ellipsoids, and spherical caps, where which regime a bubble is in at any given moment is dependent on the size of the bubble. The exact size marking the transition depends on the liquid properties and other conditions, however. Schrage [37]
has subdivided the bubble spheres and ellipsoids regions so that a total of five bubble regimes are defined, in order of increasing bubble size, as:

1. Stokes Flow Bubbles. These bubbles are small and spherical and behave like rigid spheres as if the gas inside were motionless.

2. Circulating Spheres. While these bubbles are still spherical, they can exhibit significant internal gas circulation. This can change the drag coefficient, and the analysis in this region can be more complicated than for Stokes flow bubbles.

3. Circulating Ellipsoids. For larger bubbles, a bubble will begin to distort from its spherical shape and become ellipsoidal. This will further increase the drag coefficient.

4. Oscillating Ellipsoids. Beyond a certain size, ellipsoidal bubbles cease to rise rectilinearly and instead exhibit an oscillation or zigzagging motion while rising. High Morton number liquids apparently do not exhibit this behavior.

5. Spherical Caps. These represent the largest size of bubbles before breakup occurs. The shape of a spherical cap bubble is, as the name suggests, similar to a segment of a sphere. An example of this shape is shown in Figure 2.14. These bubbles are characterized by a constant drag coefficient of 2.6 and a subtending half-angle of roughly 52°.
These classifications are based in large part on the classical work of Haberman and Morton [43], which characterized various bubble shapes during experiments of air bubbles in water. By plotting the terminal velocity of bubbles as a function of their equivalent radius one can show the relationship between bubble regime and terminal velocity, as in Figure 2.15. It should be noted, however, that such a plot is only valid for a given fluid, and that the data in Figure 2.15 was developed for water and as such cannot be used for studying bubbles in other liquids.
Figure 2.15 Bubble Regimes [37]

Bubble shapes and dynamics are complex topics, and a more complete treatment can be found in Clift et al. [44]. Those authors present a chart with various bubble regimes for bubbles freely rising or falling, allowing prediction of the bubble regime based on any two of Reynolds number, Eotvos number, or Morton number in Figure 2.16. The solid lines divide the three main regimes (spherical, ellipsoid, cap), where spherical bubbles are to the left and bottom, ellipsoids are in the upper middle, and cap-shaped bubbles are in the upper right.
Figure 2.16 Bubble Regime Chart [44].
2.9. Metallurgical Experiments

While thus far there have been few experiments conducted explicitly to study aspects of a CNTP system, particularly using liquid metals, there are a number of experimental investigations of bubble flows in liquid metals which have been conducted for the metallurgical industry. One technique for studying bubble motion and characteristics in liquid metal baths has been to use X-ray imaging on thin boxes of liquid metal with bubble injection [45,46]. This approach allows one to get relatively high-resolution images of the bubbles as they rise through a liquid metal pool, determining the size and shape of bubbles. This technique could be useful in order to validate or develop models of bubble behavior in a CNTP system, and is currently being used in an ongoing research effort at UAH which seeks to investigate the phenomenon in a CNTP system by using liquid Galinstan as a simulant for molten uranium [47].

Additionally, previous experiments have been conducted to develop heat transfer relationships between bubbles and liquid metals. Tokunaga et al. [48] performed an experiment to develop a Nusselt number correlation for bubbles in liquid metals using cooled nitrogen and heated Wood’s metal. The experimental apparatus for this study is shown below in Figure 2.17. The temperature of a bubble was measured directly using a micro-thermocouple at different elevations within the molten metal bath, and from that data a Nusselt number correlation was developed. This will be discussed further in Chapter 3.
2.10. Summary

The literature suggests that significant $I_{sp}$ gains can be realized with a liquid-fuel NTP system operating at high temperatures; however, little work has thus far been done to demonstrate how the high temperature gradients required across the annulus could be achieved. This work seeks to explore this question by establishing a model to predict the temperature distribution within a class of CNTP reactor designs that assume a liquid uranium annulus with a silicon carbide retaining wall. In addition to the literature on CNTP reactors reviewed in this chapter, engineering models of bubble dynamics and heat transfer not already introduced in this chapter will be sourced from the literature in their respective fields. Those sources will be cited in Chapter 3 as the models are introduced.
CHAPTER 3. METHODOLOGY

This chapter will describe the conceptual and mathematical framework of the problem and an overview of how the solution was carried out in MATLAB. Figure 3.1 gives a schematic view of a rotating CFE (geometry not to scale) which represents the axisymmetric domain of the model. The region under consideration by the model is subtended by an angle $\Delta \theta$. The finite-difference approach calls for this region to be split up into a series of computational cells in the radial direction, each with a small radial thickness. This region spans both the liquid uranium annulus and the porous silicon carbide frit that forms the wall of the CFE as shown in Figure 3.1. It is assumed that the temperature and other properties are uniform in the azimuthal direction, and heat transfer in the azimuthal direction can be neglected.
3.1. Alternate Designs

A number of different preliminary CNTR designs with varying numbers of CFE’s, geometric dimensions, and materials have been proposed. Because of the numerous benefits of having a multi-CFE configuration as mentioned by Nelson et al. [17], not least of which is the benefit to the neutronics, it was decided to investigate a design which contained 19 CFE’s. The materials and regions used for the thermal and neutronics analysis are those which were selected in the neutronics model parameters from Gates et al. [24]. Three different configurations were identified and modeled for this study, using the same number of CFE’s and the same material regions, but altering the sizes of the CFE’s. These designs are summarized in Table 3.1. Design 1 is based on the parameters from Gates et al. [24] and Designs 2 and 3 are alterations from Design 1, with larger CFE’s.
Table 3.1 Alternative CFE Configurations

<table>
<thead>
<tr>
<th>CFE Design #</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inner radius of uranium annulus [cm]</td>
<td>3</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Outer radius of uranium annulus [cm]</td>
<td>4.5</td>
<td>5.5</td>
<td>5.5</td>
</tr>
<tr>
<td>Outer radius of containment wall (frit), [cm]</td>
<td>4.9</td>
<td>5.9</td>
<td>5.9</td>
</tr>
<tr>
<td>$V_{fuel}/L$ [Normalized to Design 1 Value]</td>
<td>1</td>
<td>1.89</td>
<td>1.27</td>
</tr>
<tr>
<td>Origin of Design</td>
<td>Gates et al. [24]</td>
<td>Derived from 1</td>
<td>Derived from 1</td>
</tr>
</tbody>
</table>

3.2. Basic Assumptions

The key simplifying assumption in this analysis is that the liquid uranium will be modeled as a solid with the thermophysical properties of the liquid at the local temperature. Simulating the uranium annulus as a solid allows the problem to be computationally tractable as a one-dimensional conduction problem. With this assumption, the momentum equation for the uranium or for the hydrogen is not included in the model. The hydrogen gas propellant is modeled as moving through the solid matrix and exchanging internal energy as it progresses from the outer wall to the free surface at the interior. The properties of each material are evaluated locally as functions of the appropriate thermodynamic variables. As such, the model for the uranium is that of a variable-property solid in an axisymmetric coordinate system with internal energy generation from nuclear decay and internal energy transport to the hydrogen.

3.3. Energy Balance

For each computational cell, there are two unknowns: the temperature of the solid uranium or the silicon carbide frit that makes up the computational cell, as well as the temperature of the hydrogen propellant passing through each computational cell.
Therefore, two equations are needed for each computational cell. The energy balance for the solid phase in each cell can be written as:

\[
\frac{d}{dt} \int_{V_c} \rho e dV + \int_{\partial V_c} \rho \vec{V}_{rel} \cdot d\vec{A} = Q_{\text{net in}} + W_{\text{net in shaft}}. \tag{3.1}
\]

Given that nuclear decay is a driving consideration in this work, we will split the unsteady (first) term into two terms: one for internal energy, \( u \), and one for the nuclear decay, \( \dot{E}_{gen} \). The enthalpy in the advective term is given the symbol \( i \), and there is no shaft work in the problem. The energy balance then becomes

\[
\frac{d}{dt} \int_{V_c} \rho u dV - \dot{E}_{gen} + \int_{\partial V_c} \rho i \vec{V}_{rel} \cdot d\vec{A} = Q_{\text{net in}}. \tag{3.2}
\]

We also assume each cell is in steady state so there is no time-dependent change in the internal energy in each cell, so that the first term is zero. Here, \( Q_{\text{net in}} \) represents the net heat transfer via conduction into a computational cell from adjacent computational cells, and the advection term accounts for the internal energy loss to the hydrogen propellant moving through each cell. The advection of energy out of a cell is determined by equating the enthalpy outflow from the cell due to gas flow to an expression of Newton’s Law of Cooling applied to the gas inside each cell:

\[
\int_{V_c} \rho i \vec{V}_{rel} \cdot d\vec{A} = m_{\text{cell}} (i_{\text{out}} - i_{\text{in}}) = h_{g,m} A_{\text{tot,m}} (T_m - T_{g,m}). \tag{3.3}
\]

and

\[
m_{\text{cell}} = \dot{m} \left( \frac{\Delta \theta}{2\pi} \right). \tag{3.4}
\]

Here, \( T_m \) is the temperature of the uranium in each cell, \( m \), \( T_{g,m} \) is the gas temperature in cell \( m \), of the propellant, \( h_{g,m} \) is the heat transfer coefficient of the
propellant, $A_{tot,m}$ is the total surface area of propellant in the computational cell (in the uranium fuel, this is the total surface area of bubbles; in the frit, this is the total surface area of the propellant channels in the cell).

If $(T_m - T_{g,m})$ is positive, the energy flow is out of the uranium (or the frit) and into the gas. The energy balance for a uranium or a frit cell is now:

$$h_{g,m}A_{tot,m}(T_m - T_{g,m}) = \dot{Q}_{cond} + \dot{E}_{gen}.$$  \hspace{1cm} (3.5)

Fourier’s law describes the conduction between cells as

$$\dot{Q}_{cond} = -kA \frac{\partial T}{\partial r}.$$  \hspace{1cm} (3.6)

which is approximated for cell $m$ by finite difference for variable conductivity and as

$$\dot{Q}_{cond} = -kA_{cell\ interface} \frac{(T_m - T_{m-1})}{\Delta r}, \text{ where } k = k(T_m).$$  \hspace{1cm} (3.7)

A first-law expression is needed for the gas flow as well. Equation 3.1 applied to the gas phase in each cell yields:

$$\frac{d}{dt} \int_{V_u} \rho udV + \int_{S_s} \rho \vec{V}_{rel} \cdot \vec{d} = \dot{Q}_{net}.$$  \hspace{1cm} (3.8)

The gas phase is in steady state in each cell, and the resulting balance of the advection and heat transfer terms can be written as

$$\bar{m}_{cell}c_{p,g,m}(T_{g,m} - T_{g,upstream}) = h_{g,m}A_{tot,m}(T_m - T_{g,m}),$$  \hspace{1cm} (3.9)

assuming the gas leaves with the gas temperature attained in cell $m$, $T_{g,m}$, and enters with the gas temperature of the upstream cell, $T_{g,upstream}$. The energy gain to the gas is a loss to the solid.
This solution uses a finite-difference method to arrange the equations as a matrix equation of the form $AT = C$, where $A$ is a $2M \times 2M$ array, and both $T$ and $C$ are $2M \times 1$ vectors where $M$ is the total number of computational cells. The index of the current cell is $m$, increasing in the positive radial direction from $m = 1$ at the innermost cell of the uranium fuel to $m = M$ at the outermost cell of the porous frit. The number of cells within the uranium fuel annulus only is given by $N$. The cells are shown in the diagram in Figure 3.2 below. Note that the cells are constructed such that the innermost and outermost cells are half cells with their nodes placed on the boundaries of the domain where a convective boundary condition exists. In the following equations, $R_m$ is used to denote the computational cell nodes, while $r_m$ is used to denote the interface between computational cells. The following example equations and diagram in Figure 3.2 are done for $M = 5$ cells.
Figure 3.2 Computational cells for Finite-Difference Analysis

For \( m = 1 \), the cell is a half-cell that borders the gas core of the engine. For this cell, there is conduction into one radial face and convection to the core gas at the other face. Eq. 3.5 becomes:

\[
h_{g,1}A_{tot,1}(T_1 - T_{g,1}) = h_i(R_i \Delta \theta L)(T_i - T_1) + k_1(r_1 \Delta \theta L) \left( \frac{(r_2 - r_1)}{\Delta R_L} \right) + \dot{Q}_{N,1} \tag{3.10} \]

where the distance between cell centers in the liquid uranium region is given as \( \Delta R_L \). This construction is used throughout the discretization of the domain in order to accommodate changes in element thickness when the system transitions to the frit used to form the outer containing wall. Based on Figure 3.2, the position of the first node is

\[
r_1 = R_i + \Delta r_1. \tag{3.11} \]
The volume of the first node is

\[ V_1 = \left( \frac{\Delta \theta}{2\pi} \right) \pi \left[ r_1^2 - r_i^2 \right] L = \left( \frac{\Delta \theta L}{2} \right) \left[ r_1^2 - r_i^2 \right] \quad (3.12) \]

The volumetric heating term due to nuclear decay is given as:

\[ \dot{Q}_{N,1} = V_1 \dot{q}_{N,1} , \quad (3.13) \]

where the generation rate per unit volume, \( \dot{q}_{N,1} \), local to the cell of interest is provided from a neutronics model developed by Dr. William Walters as part of the larger NASA project.

Rearranging terms to group parameters, Eq. 3.10 becomes:

\[ [\alpha_0 + \alpha_1 + \beta_1] T_1 - \alpha_1 T_2 - \beta_1 T_{g,1} = \alpha_0 T_i + \dot{q}_{N,1} V_1 \quad (3.14) \]

where

\[ \alpha_0 = h_i R_i \Delta \theta L \quad (3.15) \]

\[ \alpha_1 = k_1 \left( r_1 \Delta \theta L \right) \left( \frac{1}{\Delta R_L} \right) \quad (3.16) \]

\[ \beta_1 = h_{g,1} A_{tot,1} \quad (3.17) \]

For the energy balance in the gas phase, Eq. 3.9 becomes

\[ \dot{m} \left( \frac{\Delta \theta}{2\pi} \right) c_{p,g,1} (T_{g,1} - T_{g,2}) = h_{g,1} A_{tot,1} (T_i - T_{g,1}) . \quad (3.18) \]

This equation is rearranged to group parameters so that

\[ Y_1 \equiv \frac{2\pi h_{g,1} A_{tot,1}}{\Delta \theta m c_{p,g,1}} , \quad (3.19) \]

and Eq. 3.18 becomes
\[-\gamma_1 T_1 + (\gamma_1 + 1)T_{g,1} - T_{g,2} = 0 \quad (3.20)\]

For \( m = 2 \), the cell is in the interior of the fuel annulus. For interior cells, there is conduction into both radial faces. Eq. 3.5 becomes:

\[
h_{g,2}A_{tot,2}(T_2 - T_{g,2}) = k_1(r_1\Delta\theta L)\frac{(T_1 - T_2)}{\Delta R_L} + k_2(r_2\Delta\theta L)\frac{(T_3 - T_2)}{\Delta R_L} + \dot{Q}_{N,2} \quad (3.21)
\]

Based on Figure 3.2, the position of the second node is \( r_2 = r_1 + \Delta r_2 \), and the volume of the second node is

\[
V_2 = \left(\frac{\Delta \theta L}{2}\right) [r_2^2 - r_1^2]. \quad (3.22)
\]

The volumetric heating term due to nuclear decay is given as in Eq. 3.13. Rearranging terms to group parameters, Eq. 3.21 becomes:

\[-\alpha_1 T_1 + [\alpha_1 + \alpha_2 + \beta_2]T_2 - \alpha_2 T_3 - \beta_2 T_{g,2} = \dot{Q}_{N,2}V_2 \quad (3.23)\]

where

\[
\alpha_2 = \frac{k_2(r_2\Delta\theta L)}{\Delta R_L} \quad (3.24)
\]

\[
\beta_2 = h_{g,2}A_{tot,2} \quad (3.25)
\]

For the energy balance in the gas phase, Eq. 3.9 becomes

\[
\dot{m}\left(\frac{\Delta \theta}{2\pi}\right)c_{p,g,2}(T_{g,2} - T_{g,3}) = h_{g,2}A_{tot,2}(T_2 - T_{g,2}) \quad (3.26)
\]

This equation is rearranged to group parameters so that it becomes

\[-\gamma_2 T_2 + (\gamma_2 + 1)T_{g,2} - T_{g,3} = 0, \quad (3.27)\]

where \( \gamma_2 \) is defined as in Eq. 3.19 but for cell 2.
The procedure for \( m = 3 \), as another interior cell in the fuel annulus, follows the same approach. For \( m = 4 \), the cell is in the interior of the porous frit. The only two differences between the procedure for these cells and the interior cells of the fuel annulus, are that the convective heat transfer to the propellant occurs across the flow channel surface area, instead of the bubble surfaces; and that there is no nuclear heat generation term in the porous frit. Equation 3.5 becomes

\[
h_{g,4} A_{tot,4} (T_4 - T_{g,4}) = k_3 (r_3 \Delta \theta L) \frac{(T_3 - T_4)}{(\Delta R_L + \Delta R_s)} + k_4 (r_4 \Delta \theta L) \frac{(T_5 - T_4)}{\Delta R_s}
\]

where the distance between cell centers in the solid frit region is given as \( \Delta R_s \). The distance between the nodes of the last liquid cell and the adjacent solid cell is therefore the average of \( \Delta R_L \) and \( \Delta R_s \). Based on Figure 3.2, the position of the fourth node is \( r_4 = r_3 + \Delta r_4 \).

Rearranging terms to group parameters, Eq. 3.28 becomes:

\[
-a_3 T_3 + [a_3 + a_4 + \beta_4] T_4 - a_4 T_5 - \beta_4 T_{g,4} = 0
\]

where

\[
a_3 = k_3 (r_3 \Delta \theta L) \frac{2}{\Delta R_L + \Delta R_s},
\]

\[
a_4 = \frac{k_4 (r_4 \Delta \theta L)}{\Delta R_s},
\]

\[
\beta_4 = h_{g,4} A_{tot,4}.
\]

For the energy balance in the gas phase, Eq. 3.9 becomes

\[
\dot{m} \left( \frac{\Delta \theta}{2\pi} \right) c_{p,4} (T_{g,4} - T_{g,5}) = h_{g,4} A_{tot,4} (T_4 - T_{g,4})
\]

(3.33)
This equation is rearranged to group parameters so that

\[ \gamma_4 = \frac{2\pi h_{g,4} r_{c,4} A_{g,4}}{\Delta \theta \dot{m}_{c,4}} \tag{3.34} \]

and Eq. 3.33 becomes

\[ -\gamma_4 T_4 + (\gamma_4 + 1)T_{g,4} - T_{g,5} = 0. \tag{3.35} \]

For \( m = 5 \), the cell is in the outermost section of the porous frit. Here, there is conduction on the interior cell face and a convective condition on the exterior cell face. Once again, there is no nuclear heat generation term. Equation 3.5 becomes

\[ h_{g,5}A_{tot,5}(T_5 - T_{g,5}) = k_4 (r_4 \Delta \theta L) \frac{(T_4 - T_5)}{\Delta R_4} + h_{g,\infty} (R_\theta \Delta \theta L)(T_\infty - T_5) \tag{3.36} \]

Based on Figure 3.2, the position of the fifth node is \( r_5 = r_4 + \Delta r_5 \). Rearranging terms to group parameters, Eq. 3.36 becomes:

\[ -\alpha_4 T_4 + [\alpha_4 + \alpha_5 + \beta_5]T_5 - \beta_5 T_{g,5} = \alpha_5 T_\infty \tag{3.37} \]

where

\[ \alpha_5 = h_{\infty} (R_\theta \Delta \theta L), \tag{3.38} \]

\[ \beta_5 = h_{g,5}A_{tot,5}. \tag{3.39} \]

For the energy balance in the gas phase, Eq. 3.9 becomes

\[ \dot{m} \left( \frac{\Delta \theta}{2\pi} \right) c_{p,g,5}(T_{g,5} - T_{entry}) = h_{g,5}A_{tot,5}(T_5 - T_{g,5}). \tag{3.40} \]

This equation is rearranged to group parameters with \( \gamma_5 \) of the same form as \( \gamma_4 \). Equation 3.40 becomes

\[ -\gamma_5 T_5 + (\gamma_5 + 1)T_{g,5} = T_\infty. \tag{3.41} \]
An example matrix for $M = 5$ is assembled as $AT = C$, where

$$A = $$

$$
\begin{pmatrix}
\alpha_0 + \alpha_1 + \beta_1 & -\alpha_1 & 0 & 0 & 0 & -\beta_1 & 0 & 0 & 0 & 0 \\
-\alpha_1 & \alpha_1 + \alpha_2 + \beta_2 & -\alpha_2 & 0 & 0 & 0 & -\beta_2 & 0 & 0 & 0 \\
0 & -\alpha_2 & \alpha_2 + \alpha_3 + \beta_3 & -\alpha_3 & 0 & 0 & 0 & -\beta_3 & 0 & 0 \\
0 & 0 & -\alpha_3 & \alpha_3 + \alpha_4 + \beta_4 & -\alpha_4 & 0 & 0 & 0 & -\beta_4 & 0 \\
0 & 0 & 0 & -\alpha_4 & \alpha_4 + \alpha_5 + \beta_5 & 0 & 0 & 0 & 0 & -\beta_5 \\
0 & 0 & 0 & 0 & 0 & \gamma_1 + 1 & -1 & 0 & 0 & 0 \\
0 & -\gamma_1 & 0 & 0 & 0 & 0 & \gamma_2 + 1 & -1 & 0 & 0 \\
0 & 0 & -\gamma_2 & 0 & 0 & 0 & 0 & \gamma_3 + 1 & -1 & 0 \\
0 & 0 & 0 & -\gamma_3 & 0 & 0 & 0 & 0 & \gamma_4 + 1 & -1 \\
0 & 0 & 0 & 0 & -\gamma_4 & 0 & 0 & 0 & 0 & \gamma_5 + 1 \\
\end{pmatrix}
$$

(3.42)

$$T = \begin{pmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_{g,1} \\ T_{g,2} \\ T_{g,3} \\ T_{g,4} \\ T_{g,5} \end{pmatrix},$$

(3.43)

and

$$C = \begin{pmatrix} \alpha_0 T_1 + \dot{q}_{N,1} V_1 \\ \dot{q}_{N,2} V_2 \\ \dot{q}_{N,3} V_3 \\ 0 \\ \alpha_5 T_\infty \\ 0 \\ 0 \\ 0 \\ 0 \\ T_{entry} \end{pmatrix}.$$  

(3.44)
From the above analysis, it is obvious that there are a number of parameters which must be determined in order to accurately find the temperature distribution throughout the uranium layer. These include:

- Uranium properties:
  - Density
  - Dynamic viscosity
  - Surface tension
  - Thermal conductivity

- Silicon carbide properties:
  - Thermal conductivity

- Hydrogen properties:
  - Density
  - Specific heat capacity
  - Dynamic viscosity
  - Thermal conductivity

- Nuclear heat generation

- Heat transfer coefficients:
  - Between bubbles and liquid fuel
  - Between porous frit and propellant passing through channels
  - Between outer wall of porous frit and propellant gas in clearance gap

- Bubble surface area

Additionally, a calculation of the pressure at each computational cell is required in order to determine the properties of the propellant listed above.
3.4. Pressure in Molten Uranium

The local pressure in the liquid uranium layer has a significant impact on the properties of the hydrogen as it bubbles through the uranium. A core pressure, \( p_0 \), was defined for the gas-filled central region of the cylinder and a differential equation was derived for the pressure as a function of radius in the liquid annulus. A differential element of thickness \( dr \) in the annulus (similar to one of the finite cells shown in Figure 3.2) contributes a body force \( dF \) due to the centrifugal acceleration of the spinning medium. For a liquid medium with a variable gas void fraction \( X \), and spinning at an angular velocity, \( \omega \), the force contributed by a differential annular element at radial distance, \( r \), is:

\[
dF = (1 - X)(\rho_l dV)(r\omega^2) = (1 - X)\rho_l(2\pi Lrd)(r\omega^2). \quad (3.45)
\]

The differential pressure arising from this force is:

\[
dp = dF/\!\!\!dA = dF/2\pi rL , \quad (3.46)
\]

so that

\[
dp = (1 - X)\rho_l\omega^2rdr. \quad (3.47)
\]

Integrating, we have:

\[
\int_{p_0}^{p_m} dp = \int_{R_i}^{R_m} (1 - X)\rho_l\omega^2rdr . \quad (3.48)
\]

In general, both \( \rho_l \) and \( X \) are functions of \( r \). To obtain a simple closed-form solution for the pressure at radial position \( R_m \), we can imagine a medium where both values are uniform so that Eq. 3.48 yields:

\[
p_m - p_0 = \frac{1}{2} (1 - X)\rho_l\omega^2(R_m^2 - R_i^2) \quad (3.49)
\]
To include the variability of $\rho_l$ and $X$ with $r$, a numerical integration is required. Here, the trapezoid rule gives:

$$p_m - p_0 \approx \sum_{i=2}^{m} \frac{z_i + z_{i-1}}{2} \Delta r,$$  \hspace{1cm} (3.50)

where

$$z_i = (1 - X_i)\rho_{l,i} \omega^2 R_i$$  \hspace{1cm} (3.51)

and the cell counter, $m$, is limited to those cells in the liquid annulus as opposed to the frit. Note that for $m = 1$ the node lies on the inner surface of the annulus where $p_1 = p_0$. For this reason, the summation must begin at $m = 2$, the first node entirely within the annulus.

In order to verify the above numerical formulation, it is helpful to compare the results to those obtained in a simpler case with exact formulas. The sample calculation is performed for the pressure in a CFE with a 3 cm inner radius and 4.5 cm outer radius. For simplification, the void fraction is assumed to be zero throughout the uranium layer, and the uranium density is treated as a constant with the value at melting point of 17,320 kg/m$^3$ [49]. This is the uniform-property case described by Eq. 3.49. Assuming a rotation speed of 7000 rpm and a core pressure of 10,000 kPa, the exact value of pressure at the outer radius of the uranium annulus is then:

$$p = p_0 + \frac{1}{2} \rho_l \omega^2 (R_o^2 - R_i^2) = 10\,000 \text{ kPa} + \frac{1}{2} \left( 17320 \frac{kg}{m^3} \right) \times \left( \frac{7000 \text{ Rot}}{\text{min}} \times \frac{2\pi \text{ rad}}{\text{Rot}} \times \frac{1 \text{ min}}{60 \text{ s}} \right)^2 \left[ (0.045 \text{ m})^2 - (0.03 \text{ m})^2 \right] \times \frac{1 \text{ kPa}}{1000 \text{ Pa}} = 15\,235 \text{ kPa}$$  \hspace{1cm} (3.52)
The solution from the numerical formulation can then be calculated. Note that since for all computational cells the void fraction is zero and the liquid density is constant:

\[ z_m = \rho_l \omega^2 R_m. \]  \hspace{1cm} (3.53)

Then Eq. 3.50 becomes:

\[ p_m \approx p_0 + \rho_l \omega^2 \Delta r \sum_{i=2}^{l=m} \frac{R_{i-1}+R_i}{2}. \]  \hspace{1cm} (3.54)

For an example of 100 cells across the 15 mm uranium annulus, \( \Delta r = \frac{15 \text{ mm}}{100-1} = 0.1515 \text{ mm} \), and the value of \( p_N \) at the last node in the annulus, \( R_N \), is 15,325 kPa.

However, if a varying void fraction is introduced, the difference between the two methods become obvious. For the same parameters, but now with a void fraction that varies linearly from 0.4 at the inner radius to 0.1 at the outer radius, the numerical solution is recalculated. Note that \( z \) is now given by Eq. 3.51. Then Eq. 3.50 produces a value of \( p_N \) of 13,979 kPa.

In a similar vein, we now introduce a variable density that varies linearly from 11,700 kg/m\(^3\) (uranium density at \( T = 5000 \text{ K} \)) at the inner radius to 17,320 kg/m\(^3\) (density at \( T = 1405 \text{ K} \)) at the outer radius. Eqs. 3.50 and 3.51 now produce a value of \( p_N \) of 13,418 kPa for a 100-cell annulus.

The pressure distributions across the entire uranium annulus for both the closed-form solution to the first example of uniform material properties and for the last example where both \( \rho_l \) and \( X \) are variable are compared in Figure 3.3.
Figure 3.3 Example Pressure Distributions in the Molten Uranium Annulus

Figure 3.3 illustrates the large reduction in pressure drop produced by the expected variations in liquid density with temperature and void fraction across the annulus. This reduction is the result of less liquid material required to fill the annulus in the presence of a significant gas volume and a lower average liquid density. It is therefore important to iterate the solution to the problem so that the local computed liquid temperature and the computed void fraction can properly affect the local pressure.

While the above equations give a method for determining \( p \), the hydrostatic pressure in the liquid fuel, the actual pressure of the propellant within the bubbles will be slightly larger. This is due to the pressure drop across a bubble interface due to surface tension, and is given by the Young-Laplace equation for a cell \( m \):

\[
\Delta p = \frac{2 \gamma}{r}
\]
\[ p_{g,m} = p_{l,m} + \frac{2\sigma_m}{a_m}. \]  \hspace{1cm} (3.55)

Where \( \sigma_m \) is the surface tension at cell \( m \) and \( a_m \) is the equivalent bubble radius at cell \( m \). Using typical values of \( \sigma_m \) and \( a_m \) gives a typical pressure difference of roughly:

\[ p_{g,m} - p_{l,m} = \frac{2\sigma_m}{a_m} = \frac{2(1.42 \text{ N/m})}{0.0004 \text{ m}} = 7.1 \text{ kPa}, \]  \hspace{1cm} (3.56)

which, relative to the total pressure of the fuel annulus, is not a significant difference. However, this calculation will still be used in this model to calculate the actual pressure of the gaseous propellant based on the local liquid pressure.

It should also be noted here that in the model created in this work, the core pressure \( p_0 \) is defined as an input to the model for simplicity. In reality however, the pressure in the core will be equal to the pressure generated by the propellant turbopump system minus any losses in pressure from the exit of the pumps to the point that the propellant bubbles reach the core of a CFE. In other words, from the example above for a core pressure of 10 MPa, the turbopump would have to produce a pressure equal to the gas pressure of the bubbles at the CFE at the wall (roughly 14 MPa), plus the pressure drop from friction losses and turbine expansion at all points upstream of the CFE injectors.

3.5. Material Properties

Property tables of the materials in the reactor, particularly the metallic uranium fuel, silicon carbide porous frit, and hydrogen propellant were located and incorporated into the model. These properties include the density and dynamic viscosity of uranium and hydrogen, specific heat capacity of hydrogen, and the thermal conductivity of uranium and
silicon carbide. For the most part, properties are tabulated as functions of temperature and/or pressure.

Identification of property data at the high operating temperatures of the reactor was somewhat of a challenge. For uranium, it was difficult to find properties throughout the range of temperatures considered in the study. Kirillov reports correlations of thermophysical properties for a large number of materials used in nuclear engineering, including properties of molten uranium [49]. However, these values are not provided for the complete temperature range under consideration. In cases where the properties are not available for the entire temperature range, the properties are assumed to be constant beyond the highest temperature available instead of extrapolating (with the exception of the hydrogen viscosity and thermal conductivity correlations, which are extrapolated beyond the given temperature of 3500 $K$). The following data reported in Table 3.2 was reported by Belashchenko et al., and provides density data for uranium in a much wider temperature range [50].

<table>
<thead>
<tr>
<th>$T$ [K]</th>
<th>1406</th>
<th>1500</th>
<th>2000</th>
<th>2500</th>
<th>3000</th>
<th>3500</th>
<th>4000</th>
<th>4500</th>
<th>5000</th>
<th>6000</th>
<th>7000</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho_t$ [kg/m$^3$]</td>
<td>17226</td>
<td>17060</td>
<td>16180</td>
<td>15330</td>
<td>14530</td>
<td>13760</td>
<td>13030</td>
<td>12300</td>
<td>11700</td>
<td>10400</td>
<td>9200</td>
</tr>
</tbody>
</table>

A linear fit can be applied to the data in Table 3.2, which yields:

$$\rho_t \ [kg/m^3] = 19022 - 1.4486T$$ (3.57)
with $R^2 = 0.9949$. The dynamic viscosity was also reported by Kirillov from 1405 $K$ to 2973 $K$ [49]:

$$ln \mu_t = -5.9307 + 0.6557ln T + \frac{4134}{T}$$

(3.58)

where $\mu$ is in $mPa \cdot s$ and $T$ is in $K$.

The surface tension was reported by Kirillov from 1405 $K$ to 2100 $K$ as [49]:

$$\sigma [N/m] = 2.1275 - 3.365 \times 10^{-4}T$$

(3.59)

with an uncertainty of $\pm 0.05 \ N/m$. The thermal conductivity of molten uranium is reported in Kirillov [49] as 13.7 $W/mK$ at the melting point of uranium, approximately 1405 $K$. Unfortunately, data was not available for conductivity at higher temperatures, so this value was treated as constant. However, other studies have found that the electrical resistivity of molten uranium increases with increasing temperature [51–53], meaning that the electrical conductivity decreases with temperature. Since the thermal conductivity of metals is primarily proportional to the electrical conductivity via the Wiedemann-Franz law [54], it is expected that the thermal conductivity of molten uranium will decrease with temperature. Therefore, the assumption of a constant thermal conductivity beyond the melting point should be conservative. However, when considering conduction throughout the fuel region, it should be noted that the significant void fractions will serve to reduce heat transfer and insulate the fuel regions with high void fractions. It was decided that the best way to account for this effect was to reduce the effective thermal conductivity at each cell by the local void fraction. Therefore, this effective thermal conductivity for a given cell is:
\[ k_{l, \text{eff}, m} = k_l(1 - X_m), \]  \hspace{1cm} (3.60)

where \( k_l \) is the nominal thermal conductivity of the molten uranium, 13.7 \( W/mK \) in this case.

The thermal conductivity of silicon carbide, as well as other properties, appears to be highly dependent on processing technique and polymorph structure. Liu and Lin [55] report measured thermal conductivities for a selection of different polymorphs of silicon carbide, and a representative sample, composed of 5\% (by volume) 3C, 87.3\% 6H, and 7.7\% 4H, with a porosity of 1–1.3\%, and with grain sizes in the range of 1–3 \( \mu m \), has the following thermal conductivity at different temperatures (estimated based off of chart provided) in Table 3.3:

<table>
<thead>
<tr>
<th>( T ) [K]</th>
<th>297.3</th>
<th>369.75</th>
<th>469.8</th>
<th>569.85</th>
<th>669.9</th>
<th>769.95</th>
<th>866.5</th>
<th>970.05</th>
<th>1070.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k_s ) [W/mK]</td>
<td>85.5</td>
<td>81.0</td>
<td>71.6</td>
<td>64.9</td>
<td>60.1</td>
<td>50.6</td>
<td>49.5</td>
<td>45.6</td>
<td>43.1</td>
</tr>
</tbody>
</table>

Performing a 2\textsuperscript{nd} order polynomial fit of the above data gives, for 300 to 1070 \( K \):

\[ k_s \ [W/mK] = 5 \times 10^{-5}T^2 - 0.12T + 117.93, \]  \hspace{1cm} (3.61)

with \( T \) in \( K \) and with \( R^2 = 0.9939 \). For frit temperatures above 1070 \( K \) the thermal conductivity is evaluated at 43.1 \( W/mK \). Although notconsidered in this study, it is known that neutron irradiation can have a significant impact on the thermal conductivity.
of silicon carbide. This effect, including a number of additional studies on silicon carbide properties, are summarized in Snead et al. [56].

For zirconium carbide, Katoh et al. [57] summarize various studies of thermophysical properties. As for silicon carbide, the thermal conductivity is dependent on processing techniques as well as impurities and the stoichiometric ratio of carbon to zirconium. However, as a rough approximation, Katoh et al. [57] reports a value from Grossman [58] of 26 W/mK at approximately 1500 K. Although the conductivity does increase with temperature, because the zirconium carbide region is so small and has a target temperature of 1500 K this value will be used as a constant.

For hydrogen, the density was found from tabulated values reported by Patch [59] (using spin-equilibrated hydrogen) as a function of temperature and pressure. A subfunction was written as part of the current model which will interpolate between both temperature and pressure from this data to find the density. Patch’s work also reports the specific heat capacity of hydrogen for various temperatures and pressures, and a comparable subfunction with the same interpolation approach is used to determine specific heat capacities of hydrogen in the model.

A note needs to be made about the specific heat of hydrogen at the temperatures under consideration in this study. The study by Patch showed that the specific heat displays two “spikes” in magnitude as the temperature is increased. This effect can be seen in Figure 3.4. The first spike seems to be in the vicinity of high levels of hydrogen dissociation, and the second spike is in the vicinity of high levels of hydrogen ionization. At the temperatures and pressures under consideration in this study, the first spike must be considered but the second is beyond the conditions in this study.
The specific heat capacity results can depend on the source used as they are all the results of property model computations as opposed to laboratory measurements. For this reason, care must be taken when selecting a source for property data. For example, the fluid property package “CoolProp” [60] yields significantly lower specific heat capacities for normal hydrogen above 2500 K compared to Patch. The specific heat capacity from CoolProp at 100 atm from 1000 K to 10,000 K is compared to the data from Patch at 30, 100, and 300 atm in Figure 3.5. The CoolProp data does not display the spike in specific heat that the data from Patch does from about 2500 K onwards. CoolProp states the limit for the intended use of their values to be 1000 K, however, and the values given by their website appear to be extrapolated beyond this point. Meanwhile, the data from Kubin and Presley [61], which is also plotted in Figure 3.5 for 100 atm, seems to agree fairly well with the data from Patch although the spike in specific heat is slightly offset by comparison.
Figure 3.4 Constant-Pressure Specific Heat Capacity from Patch [59]
Charmeau reports the dynamic viscosity and thermal conductivity of hydrogen [62]. The dynamic viscosity for pressures above 1 \( MPa \) and temperatures from 200 to 3500 \( K \) is:

\[
\mu_g \ [Pa \cdot s] = -1.44 \times 10^{-12}T^2 + 1.69 \times 10^{-8}T + 4.64 \times 10^{-6} \quad (3.62)
\]

The thermal conductivity is given for temperatures below 2000 \( K \) as:

\[
k_g \ [W/mK] = 3.54 \times 10^{-4}T + 9.13 \times 10^{-2} \quad (3.63)
\]

For temperatures above 2000 \( K \), the conductivity is pressure and temperature dependent.

For temperatures between 2000 \( K \) and 3500 \( K \),
\[ k_g \ [W/mK] = a_1 T^2 + a_2 T + a_3 \]  
(3.64)

where

\[ a_1 \ [W/mK^3] = 2.43 \times 10^{-21} p_g^2 - 9.28 \times 10^{-14} p_g + 1.46 \times 10^{-6}, \]  
(3.65)

\[ a_2 \ [W/mK^2] = -1.04 \times 10^{-17} p_g^2 + 3.98 \times 10^{-10} p_g - 5.87 \times 10^{-3}, \]  
(3.66)

\[ a_3 \ [W/mK] = 1.11 \times 10^{-14} p_g^2 - 4.24 \times 10^{-7} p_g + 6.72. \]  
(3.67)

Note that \( p_g \) is given in \( Pa \) for Eqs. 3.65–3.67.

3.6. Nuclear Heat Deposition

The heat deposition from the nuclear fission processes has been modeled by Dr. William Walters [63,64] at the Pennsylvania State University, a collaborator in the larger research project which supports this effort. For the purposes of neutronics calculations, this model uses the materials defined in the baseline configuration from Gates et al. [24], with slight variations of the dimensions for the alternative designs mentioned in Table 3.1. The baseline design dimensions and materials are given in Tables 3.4 and 3.5.
The model was created in OpenMC, an open-source Monte Carlo software [65], and uses continuous energy neutron cross-sections while simulating thousands of particle histories. This computation was performed over 50 computational cells, and the power generated at each computational cell was tallied and normalized to a 10 MW total CFE power level. This normalized power level is accounted for in the curve fits as in Eq. 3.68.
For each design from Table 3.1, these calculations were performed for each individual CFE in the 19-CFE configuration. For reference, the CFE’s are numbered based upon their location in the cluster, as in Figure 3.6. However, the heat deposition as a function of radius follows the same general trend for all CFE’s in a reactor. For example, Figure 3.7 shows the power generation data for CFE 1 (on the outer ring of fuel elements), CFE 5 (on the inner ring), and CFE 10 (the center fuel element) for Design 1. While CFE’s 5 and 10 are almost identical, CFE 1 is skewed towards more power generation at the outer radius. Because this scenario represents the greater challenge in terms of maintaining appropriate temperatures at the wall, CFE 1 is the CFE chosen for investigation in this thermal model.

Figure 3.6 Numbering of CFE’s for Neutronics Model
A 5th-order polynomial fit was applied to the nuclear energy deposition data as a function of radial position and is reported in generic form in Eq. 3.68 below, where $r$ is the radial position measured in cm, $\hat{Q}_{gen}$ is the total power level of the CFE in MW, and $\hat{q}_N$ is the volumetric heating term from the nuclear fission process measured in $W/m^3$. Table 3.6 reports the coefficients for the curve fits in different designs. Note that the leading fraction in Eq. 3.68 is necessary to adjust for the fact that the CFE power level assumed for a given simulation may be different from the 10 MW total power assumed in the neutronics calculations. If the CFE is operated at the 10 MW power level, the fraction goes to unity.
\[ \hat{q}_N = \frac{\hat{q}_{gen}}{10} (c_5 r^5 + c_4 r^4 + c_3 r^3 + c_2 r^2 + c_1 r + c_0). \]  

(3.68)

<table>
<thead>
<tr>
<th>Design #</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>(c_5)</td>
<td>8,370.894</td>
<td>572.882</td>
<td>6,023.773</td>
</tr>
<tr>
<td>(c_4)</td>
<td>–150,353.35</td>
<td>–11,396.66</td>
<td>–137,714.26</td>
</tr>
<tr>
<td>(c_3)</td>
<td>1,077,768.92</td>
<td>90,193.75</td>
<td>1,257,534.56</td>
</tr>
<tr>
<td>(c_2)</td>
<td>–3,852,036.55</td>
<td>–354,512.14</td>
<td>–5,731,600.85</td>
</tr>
<tr>
<td>(c_1)</td>
<td>6,862,317.23</td>
<td>691,570.65</td>
<td>13,036,404.19</td>
</tr>
<tr>
<td>(c_0)</td>
<td>–4,871,942</td>
<td>–534,556</td>
<td>–11,834,090</td>
</tr>
</tbody>
</table>

Table 3.6 Nuclear Heat Deposition Curve Fit Coefficients

However, the neutronics model from which the curve fit is derived was created assuming a uniform void fraction, with the value for each design given in Table 3.1. It was later determined that, far from being a constant value, the void fraction increases approximately linearly from the outermost cells to the innermost cells. This is primarily due to the effect of constricting geometry as the radius decreases, as well as the expansion of the propellant with increasing temperature. This necessitated adjusting the power production at each cell by the local void fraction, multiplying it by the term \( \frac{(1-X_m)}{0.5} \), where \( X_m \) is the local void fraction. Doing this, however, changes the total power level; therefore, another constant, \( F_N \), must be added to the formula to normalize the total power to the desired level. Since \( F_N \) depends on the void fraction distribution, which emerges from the model, the exact value cannot be predicted. Instead, \( F_N \) is recalculated/adjusted for each
model iteration, $j$. The value at a given iteration is designated, then, as $F_{N,j}$, and defined as:

$$F_{N,j} = \frac{\Delta \theta}{2\pi} \left[ \sum_{m=1}^{N} (v_m d_{N,m}) \right]_{j-1} F_{N,j-1}.$$  

(3.69)

The actual volumetric energy generation then is:

$$\dot{q}_N = F_{N,j} \frac{Q_{gen}}{10} \left( \frac{1 - x_m}{0.5} \right) \left( c_5 r^5 + c_4 r^4 + c_3 r^3 + c_2 r^2 + c_1 r + c_0 \right).$$  

(3.70)

3.7. Bubble Injection

In order to estimate the volume and surface area of the bubbles in each computational cell in the annulus, it is necessary to calculate the size of the bubbles upon injection into the liquid uranium. The volume of a bubble at injection is found by modeling the formation of a bubble at an orifice with constant flow. Different injection models exist, and for the present work a two-step model derived by Ruff [66] was selected. In this model, the bubble sits at the orifice as it grows until the lifting forces on the bubble exceed the restraining forces. A schematic of the bubble growth process is shown in Figure 3.8.

Ruff’s model divides bubble growth into two sections. The first section, represented by Figure 3.8 (A), models the initial bubble growth as the bubble first develops and continues to grow while still held in place at the surface of the orifice. Eventually the bubble will have grown large enough that the lifting forces are in equilibrium with the restraining forces at the volume $V_e$. Beyond this point, the lifting forces overcome the restraining forces acting on the bubble, causing the bubble to rise as in Figure 3.8 (B). However, at this stage the bubble is still connected to the orifice with a “neck” which allows the bubble to continue to grow due to the incoming gas flow rate. Once the bubble has
lifted a certain distance from the orifice plate, assumed in the Ruff model to be equal to the radius of the bubble at the end of stage (A), the bubble will completely separate from the orifice at which time another bubble begins to form, as in Figure 3.8 (C). The increase in volume during stage (B) is defined as \( \Delta V \). Therefore, the volume of each bubble when it is released from the orifice, \( V_{B,N} \), is defined as:

\[
V_{B,N} = V_e + \Delta V .
\]  

(3.71)

Figure 3.8 Bubble Growth While Attached to Orifice

The actual derivation of Ruff’s model is quite complex, and the complete details can be found in [66]. However, the model is summarized by Hsu et al. [67]. The equation for the bubble equilibrium volume \( V_e \) at the end of stage (A) is:
\[ V_e^{5/3} = 0.05773 \frac{Q^2}{g} + 2.418 \left( \frac{\mu_l}{\rho_{lg}} \right) Q V_e^{1/3} + \left( \frac{\pi d_c g}{\rho_{lg}} \right) V_e^{2/3} + 0.2041 \left( \frac{\mu_l}{\rho_{lg}} \right)^{1/2} \frac{Q^{3/2} V_e^{1/6}}{g}. \] 

(3.72)

Equation 3.72 can be solved iteratively to find \( V_e \) and the Newton-Raphson method was used in this work. Note that the gas flow rate, \( Q \), is defined per channel using the mass flow rate in a single channel and the gas density at the injection cell where \( m = N \) such that:

\[ Q = \frac{m}{n_c \rho_{lg} N}. \] 

(3.73)

Also, \( g \) is defined as the local centripetal acceleration at the orifice (the radial position \( r_s \)):

\[ g = r_s \omega^2. \] 

(3.74)

Next, \( \Delta V \) is defined by

\[ \Delta V = Q t_d, \] 

where \( t_d \) is the amount of time that the bubble is in the detachment phase, \( i.e., \) stage (B), from Figure 3.8. This time can be found from:

\[ t_d = \left( \frac{Q^{1/5}}{g^{3/5}} \right) \left[ 1 + 4 \left( \frac{\mu_l}{\rho_{lg}^{1/5} Q^{3/5}} \right)^{3/4} \right]. \] 

(3.76)

After a bubble is injected into the uranium, we then assume the mass of each bubble remains constant while it traverses the fuel annulus. This assumption may not be accurate if the bubbles undergo any breakup during the traversal through the uranium layer, or if uranium evaporates into, or is entrained in, the bubbles. While these phenomena are not
components of this model, future studies may be required to investigate them as part of an expansion of this model (see Chapter 5). The mass of a bubble is found by:

\[ m_B = V_{B,N} \rho_{g,N}. \]  

(3.77)

As the bubble passes through the fuel annulus it expands, and the volume (and from that the equivalent radius) at each point after injection is found by dividing the mass of the bubble by the local gas density:

\[ V_{B,m} = \frac{m_B}{\rho_{g,m}}. \]  

(3.78)

The equivalent radius of a bubble, \( a \), is then defined as

\[ a \equiv \left( \frac{3V_B}{4\pi} \right)^{1/3}. \]  

(3.79)

For typical design values the Ruff bubble injection model will yield, from Eqs. 3.71 and 3.79, an equivalent bubble radius on the order of about 0.3 \( mm \) immediately after injection. These small bubble sizes seem to be due in part to the very high buoyant forces on the bubbles caused by the high cylinder revolution rate, as using a value of \( g = 9.81 \ m/s^2 \) (gravitational acceleration on Earth) in the Ruff model will yield an equivalent radius an order of magnitude larger. As will be shown in the following discussions, small bubble sizes will yield a greater total bubble surface area and larger heat transfer coefficients, both of which will significantly increase the ability of the bubbles to extract heat from the uranium liquid.
3.8. Bubble Surface Area

Next, we come to the total surface area of bubbles in a computational cell. A diagram showing two computational cells with bubbles passing through is shown in Figure 3.9.

![Figure 3.9 Bubbles Passing Through Computational Cells within the Fuel Annulus](image)

At this point in the development, we must make assumptions about the morphology of the bubbles as this will allow us to evaluate variables such as surface area and rise velocity. In keeping with the approach used by the past research from Princeton [17,19], we adopt the assumption that (1) once the bubbles detach they quickly evolve into cap-shaped bubbles, and (2) thereafter, the bubbles travel at the terminal velocity computed for a cap-shaped bubble exposed to the local environment at a given radius. The assumption
of spherical cap bubbles is useful because the velocity for these bubbles is generally independent of the local liquid properties [68].

It was previously stated that, using Figure 2.16, it is possible to predict the bubble morphology based on a combination of two of the Reynolds number, Morton number, and Eötvös number (also referred to as the Bond number). These are defined for a bubble, in respective order, as:

\[ Re_B = \frac{u_B d_B}{v_g}, \]  

(3.80)

\[ M = \frac{g \mu_B (\rho_l - \rho_g)}{\rho_l^2 \sigma^3}, \]  

(3.81)

\[ Eo = \frac{g (\rho_l - \rho_g) d_B^2}{\sigma}. \]  

(3.82)

Since the Reynolds number depends on the velocity of the bubble, which is dependent on the bubble morphology, the Morton and Eotvos numbers will be used to approximate the morphology that the bubbles in a CNTR occupy. These numbers are recorded for the optimized run for Design 1, with run parameters recorded in Table 4.1. From this run, \( \log M \) varies from approximately −9.7 at bubble injection to −11.2 at the inner fuel surface, while \( Eo \) varies from 40.4 to 68.7 in the same region. Based on Figure 2.16, this should put the bubbles in the spherical cap regime and the assumption of spherical cap geometry appears to be justified.

The terminal velocity of a cap-shape bubble has previously been shown in the classic work by Davies and Taylor [18] to be:

\[ u = \frac{2}{3} \sqrt{r_B g}. \]  

(3.83)
Where \( g \) is the centripetal acceleration, and \( r_B \) is the radius of curvature of the spherical cup bubble, which is related to the equivalent spherical radius of the bubble by [19]:

\[
r_B = 2.179a.
\] (3.84)

Therefore, the terminal velocity can be rewritten:

\[
u = \frac{2}{3} \sqrt{(2.179a)(R\omega^2)} = 0.984\omega\sqrt{aR}.
\] (3.85)

The total bubble surface area within a cell is equal to the number of bubbles in the cell, multiplied by the surface area of each individual bubble:

\[A_{tot,m} = n_{B,m}A_{B,m}.
\] (3.86)

The surface area for a spherical cap bubble is [69]:

\[A_{B,m} = 20.728a^2.
\] (3.87)

The number of bubbles in a given computational cell can be estimated by the following means. First, the mass flow rate through an individual cell can be converted into the volume flow rate of propellant through a cell by dividing it by the density of the propellant at that point. Next, this volume flow rate can be divided by the volume of an individual bubble in that cell, given from Eq. 3.78, to calculate the number of bubbles per second passing through a cell. Finally, this value is multiplied by the amount of time it takes a single bubble to traverse a cell, which is equal to the radial length of the current computational cell divided by the bubble velocity at that cell. The resulting expression is shown in Eq. 3.88.

\[
n_{B,m} = \dot{m}\left(\frac{\Delta\theta}{2\pi}\right)\left(\frac{1}{\rho_{g,m}}\right)\left(\frac{1}{V_{B,m}}\right)\left(\frac{\Delta r_m}{u_{B,m}}\right) = \frac{\dot{m}\Delta\theta\Delta r_m}{2\pi\rho_{g,m}V_{B,m}u_{B,m}}.
\] (3.88)
Therefore, the total bubble surface area within a cell becomes

\[ A_{\text{tot},m} = 20.728 \frac{\dot{m} \Delta \theta \Delta r_m a^2}{2 \pi \rho_{g,m} V_{B,m} u_{B,m}}. \]  

(3.89)

3.9. Void Fraction

The void fraction, which has been used in multiple calculations above, is defined as the total volume of the bubbles in a given cell divided by the geometric volume of that cell. Using the previous development of the bubble number and size, it can now be expressed for each cell as:

\[ X_m \equiv \frac{n_{g,m} V_{B,m}}{V_m} = \frac{\dot{m} \Delta \theta \Delta r_m}{2 \pi \rho_{g,m} u_{B,m} \left( \frac{1}{\pi \left( r_m^2 - r_{m-1}^2 \right)} \left( \frac{4\theta_n}{2\pi} \right) \right)} = \frac{\dot{m} (r_m - r_{m-1})}{\pi \rho_{g,m} u_{B,m} \left( r_m^2 - r_{m-1}^2 \right)}, \]  

or

\[ X_m = \frac{\dot{m}/(2\pi)}{\rho_{g,m} u_{B,m} (r_m + r_{m-1})/2}. \]  

(3.90)

While the terms in the numerator of Eq. 3.91 are constants for a given gas mass flow rate, the terms in the denominator vary with radius and with other system parameters and can cause the void fraction to vary in unanticipated ways. First, it is noted that \( X_m \) increases with decreasing cell volume, \( V_m \). This means that at the inner cells of the fuel annulus the void fraction will be higher, since the radii of the cells there are smaller. Secondly, notice that \( X_m \) decreases with increasing bubble velocity, \( u_{B,m} \). This represents the fact that, if the bubble velocity increases, the individual bubbles will have a shorter residence time in a computational cell and therefore fewer bubbles will exist there at a time. Finally, \( X_m \) is also inversely proportional to \( \rho_{g,m} \). Since the density of the propellant will decrease with increasing temperature, the void fraction will go up as the propellant gets
hotter towards the center of the annulus. These effects all combine such that there is a substantial monotonic increase from low void fractions at the injection sites on the outer radius of the fuel annulus to high void fractions at the inner radius. This will be shown graphically in Chapter 4.

3.10. Bubble Heat Transfer

The convection coefficient for the interior of the bubble, $h_g$, must be known in order to evaluate the heat transfer to/from the propellant while it is bubbling through the liquid uranium. Tokunaga et al. [48] present a correlation for the bubble Nusselt number,

$$ Nu_B = 1.1 \left[ Pe/(1 + \kappa) \right]^{0.7} $$

where $\kappa$ is the viscosity ratio defined as

$$ \kappa \equiv \frac{\mu_g}{\mu_i} $$

and the bubble Nusselt number is defined on the gas-side properties,

$$ Nu_B \equiv \frac{h_g d_B}{k_g} $$

In this definition, $d_B$ is the bubble diameter and $k_g$ is the thermal conductivity of the gas inside the bubble. Tokunaga et al. found that the liquid-side heat transfer coefficient was much larger than the gas-side coefficient so that $h_g$ is the limiting value for the heat transfer rate into the bubble.

The Peclet number for the bubbles is defined as:

$$ Pe \equiv Re_B Pr_g $$
where the bubble Reynolds number was defined in Eq. 3.80 and the Prandtl number for the bubble is defined on gas properties,

\[ Pr_g = \frac{c_p g \mu_g}{k_g}. \]  

(3.96)

Note that \( Re_B \) uses the bubble rise velocity as the kinetic scale but otherwise uses gas properties for the viscous scale. Here, the bubble rise velocity can also be understood as a scale for the circulation speed within the bubble through a no-slip boundary at the bubble surface.

It should be noted that this correlation yields very high values of heat transfer to the bubbles. For example, at bubble injection typical values for Reynolds and Prandtl numbers are roughly \( Re_B \approx 300 \) and \( Pr_g \approx 0.68 \). This would yield a Peclet number of \( Pe = 204 \). Also, since the viscosity of hydrogen gas is about two orders of magnitude lower than that of molten uranium, \( \kappa \) is close to zero and can be ignored in a rough calculation. Therefore, the Nusselt number from Eq. 3.92 should be approximately

\[ Nu_B \approx 1.1(Pe)^{0.7} = 1.1(204)^{0.7} = 45.5. \]  

(3.97)

Additionally, the conditions in the CFE yield very small bubble sizes at injection, with equivalent diameters around 0.6 \( mm \). A typical value of the hydrogen thermal conductivity at injection is roughly 0.4 \( W/m/K \). Putting these numbers together, the heat transfer coefficient for a bubble at injection can be calculated by rearranging Eq. 3.94:

\[ h_g = \frac{Nu_B k_g}{d_B} = \frac{(45.5)(0.4 W/m \cdot K)}{0.0006 m} \approx 30,300 W/m^2K. \]  

(3.98)

Due to the combination of this extremely high heat transfer coefficient and the fact that the individual bubbles are so small that their aggregate surface area is very high, the
bubbles will come into a local thermal equilibrium with the surrounding liquid uranium very quickly. This will be shown in more detail in Chapter 4, and agrees very well with the observations from Nelson et al. [17].

3.11. Pressure Drop and Heat Transfer in Silicon Carbide Frit

The propellant flow through the silicon carbide frit is modeled as flow through a set of straight, circular channels aligned in the radial direction. The current design assumes these channels would have a diameter, \( d_c = 0.5 \) mm, and a spacing of \( \eta = 2 \) mm between channels both in the azimuthal and axial directions. The spacing is measured on a rectangular grid at the outer radius of the frit. The number of channels can be calculated based on the respective ratios of the circumference and the length of a CFE to the channel spacing. In equation form, this can be given as:

\[
n_c = \left\lfloor \frac{2\pi R_o}{\eta} \right\rfloor \left\lfloor \frac{L}{\eta} \right\rfloor,
\]

where the term for the spacing in the circumferential direction and the term for the spacing in the axial direction are each rounded down to the nearest whole number so that a whole number of channels is obtained. For the baseline geometry, then, the number of channels is approximately:

\[
n_c = \left\lfloor \frac{2\pi (0.049 \text{ m})}{0.002 \text{ m}} \right\rfloor \left\lfloor \frac{0.84 \text{ m}}{0.002 \text{ m}} \right\rfloor = 64,260.
\]

The Reynolds number at each channel within the frit is defined as:

\[
Re_{D,m} = \frac{4\dot{m}}{\pi n_c d_c \nu_{g,m}}.
\]
The mass flow rate is for the entire cylinder, so it must be divided by the number of channels in order to get the mass flow rate for an individual channel. The Reynolds number can be used to determine if the flow is in the laminar or turbulent regime. The transition region from laminar to turbulent is taken to start at \( Re_D > 2,300 \). However, it was found in all simulation runs that the Reynolds number is significantly lower than this; therefore, the flow was taken to be laminar.

It is next necessary to determine if the flow becomes fully developed over the length of the channel within the frit. For laminar flow, the hydrodynamic entry length can be found from the general expression [70]:

\[
\left( \frac{x_{fd,h}}{d_c} \right) \approx 0.05 Re_D. \tag{3.102}
\]

For the baseline geometry, a typical value for the Reynolds number is \( Re_D \approx 500 \). This yields a hydrodynamic entry length of:

\[
x_{fd,h} \approx 0.05 Re_D d_c = 0.05(500)(0.5 \text{ mm}) = 12.5 \text{ mm}. \tag{3.103}
\]

By contrast, the thermal entry length can be found for a similar expression incorporating the Prandtl number [70]:

\[
\left( \frac{x_{fd,t}}{d_c} \right) \approx 0.05 Re_D Pr_g. \tag{3.104}
\]

Again, for the baseline design, a typical value for the Prandtl number of the hydrogen entering the flow channels is \( Pr_g \approx 0.68 \). This would then give a thermal entry length of roughly:

\[
x_{fd,t} \approx 0.05 Re_D Pr_g d_c = 0.05(500)(0.68)(0.5 \text{ mm}) = 8.5 \text{ mm}. \tag{3.105}
\]
Both of these entrance region estimates are much longer than the length of the propellant channels which is also the thickness of the frit, or 4 mm. Therefore, the channel flow within the frit is entirely an entrance length problem. The heat transfer coefficient can be written in terms of the Nusselt number as:

\[ h_g = \frac{Nu_g k_g}{d_c}. \]  

(3.106)

To determine the Nusselt number, a variety of correlations could be used. These depend on a number of flow conditions, namely: whether the local hydrodynamic and thermal boundary layers are still developing (combined flow problem), the thermal boundary layer only is still developing (thermal entry length problem), or the flow is fully developed. Additionally, different correlations exist depending on whether or not the flow is laminar or turbulent.

3.11.1. Laminar, Fully Developed Flow

For laminar flow in the fully developed region, there are two simple situations typically given in the literature which each give a constant Nusselt number. First, if the heat flux in a circular tube is constant, the Nusselt number is

\[ Nu_D = \frac{h_g d_c}{k_g} = 4.36. \]  

(3.107)

Alternatively, if the surface temperature of the channel is constant, the Nusselt number is

\[ Nu_D = 3.66. \]  

(3.108)

Given the conductivity of the silicon carbide, around 45 W/mK, and given there is no volumetric heat generation within the frit, the uniform temperature surface boundary condition is selected.
3.11.2. Laminar, Developing Flow

In the developing region of the flow, the heat transfer is higher than either of these values and approaches the developed value asymptotically with axial distance. Kays [71] presents theoretical data for the local Nusselt number in the thermally developing region as a function of \( x^+ \), which is defined as

\[
x^+ \equiv \frac{2(x/d_c)}{Re_d Pr_g}.
\]

(3.109)

where \( x \) is the distance from the channel entrance to the point under consideration. In our geometry, for cell \( m \), it would be:

\[
x_m = R_o - R_m.
\]

(3.110)

A power law fit to the data from Kays for the region of \( x^+ = 0.001 \) to 0.10 provides fairly good results:

\[
Nu_D \equiv \frac{h d_c}{k_g} \approx 1.8684(x^+)^{-0.269}.
\]

(3.111)

This data fit is used for convection in the frit region, as long as \( x < x_{fd,h} \). For \( x \geq x_{fd,h} \), the fully developed \( Nu_D = 3.66 \). Since the node at the outermost computational cell is on the outer radius of the frit (see Figure 3.2), \( x^+ \) is zero at the outermost cell meaning that \( Nu_D \) would be undefined there. Therefore, the value of \( Nu_D \) at this point is set equal to the value at the adjacent downstream node. While this selection underestimates the initial value for Nusselt number, the difference should be negligible for large numbers of cells in the frit region.
The pressure drop as the propellant flows down the channels is based on a friction factor, \( f \), and is given by the following equation:

\[
p_{g,m} = p_{g,\text{upstream}} - \frac{\rho_{g,m} \Delta r u_{g,m}^2}{2d_c} f_m = p_{g,\text{upstream}} - \frac{8\Delta r m^2}{\pi^2 \rho_{g,m} d_c^5 n_c^2} f_m \tag{3.112}
\]

Where the friction factor for laminar flow at cell \( m \) is given as:

\[
f_m = \frac{64}{Re_{\rho,m}} \tag{3.113}
\]

The surface area of one channel segment contained within a given computational cell is:

\[
A_{c,m} = \pi d_c \Delta r \tag{3.114}
\]

The total surface area of channel segments within a computational cell is:

\[
A_{\text{tot},m} = n_c A_{c,m} \frac{\Delta \theta}{2\pi} \tag{3.115}
\]

To implement the channel heat transfer model in the code the channel heat transfer coefficient within the frit, \( h_g \), is estimated from Eq. 3.108 or 3.111, as the case may be, for each computational cell.

### 3.12. Heat Transfer in Clearance Gap

This section discusses the convective heat transfer occurring within the clearance gap outside of the CFE (see Figure 3.1). The convection in this region is modeled by assuming it is Taylor-Couette flow; that is, the fluid motion is in the direction of the cylinder rotation, and there is no flow in the axial direction. The addition of axial flow, which would be regarded as Taylor-Couette-Poiseuille flow, may be examined in later studies. Fénot et al. [72] have summarized a number of studies of Taylor-Couette flow,
reporting observations and various heat transfer correlations. We assume the outer wall of
the clearance gap (the moderator surface) is adiabatic. That is, all the energy lost by the
moving inner wall goes to increase the enthalpy of the hydrogen flowing in the gap. We
apply this assumption of an adiabatic outer surface in order to constrain our analysis to the
CFE itself and the hydrogen flowing into the CFE.

One of the key dimensionless numbers in these correlations is the Taylor number,
where:

\[ \tau = \frac{\omega^2 R_o (D_h/2)^3}{v^2}. \]  \hspace{1cm} (3.116)

and

\[ D_h = 2(R_{gap} - R_o). \]  \hspace{1cm} (3.117)

where \( R_{gap} \) is the outer radius of the clearance gap and \( R_o \) is the outer radius of the CFE.
The critical Taylor number, \( \tau_{cr} \), is typically reported as 1708, which marks the appearance
of Taylor vortices in the flow [72]. However, the fluid motion in this regime is still orderly,
and the transition to true turbulent flow does not occur until the ratio \( \tau / \tau_{cr} \approx 1300 \), or
\( \tau \approx 2 \times 10^6 \). Under the assumption of a Taylor flow in the clearance gap, a CNTP
reactor (7000 rpm, clearance gap of 2 mm, gas delivery temperature of 300 K, and core
pressure of 10 MPa) would have \( \tau \sim 10^8 \). This indicates a turbulent flow in the clearance
gap. Fénot et al. present only two correlations with good coverage of the turbulent
operating range. The more conservative of these is due to Tachibana and Fukui [73]:

\[ Nu_\infty = 0.092(\tau Pr_y)^{1/3}. \]  \hspace{1cm} (3.118)
where the Nusselt number is related to the heat transfer coefficient, $h_\infty$, on the outside of the frit by

$$Nu_\infty = \frac{h_\infty D_h}{k_g}. \quad (3.119)$$

The propellant properties are evaluated at $T_\infty$ and $p_{g,M}$. Typical values of $h_\infty$ are near 2900 $W/m^2K$ for $Nu_\infty$ near 60. The rise in the gas temperature in the clearance volume to a gas temperature entering the frit, $T_{g,M}$, is given by

$$m c_{p,g,\infty} (T_{g,M} - T_\infty) = h_\infty A_M (T_M - T_\infty). \quad (3.120)$$

where $A_M$ is the outer surface area of the frit and $T_M$ is the temperature of that surface. This approach borrows the heat transfer coefficient from the heated Taylor flow as shown and assumes that the entire frit surface (which is the inner surface of the Taylor problem) is available for heat transfer to the gas before it exists the clearance gap through the channels in the frit. Also, the driving temperature difference here is $T_M - T_\infty$ whereas it is the temperature across the clearance gap in the Taylor problem. These differences are acknowledged here, and the likelihood is that they cause something of an overestimate in the heat transfer to the gas while it is in the clearance volume. However, we know of no better approach as of this writing.

3.13. Implementation

This chapter has presented the computational framework and the thermo-physical models that will be employed in a computer code for the computation of

- the uranium and hydrogen bubble temperatures as a function of radial position in the annulus,
the silicon carbide and hydrogen gas temperatures in the frit and the gas temperature in the clearance gap outside the fit, and

- the energy budgets in the uranium annulus and in the frit.

The code will be implemented in MATLAB Version R2020a and executed on a standard Microsoft Windows computer. For all runs, 400 cells were used. Doubling the number of cells resulted in only a 0.03% change in the maximum fuel temperature, so 400 cells was taken to be a sufficiently refined grid. Additionally, the numerical iterations on the temperature solution were taken to be converged after the maximum change in temperature at any given cell between iterations became less than 0.01%. Chapter 4 will present results for the three designs introduced and a discussion of those results.

3.14. Limited Model Validation

The issue of model validation is difficult to address for this model. No experimental data for a full CNTP-like system exists for comparison. An alternative is to validate against a closed-form solution. While there is no general closed-form solution applicable to all of the processes that have been modeled in a CNTP reactor, this model can be simplified such that it can be compared to a closed-form solution for a simple scenario. The closed-form solution for an annular ring with Type 1 (fixed temperature) boundary conditions on the inner and outer radius with no internal generation was selected for comparison to this study. The closed-form solution to the temperature as a function of radius was given by Mills [74] as:

\[
\frac{T_1 - T}{T_2 - T_1} = \frac{\ln(R/R_1)}{\ln(R_2/R_1)},
\]

(3.121)
where $T_1$ and $R_1$ are the temperature and radius, respectively, at the inner surface and $T_2$ and $R_2$ are the corresponding values at the outer surface. To compare solutions, the computational model has the mass flow rate and power generation level set to zero (so that there are no internal energy generations or losses in the cells). Additionally, the conductivity in both the fuel and frit regions was set to be identical at 13.7 $W/mK$ so that the material in both regions would conduct heat the same. For this example, the inner and outer radii of Design 1 from Table 3.1 are used along with an inner surface temperature of $3000 \, K$ and an outer surface temperature of $500 \, K$. The resulting temperature profiles from both the closed-form expression and the MATLAB model, using 400 cells, are plotted in Figure 3.10.

![Figure 3.10 Comparison of Model Output to a Closed-Form Solution for a Simple Case](image)
It can be seen from Figure 3.10 that the temperature profiles are identical. The curves were plotted in two separate windows as otherwise the curves would lie on top of one another and be indistinguishable. While this comparison does not test parts of the model which deal with two-phase flow or nuclear energy generation, it does show that the matrix formulation and linear algebra of the basic solution procedure are accurate.

Additionally, Mills also records that the total power passing through an annulus with no internal generation and Type 1 boundary conditions can be expressed by the following equation:

$$
\dot{Q} = \frac{2\pi (T_1 - T_2)}{\ln(R_2/R_1)}, \quad (3.122)
$$

where $k$ is the thermal conductivity of the annular region and $L$ is the length of the annulus. For the geometry and temperatures described above, this yields:

$$
\dot{Q} = \frac{2\pi (13.7 \text{ W/mK})(0.84 \text{ m})(3000 \text{ K} - 500 \text{ K})}{\ln\left(\frac{0.049 \text{ m}}{0.03 \text{ m}}\right)} = 368,444 \text{ W}. \quad (3.123)
$$

This equation should be equal to the power passing through any circumferential control surface in the numerical model. Applying Fourier’s Law to compute the power transferred from the innermost cell (of $2\pi$ arc length) to the neighboring cell gives:

$$
\dot{Q}_{\text{cond,1}} = \left(13.7 \frac{\text{W}}{\text{mK}}\right)(2\pi \cdot 0.84 \text{ m} \cdot 0.030955 \text{ m}) \frac{(3000 \text{ K} - 296 \text{ K})}{(1.91083 \times 10^{-4}\text{ m})} = 368,444 \text{ W}. \quad (3.124)
$$

This agreement is expected given the successful comparison of the temperature profiles.
CHAPTER 4. RESULTS AND DISCUSSION

This chapter presents the results of the model simulations of the CNTP reactor for all three design cases described in Chapter 3. It also presents a discussion of the key results and findings regarding the CNTP concept. Results described as “optimized” were found by running simulations with some identified parameters (such as containing-wall temperature or maximum void fraction) held fixed while other parameters were varied to produce the best outcome for the fixed parameters. Six sets of data will be discussed, and in each of the first three sets the runs examined are those for which the maximum containing wall temperature is restricted to 1500 °K or below, and the maximum void fraction (which occurs at the inner radius) is restricted to 0.4. The six cases are described as follows:

- First, the detailed results of an optimized run with the baseline geometry are presented. Then these results are then compared to the results produced by the other two geometries with the same parameters from the optimized baseline geometry applied to the other two geometries.
- Second, the optimized performance is identified and presented for each of the three designs, and those results are compared.
- Third, all three designs are run with parameters that cause the core temperature to reach 5,000 °K while keeping the constraint on void fraction but releasing the constraint on wall temperature.
- Fourth, Design 3 is run with different assumed core pressures ranging from 5 MPa to 20 MPa. The input parameters are optimized for each value of the core pressure.
In the fifth set of runs, all three designs are optimized for an assumed constant-power density distribution of the nuclear heat generation \(i.e.,\) without using the neutronics calculations from Penn State.

Finally, runs are performed at a lower cylinder rotation speed to document the effect of rotation speed on the model output parameters.

### 4.1. Reduced-Order Modeling

Before the results from the MATLAB model are presented, a pair of reduced-order models are presented to help the reader gain insight into the results. An assumed maximum of 40\% on void fraction limits the mass flow rate for a given desired core temperature. This can be demonstrated by evaluating the void fraction at the inner annulus radius, \(X_0\).

Following Nelson et al. [17], a modified form of their expression is

\[
X_0 = \frac{m}{A_w u_0 \rho_{g,0}} = \frac{m}{(2\pi R_i)(0.984 \omega_0/\alpha R_i)} \left( \frac{R_u T_g,0}{p_0 M} \right) = \frac{m R_u T_g,0}{6.18 R_i^{3/2} L p_o M \omega_0/\alpha_0} \quad (4.1)
\]

where \(R_u\) is the universal gas constant, \(M\) is the molecular weight of hydrogen, and \(u_0\), \(T_{g,0}\), \(\rho_{g,0}\), and \(a_0\) are the bubble velocity, propellant temperature, propellant density, and bubble equivalent radius, respectively, at the inner surface of the fuel. Note that this derivation assumes that the hydrogen gas behaves as an ideal gas in order to calculate the density as an explicit function of temperature and pressure. This is not exactly true but is close enough to be a good first approximation.

Eq. 4.1 can be used to see the impact of pressure on allowable mass flow rates for a certain void fraction constraint. The equation is plotted in Figure 4.1 as a function of mass flow rate and for various values of core pressure. This graph assumes that \(T_{g,0}\) is 5000 \(K\), \(R_i\) is 0.03 \(m\), \(a_0\) is 0.45 \(mm\) (a representative value from the MATLAB model...
runs), $\omega$ is a rotation speed of 7000 rpm (converted to 733 rad/s), and $M$ is 2.0158 kg/kmol. Note that for low core pressures, only very minimal mass flow rates can be maintained without exceeding a 40% void fraction.

![Figure 4.1 Void Fraction as a Function of Mass Flow Rate for Varying Core Pressures](image)

An additional reduced-order model, based on a closure of the First Law of Thermodynamics, is shown below in Eq. 4.2:

$$Q_{gen} = \dot{m}c_{p,g}\Delta T_g,$$  \hspace{1cm} (4.2)

where

$$\Delta T_g = T_{g,0} - T_{g,\infty}.$$  \hspace{1cm} (4.3)
Equation 4.2 can also be solved for the temperature rise in the gas, $\Delta T_g$:

$$\Delta T_g = \frac{1}{c_{p,g}} \left( \frac{\dot{q}_{gen}}{m} \right). \quad (4.4)$$

The effective specific heat, $c_{p,g}$, is determined by the temperature range across the annulus and therefore is a relatively fixed number. Therefore, a desired temperature rise in the gas determines the ratio of the power generation to the mass flow rate. It follows that there are an infinite number of combinations of power and mass flow rate that will yield the required ratio for a desired temperature rise in the gas.

However, going back to Eq. 4.1, it can be seen that $\dot{q}_{gen}$ does not appear explicitly in $X_0$. Therefore, in order to keep the void fraction below a desired maximum, there must be a limit on the mass flow rate for given thermodynamic conditions, independent of the power level. Therefore, as a design tool, Eq. 4.1 can be used to determine the maximum mass flow rate. Then, Eq. 4.2 can be used to determine the corresponding power level that would be required in order to achieve the desired $\Delta T_g$.

**4.2. Procedure used to Determine the Parameter Set for the “Optimized Run”**

The approach described above can be used to obtain approximate results; however, caution should be used as Eq. 4.1 assumes that the hydrogen behaves as an ideal gas and calculates the density using the ideal gas law. In reality however, the density will be lower than expected from the ideal gas law and Eq. 4.1 will overpredict the allowable mass flow rate for a given void fraction. An additional challenge is that Eq. 4.2 expects a constant effective value $c_{p,g}$. However, as shown in Chapter 3, $c_{p,g}$ varies significantly as the temperature and pressure of the hydrogen increases across the annulus. For Eq. 4.2 to be
useful as a preliminary design tool, an effective value of $c_{p,g}$ must be determined. As will be seen later, however, a large fraction of the total power is deposited into the propellant closer to the frit wall. This means that the effective specific heat, $\bar{c}_{p,g}$, will be biased toward values present closer to the frit wall. The value can be determined by considering each computational element from the clearance gap through the frit and the annulus to be a heat exchanger obeying Eq. 4.2 independently,

$$\dot{Q}_{gen} = \dot{m}\bar{c}_{p,g}\Delta T_g = \sum_{m=1}^{M-1}(\dot{m}c_{p,g,m}\Delta T_{g,m}) + \dot{m}c_{p,g,M}(T_{g,M} - T_\infty).$$  \hspace{1cm} (4.5)

where the last term is the energy absorption in the clearance gap and $\Delta T_{g,m}$ is defined as

$$\Delta T_{g,m} \equiv T_{g,m} - T_{g,m+1}.$$  \hspace{1cm} (4.6)

Rearranging, $\bar{c}_{p,g}$ is then:

$$\bar{c}_{p,g} = \frac{1}{\Delta T_g} \left[ \sum_{m=1}^{M} c_{p,g,m}\Delta T_{g,m} + c_{p,g,M}(T_{g,M} - T_\infty) \right].$$  \hspace{1cm} (4.7)

We can now rewrite Eq. 4.2 with $\bar{c}_{p,g}$:

$$\dot{Q}_{gen} = \dot{m}\bar{c}_{p,g}\Delta T_g.$$  \hspace{1cm} (4.8)

The only temperatures appearing in the above equations are the temperatures for the gas, and not the fuel or the frit. Therefore, the constraint of 40% void fraction can be inserted into the equations above but the constraint of a 1500 $K$ frit wall temperature cannot be. This, combined with the error introduced by the fact that the density is lower than the ideal gas law predicts, means that Eqs. 4.1 and 4.2 can only be used for approximate optimization. The parameters will have to be “tweaked” by trial-and-error operation of the larger MATLAB model, changing the mass flow rate and/or power to observe how the
outputs have changed. It is helpful, however, to note that Eq. 3.9 indicates that the heat transfer from the frit wall to the propellant is increased with a larger mass flow rate. This means that larger mass flow rates will cool the frit wall more effectively, which is key to keeping the frit wall temperature at 1500 K or below. In light of this, a general procedure for obtaining optimized results for each of the three geometry designs is as follows:

1. Use Eq. 4.1, with anticipated values, to find the highest mass flow rate which does not cause the void fraction to exceed a specified limit (40% for these cases).
2. Next, for the selected $\dot{m}$ and the desired value of $\Delta T_g$, use Eq. 4.2 to calculate the necessary power level for the CFE.
3. Run the model with these values of $\dot{m}$ and $\dot{Q}_{gen}$.
4. Based on model output, adjust the variable values as needed to optimize the desired output variable (core temperature, frit temperature, etc.). Repeat (4) until an observed optimum combination is identified.

In practice, due to the assumptions embedded in Eqs. 4.1 and 4.2, the model results will be slightly unoptimized. The additional runs described in step 4 were executed within this range to manually refine the parameter selection. For example, if the wall temperature is too high but the void fraction is still under 40%, the mass flow rate can be increased slightly. Alternatively, if the temperature of the wall is below 1500 K, the power level can be increased until the wall reaches 1500 K which will also raise the core temperature. The result of this last step is what is presented in the sections that follow as an “optimized run.”
4.3. Baseline-Optimized Run for Geometry 1

The optimized run for the baseline design (Design 1) was determined for the constrained parameters as shown in Table 4.1. The model produced a core hydrogen propellant temperature of 3637 K for a maximum wall temperature of 1491 K. Additionally, the maximum void fraction is 0.392. The temperature distributions of the uranium fuel, frit, and propellant are shown in Figure 4.2.

Table 4.1 Parameters for Optimized Run for Design 1

<table>
<thead>
<tr>
<th>Fixed Parameters</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum Containing Wall Temperature</td>
<td>1500 K</td>
</tr>
<tr>
<td>Core Pressure</td>
<td>10 MPa</td>
</tr>
<tr>
<td>Pore Spacing in SiC Frit</td>
<td>2 mm</td>
</tr>
<tr>
<td>CFE Rotation Speed</td>
<td>7000 rpm</td>
</tr>
<tr>
<td>Inlet Coolant Temperature</td>
<td>300 K</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variable Parameters</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂ Mass Flow Rate</td>
<td>0.108 kg/s</td>
</tr>
<tr>
<td>Power Level</td>
<td>7 MW</td>
</tr>
<tr>
<td>Core Gas Temperature</td>
<td>3637 K</td>
</tr>
</tbody>
</table>

The propellant temperature quickly reaches the local temperature of the uranium fuel. This agrees well with the result from Nelson et al. [17] that the temperature of the propellant comes into local equilibrium with the fuel very quickly. The temperature gradient in the fuel is highest near the wall. This is expected as the frit is being effectively cooled by the hydrogen flow through many microchannels and there is no energy generation in the frit. The system responds by creating a high temperature gradient.
adjacent to the wall. This result also differs from that of Leer [26], who predicted an almost linear increase in temperature. However, this may be explained by the fact that Leer assumed a uniform energy generation rate from the fission reactions, independent of radial location. As shown previously in Figure 3.7, the power generation is expected to be highly nonuniform, and the actual generation rate must be weighted locally by the void fraction. The distribution of the void fraction for this case can be seen in Figure 4.3 below.

Figure 4.2 Temperature Distributions for Baseline Design
An energy budget can be constructed to ensure that there are no unaccounted-for energy losses or gains in the system. One can balance the power generated in the fuel with the power imparted to the propellant (over the whole volume of the CFE) as in Eq. 4.9:

$$\dot{Q}_{gen} - \dot{Q}_{bubbles} - \dot{Q}_{channels} - \dot{Q}_{gap} = 0.$$  \hspace{1cm} (4.9)

For the baseline design case with optimized parameters, this becomes:

$$7 \text{ MW} - 5.823 \text{ MW} - 0.609 \text{ MW} - 0.568 \text{ MW} = 0.$$ \hspace{1cm} (4.10)

Figure 4.4 shows the volumetric power generation/absorption (in W/cm\(^3\)) plotted as a function of radial position in the CFE. The volumetric energy generation term, from Eq. 3.70 is skewed heavily towards the outer radius due to the combination of nonuniform
neutronics and nonuniform void fraction as discussed above. Note that the quantities shown in this figure are power densities whereas the quantities shown in Eq. 4.10 are power in Watts. Given that the computational cells increase in size with increasing radius, the nonuniformity in power is actually more severe than is indicated in Figure 4.4. Equation 4.10 shows that about 17% of the power generated is absorbed in the clearance gap and the frit. The majority of the power is deposited into the propellant in the bubble stage in the annulus, and most of that occurs between the 4 cm and 4.5 cm radial positions. As a result, the temperature of the bubbles rises rapidly upon injection into the liquid fuel as shown in Figure 4.2.

Figure 4.4 Volumetric Energy Generation/Loss for Baseline Case
The need for an effective specific heat capacity in Eq. 4.2 can be readily seen from Figure 4.5, where the same energy absorption from Figure 4.4 is plotted alongside the local specific heat capacity of the hydrogen. While the specific heat is relatively constant in the clearance gap and through the frit, it more than doubles across the annulus. However, a significant amount of heat transfer occurs at radial positions greater than 4.25 cm where the specific heat is low. The mean value of $c_{p,g}$ from this run is $24.4 \, kJ/kg/K$. However, the value of the weighted specific heat, $\bar{c}_{p,g}$, from Eq. 4.7 is $19.4 \, kJ/kg/K$. It is this latter value that accurately predicts the core temperature in Eq. 4.8. This shows that using an unweighted average specific heat will overestimate the required power in Eq. 4.2.

![Figure 4.5 Volumetric Energy Loss and Specific Heat Capacity for Baseline Case](image-url)
The equivalent bubble radius and bubble velocity are plotted together in Figure 4.6. The size of the bubbles predicted in this case is quite small, with the equivalent radius at injection being roughly 0.28 mm and expanding to 0.47 mm at the inner surface. These small bubble sizes can be attributed to the high pressures in the system which compress the gas, as well as the high centrifugal acceleration which causes the bubbles to rise from the injectors before reaching a large size. Because the mass passing through the annulus is divided up into a large number of sub-millimeter bubbles, the total surface area of the bubble field is large as is the predicted heat transfer coefficient for each bubble from Eq. 3.98. The resulting temperature difference across the bubble surfaces is small everywhere except near the injection radius, and the bubbles come into a local thermal equilibrium with the fuel very rapidly after injection as seen in Figure 4.2.
Due to the high rotational speeds and resulting centrifugal acceleration, the computed bubble velocities are extremely high. The average bubble velocity in this run is 2.83 m/s. At this speed, a bubble would pass through the uranium layer in approximately 5.3 ms. From Eq. 3.85 it is seen that the bubble velocity is directly proportional to the angular velocity of the CFE. High bubble velocities may induce a large amount of mixing in the uranium annulus. Mixing will tend to homogenize the temperature distribution which would degrade the performance of the engine. While outside the limits of this study, a future investigation of mixing may be warranted to determine the severity of the issue.

The non-monotonic behavior of the bubble velocity in Figure 4.6 can be attributed to the dependence of $u$ on both $\alpha$ and $R$ from Eq. 3.85. The bubble equivalent radius results in Figure 4.6 however show that there is an inverse relationship between $\alpha$ and $R$. 

Figure 4.6 Bubble Equivalent Radius and Velocity
Therefore, the increasing value of $a$ dominates bubble velocity as a bubble passes from $R = 4.5 \text{ cm}$ to $R \approx 4 \text{ cm}$. Afterwards, the decreasing value of $R$ has a more significant impact on the bubble velocity, causing it to decrease as well.

The primary goal of achieving higher fuel (and therefore propellant) temperatures is the increase to the specific impulse of the rocket. For this case, if it is assumed that the molecular weight of the hydrogen propellant is $2.0158 \text{ kg/kmol}$ (i.e., no dissociation of H$_2$ and no other species present in the exhaust), and that $\gamma$ is 1.20 (interpolated from Patch [59] at 3637 K and 10 MPa) then the $I_{sp}$ becomes:

$$I_{sp} = \frac{1}{9.81 \text{ m/s}^2} \sqrt{\frac{2(1.20)(8314 J/kmol\cdot K)(3637 K)}{(1.20-1)(2.0158 \text{ kg/kmol})}} = 1368 \text{ s.} \quad (4.11)$$

As described in the discussion surrounding Eq. 1.2, this calculation of $I_{sp}$ is idealized in that it assumes an infinite expansion for operation in a vacuum. This calculation is also very dependent on the selection of $\gamma$; the room temperature value of $\gamma$ of 1.41 will give an $I_{sp}$ of 1035 s for example. As shown in Figure 3.5, there is a significant difference predicted by thermodynamic theory for the specific heat capacity between molecular hydrogen and hydrogen undergoing dissociation at high temperature. That difference extends to the specific heat ratio. As a result, there is some uncertainty in these $I_{sp}$ calculations and the actual $I_{sp}$ may be somewhat lower. Nevertheless, even in this idealized case the $I_{sp}$ is lower than the 1800 s which is desired for this engine [10,11]. Therefore, two other choices for the radial extent of the uranium annulus will now be explored to see if these choices will facilitate higher core temperature and $I_{sp}$. 

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4.4. Geometry 1 Parameters Applied to Geometries 2 and 3

Next, Designs 2 and 3 from Table 3.1 are run for the optimized baseline parameters which were previously described in Table 4.1. The key results from these runs for all three designs are summarized in Table 4.2. Interestingly, the temperature plots for the two additional geometries are similar to the first design. All three designs reach approximately the same temperature at the core of the annulus, while maintaining a maximum wall temperature of close to 1500 K. The temperature of the fuel and frit can be seen in Figure 4.7 while the temperatures of the propellant are plotted in Figure 4.8.

<table>
<thead>
<tr>
<th>CFE Design #</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum Temperature [K]</td>
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<td>3643</td>
<td>3641</td>
</tr>
<tr>
<td>Wall Temperature [K]</td>
<td>1491</td>
<td>1445</td>
<td>1557</td>
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<tr>
<td>Maximum Void Fraction</td>
<td>0.392</td>
<td>0.417</td>
<td>0.270</td>
</tr>
</tbody>
</table>

Where the designs differ more significantly is in void fraction. The void fraction levels of Design 2 are slightly higher than those of Design 1, but Design 3 is significantly lower as can be seen in Figure 4.9. This is due to the larger inner surface area of the fuel annulus, which means that the bubble flow is spread out over a greater cross-sectional area at the inner radius of the annulus. Because the maximum void fraction for Design 3 is lower than the 40% limit prescribed in this study, it should be possible to optimize the performance of this design with a higher mass flow rate.

The power density profiles are also shown in Figure 4.10. As was seen in Figure 3.7, the power generation is heavily skewed towards the outer radius of the fuel annulus.
The problem is exacerbated, however, by the higher void fraction at the inner radius (reducing the power generation) and being low at the outer radius (increasing the power generation). This presents a significant problem for this design, as the high power generation at the wall will tend to make the wall hot while limiting the temperature increase towards the core of the fuel annulus. Thus, if the power level is kept to values which allow for wall temperatures in the vicinity of 1500 K with the set mass flow rate then the core temperature is somewhat limited.
Figure 4.7 Fuel/Frit Temperature Profiles for Baseline-Optimized Parameters

Figure 4.8 Propellant Temperature Profiles for Baseline-Optimized Parameters
Figure 4.9 Void Fraction Profiles for Baseline-Optimized Parameters

Figure 4.10 Power Density Profiles for Baseline-Optimized Parameters
4.5. Optimized Runs for Each of the Three Geometries

Next, optimized parameters for all three designs are run and compared. These parameters and key results are summarized in Table 4.3 and plotted in Figure 4.11 through Figure 4.14. For Design 1, these are the same parameters as were presented in Table 4.1. Due to the larger inner surface radius of Design 3, the mass flow rate could be increased while keeping the void fraction at the inner surface to below 40%. The reduction in maximum void fraction with increasing inner radius can be seen in Eq. 4.1. The increased mass flow rate means that a greater power level can be used (while keeping the wall temperature to approximately 1500 K), which in turn results in a slightly higher core temperature.

<table>
<thead>
<tr>
<th>CFE Design #</th>
<th>Fixed Parameters</th>
<th>Variable Parameters</th>
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</thead>
<tbody>
<tr>
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<td>Core Pressure ([MPa])</td>
<td>Mass Flow Rate ([kg/s])</td>
</tr>
<tr>
<td>1</td>
<td>10</td>
<td>0.108</td>
</tr>
<tr>
<td>2</td>
<td>10</td>
<td>0.102</td>
</tr>
<tr>
<td>3</td>
<td>10</td>
<td>0.162</td>
</tr>
<tr>
<td></td>
<td>CFE Rotation Speed ([rpm])</td>
<td>Reactor Power per CFE ([MW])</td>
</tr>
<tr>
<td>1</td>
<td>7000</td>
<td>7</td>
</tr>
<tr>
<td>2</td>
<td>7000</td>
<td>6.8</td>
</tr>
<tr>
<td>3</td>
<td>7000</td>
<td>11.7</td>
</tr>
<tr>
<td></td>
<td>Void Fraction</td>
<td>Wall Temperature ([K])</td>
</tr>
<tr>
<td>1</td>
<td>0.392</td>
<td>1491</td>
</tr>
<tr>
<td>2</td>
<td>0.404</td>
<td>1499</td>
</tr>
<tr>
<td>3</td>
<td>0.397</td>
<td>1496</td>
</tr>
<tr>
<td></td>
<td>Wall Temperature ([K])</td>
<td>Core Temperature ([K])</td>
</tr>
<tr>
<td>1</td>
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<td>3637</td>
</tr>
<tr>
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<td>1499</td>
<td>3692</td>
</tr>
<tr>
<td>3</td>
<td>1496</td>
<td>3821</td>
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Table 4.3 Run Parameters and Key Outputs for Optimized Runs

<table>
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<td>Core Pressure [MPa]</td>
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<td>10</td>
<td>10</td>
</tr>
<tr>
<td>CFE Rotation Speed [rpm]</td>
<td>7000</td>
<td>7000</td>
<td>7000</td>
</tr>
<tr>
<td>Void Fraction</td>
<td>0.392</td>
<td>0.404</td>
<td>0.397</td>
</tr>
<tr>
<td>Wall Temperature [K]</td>
<td>1491</td>
<td>1499</td>
<td>1496</td>
</tr>
<tr>
<td><strong>Variable Parameters</strong></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Mass Flow Rate [kg/s]</td>
<td>0.108</td>
<td>0.102</td>
<td>0.162</td>
</tr>
<tr>
<td>Reactor Power per CFE [MW]</td>
<td>7</td>
<td>6.8</td>
<td>11.7</td>
</tr>
<tr>
<td>Core Temperature [K]</td>
<td>3637</td>
<td>3692</td>
<td>3821</td>
</tr>
</tbody>
</table>

Repeating the $I_{sp}$ calculation from Eq. 1.2 for Design 3 here gives:

$$I_{sp} = \frac{1}{9.81 \text{ m/s}^2} \sqrt{\frac{2(1.20)(8314 \text{ J/kmol·K})(3821 \text{ K})}{(1.20 - 1)(2.0158 \text{ kg/kmol})}} = 1402 \text{ s.} \quad (4.12)$$

This value is slightly higher than that calculated in Eq. 4.11. It should be pointed out that Design 3 with these parameters represents the highest core temperature possible while respecting the constraints of less than approximately 40% void fraction and 1500 $K$ wall temperature. In order to obtain performance beyond this case, it will be necessary to alter the design in a way not investigated by this study.
Figure 4.11 Fuel/Frit Temperature Profiles for Optimized Parameters

Figure 4.12 Propellant Temperature Profiles for Optimized Parameters
Figure 4.13 Void Fraction Profiles for Optimized Parameters

Figure 4.14 Power Density Profiles for Optimized Parameters
4.6. Runs with 5000 K Core Temperature

The previous results show that keeping the wall temperature to 1500 K and below creates a significant difficulty when trying to achieve core temperatures in the neighborhood of 5000 K. Here, the three designs are optimized for the lowest wall temperature while achieving a required maximum core temperature reaches approximately 5000 K. These results show that it may be possible to reach a temperature of 5000 K if a frit material can be identified which can withstand temperatures in excess of 1500 K.

Table 4.4 Run Parameters and Key Outputs for 5000 K Runs

<table>
<thead>
<tr>
<th>CFE Design #</th>
<th>Fixed Parameters</th>
<th>Variable Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Core Temperature [K]</td>
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<tr>
<td></td>
<td>Core Pressure [MPa]</td>
<td>10</td>
</tr>
<tr>
<td></td>
<td>CFE Rotation Speed [rpm]</td>
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</tr>
<tr>
<td></td>
<td>Reactor Power per CFE [MW]</td>
<td>9</td>
</tr>
<tr>
<td></td>
<td>Mass Flow Rate [kg/s]</td>
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<td></td>
<td>Wall Temperature [K]</td>
<td>2751</td>
</tr>
<tr>
<td></td>
<td>Void Fraction</td>
<td>0.377</td>
</tr>
</tbody>
</table>
Figure 4.15 Fuel/Frit Temperature Profiles for 5000 $K$ Target Temperature

Figure 4.16 Propellant Temperature Profiles for 5000 $K$ Target Temperature
Figure 4.17 Void Fraction Profiles for 5000 K Target Temperature

Figure 4.18 Power Density Distributions for 5000 K Target Temperature
Achieving a core temperature of 5000 \( K \) would have significant advantages for engine performance. Assuming a \( \gamma \) of 1.21 (from Patch [59] at 5000 \( K \) and 10 MPa), Eq. 1.2 gives:

\[
I_{sp} = \frac{1}{9.81 \, m/s^2} \sqrt{\frac{2(1.21)(8314 \, J/kmol\cdot K)(5000 \, K)}{(1.21-1)(2.0158 \, kg/kmol)}} = 1571 \, s \tag{4.13}
\]

Additionally, this calculation neglects the effect of dissociation on molecular weight; at 5000 \( K \), there may be a significant level of hydrogen dissociation from H\(_2\) to H, which will further increase the \( I_{sp} \). However, it should again be noted that this analysis neglects any vaporization of the fuel. As mentioned in Chapter 2, this was a significant concern of previous studies [12,16,17,19] which could reduce the \( I_{sp} \) by the inclusion of high molecular weight species in the propellant exhaust (not to mention the consumption of the fissile fuel over the course of engine operation). This effect would become more severe with increasing temperature, meaning that at some point there will no longer be an advantage to increasing the fuel temperature.

Whether or not a CFE could be constructed with a frit or containment wall that could withstand temperatures on the order of 2500 to 3000 \( K \) is not known. Although the previous studies [11,23] suggested wall temperatures of the silicon carbide frit (with zirconium carbide coating) of 1500 \( K \) and below, the actual melting points of these materials are higher. Silicon carbide dissociates at roughly 2730 \( K \) [56], while zirconium carbide has a melting point between 3150 \( K \) and 3700 \( K \) [57], depending on the stoichiometric ratio. Additionally, refractory metals such as tungsten and tantalum have melting points well in excess of 3000 \( K \), with refractory carbides having even higher melting points; the melting point of tantalum carbide, for example, is roughly 4000 \( K \).
Nevertheless, the strength of these materials may deteriorate long before these temperatures are reached, especially considering the significant structural loads imposed by high rotation speeds, and it may be impractical to fabricate or utilize them for structural purposes. Future work will be required to evaluate whether such high temperature materials will be compatible with the CNTP configuration, but they could significantly impact the feasibility of this configuration.

4.7. Design 3 with Variable Core Pressure

One of the parameters which is critical for the performance of a CNTP reactor is the core pressure; that is, the gas pressure in the center of the CFE. In this study thus far it has been assumed that this pressure is 10 MPa; this is roughly equal to 100 atm, which is one of the design pressures used by Nelson et al. [17]. While this is a high pressure, the reason for operating at high pressure can be seen from Figure 4.1 and Eq. 4.1 previously: the lower the pressure, the lower the mass flow rate which can be used. Additionally, since lower mass flow rates mean that the frit wall will not be cooled as effectively, lower core temperatures can be attained while keeping the wall temperature to 1500 K. In order to investigate the effect of changing the pressure, the next set of runs will investigate the performance of a CNTP reactor using the geometry of Design 3 at different core pressures. Each of these runs has been optimized to achieve the highest core pressure while keeping the void fraction at 40% and the frit wall temperature at 1500 K. The parameters are summarized in Table 4.5, with outputs plotted in Figure 4.19 through Figure 4.23.
Table 4.5 Run Parameters and Key Outputs for Varying Core Pressure in Design 3

<table>
<thead>
<tr>
<th>Fixed Parameters</th>
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<tbody>
<tr>
<td>CFE Rotation Speed (\text{rpm})</td>
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<td>7000</td>
<td>7000</td>
<td>7000</td>
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<td>Wall Temperature (K)</td>
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<td>1496</td>
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<td>Void Fraction</td>
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<th>Variable Parameters</th>
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<tr>
<td>Core Pressure (\text{MPa})</td>
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<td>10</td>
<td>15</td>
<td>20</td>
</tr>
<tr>
<td>Mass Flow Rate (\text{kg/s})</td>
<td>0.096</td>
<td>0.162</td>
<td>0.224</td>
<td>0.283</td>
</tr>
<tr>
<td>Reactor Power per CFE (\text{MW})</td>
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<td>11.7</td>
<td>18.7</td>
<td>25.5</td>
</tr>
<tr>
<td>Core Temperature (K)</td>
<td>3323</td>
<td>3821</td>
<td>4099</td>
<td>4278</td>
</tr>
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</table>
Figure 4.19 Fuel and Frit Temperatures for Design 3 with Variable Core Pressure

Figure 4.20 Propellant Temperatures for Design 3 with Variable Core Pressure
Figure 4.21 Void Fraction Profiles for Design 3 with Variable Core Pressure

Figure 4.22 Power Density Profiles for Design 3 with Variable Core Pressure
Clearly, the core pressure has a significant impact on the core temperatures which can be attained. Reducing the core pressure to only 5 MPa decreases the attainable core pressure by roughly 500 K, as seen in Figure 4.19 and Figure 4.20. Conversely, increasing the core pressure will increase the attainable core temperature, but with diminishing returns. It should also be remembered that the pressures varied here are the core pressures; the hydrostatic pressure distribution across the annulus for all four of these cases is plotted in Figure 4.23, which shows that the pressure in the propellant required at injection into the fuel annulus could be as much as four to five MPa higher than the desired core pressure; when additional pressure losses upstream of the CFE are also taken into account, the necessary turbopump pressure could be quite high.

Figure 4.23 Hydrostatic Pressure in Annulus for Design 3 with Variable Core Pressure
4.8. Uniform Power Density Runs

The nonuniform power distributions as seen throughout this chapter are a major challenge in achieving the desired core temperature while ensuring a survivable frit wall temperature. In order to illustrate how much of a limitation this is, the following set of runs was performed with an idealized uniform power density instead of the power distributions computed from neutronics and modified by void fraction. Table 4.6 provides the parameters and key outputs from these runs, and some of these results are plotted in Figure 4.24 through Figure 4.28.

### Table 4.6 Run Parameters and Key Outputs for Uniform Power Density Runs

<table>
<thead>
<tr>
<th>CFE Design #</th>
<th>Fixed Parameters</th>
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</thead>
<tbody>
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<td></td>
<td>Core Pressure [MPa]</td>
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<td>CFE Rotation Speed [rpm]</td>
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<td></td>
<td>Wall Temperature [K]</td>
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<td>1501</td>
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<tr>
<td></td>
<td>Void Fraction</td>
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<td>0.401</td>
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</table>

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<tr>
<td>Mass Flow Rate [kg/s]</td>
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</tr>
<tr>
<td>Reactor Power per CFE [MW]</td>
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<td>Core Temperature [K]</td>
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<td>4693</td>
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</table>
Figure 4.24 Fuel and Frit Temperatures for Uniform Power Density

Figure 4.25 Propellant Temperatures for Uniform Power Density
Figure 4.26 Void Fraction Profiles for Uniform Power Density

Figure 4.27 Power Density Uniform Levels
Figure 4.28 Volumetric Energy Generation/Loss for Design 3 with Uniform Power Density. The Power Budget is as Follows: $\dot{Q}_{\text{gen}} = 14.4 \text{ MW}$, $\dot{Q}_{\text{bubbles}} = 13.02 \text{ MW}$, $\dot{Q}_{\text{channels}} = 0.62 \text{ MW}$, $\dot{Q}_{\text{gap}} = 0.76 \text{ MW}$.

It is notable that these runs produce maximum temperatures on the order of 4500 – 4600 $K$, significantly higher than the corresponding maximum temperatures for these design0s from Table 4.3. Clearly, having a more uniform power distribution throughout the CFE is strongly desirable; however, it is not clear how this could be attained. Detailed neutronics modeling and trade studies with various reactor configurations will likely be required to determine whether or not it will be possible to create a more uniform power distribution.
4.9. Reduced Rotation Speed Run

It is acknowledged that the rotation speed assumed thus far, 7000 rpm, is a high value and could present a significant design challenge despite the fact that this value was used previously by Nelson et al. [17]. It can be seen from Eq. 4.1, however, that the void fraction has the same inverse dependence on rotation speed as on core pressure; meaning that reducing the rotation speed will have the same undesirable effect on void fraction as reducing the core pressure. Here, the performance of Design 1 is optimized for two different rotation speeds and a wall temperature of 1500 K. First, Design 1 is run with the parameters from Table 4.1, including a rotation speed of 7000 rpm. Next, design parameters are optimized for the same geometry but with a 3500 rpm rotation speed. These run parameters are shown in Table 4.6, with the results plotted in Figure 4.29 through Figure 4.32. Reducing the rotation speed by half lowers the core temperature to 3200 K, a reduction of over 400 K.

Table 4.7 Parameters with Reduced Rotation Speed

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</tr>
<tr>
<td>Wall Temperature [K]</td>
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<td>1494</td>
</tr>
<tr>
<td>Void Fraction</td>
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</table>

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<tr>
<td>Mass Flow Rate [kg/s]</td>
<td>0.108</td>
<td>0.065</td>
</tr>
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<td>Reactor Power per CFE [MW]</td>
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<td>3.3</td>
</tr>
<tr>
<td>Core Temperature [K]</td>
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<td>3198</td>
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Figure 4.29 Fuel/Frit Temperature Profiles for 3500 rpm with Baseline Geometry

Figure 4.30 Propellant Temperature Profiles for 3500 rpm with Baseline Geometry
Figure 4.31 Void Fraction Profiles for 3500 rpm with Baseline Geometry

Figure 4.32 Power Density for 3500 rpm with Baseline Geometry
4.10. Lagrangian Analysis of Bubble Temperature

One of the prominent features of the MATLAB model results is the tendency of the gas temperature to rapidly increase toward the liquid uranium temperature over a short distance from the outer wall and thereafter the temperature difference between gas and liquid is on the order of tens of degrees Kelvin until the inner radius is reached. The observation then is that most of the heat transfer is accomplished across a small local temperature difference as the bubbles cross the annulus. To verify the reasonableness of this result, we turn in this section to a Lagrangian coordinate model of the bubble heat transfer where we attach our coordinate system to a simplified model of one bubble and observe the energy gain as the bubble moves through the liquid. The energy content and temperature of the bubble changes in time in response to the change in the surroundings of the bubble as the liquid around the bubble translates by the “stationary” bubble. In this case, those surroundings include the liquid temperature and the local gradient in the liquid temperature.

We begin by establishing a control surface around the surface of the bubble and writing the energy equation for the bubble control volume:

\[
\frac{d}{dt} \int_{cv} \rho e dV + \int_{cs} \rho \dot{V}_{rel} \cdot d\vec{A} = \dot{Q}_{net \ in} + \dot{W}_{net \ in\ shaft}.
\]  

(4.14)

Assuming there is no mass flux across the bubble surface and no work done on the bubble due to expansion (for simplicity a fixed-volume bubble) we have

\[
\frac{d}{dt} \int_{cv} \rho e dV = \dot{Q}_{net \ in}.
\]  

(4.15)

Introducing the heat capacity of a uniform-property bubble and Newton’s Law of Cooling, we have
\[
\frac{d}{dt} \left( \rho V c_{v,g} T_g \right) = h_B A_B \left( T_l - T_g \right). \tag{4.16}
\]

Next, we assume that \( \rho, V, c_{v,g}, A_B, \) and \( h_B \) are constants and group those constants. An ordinary differential equation can be written as

\[
\left[ \frac{\rho g V B c_{v,g}}{h_B A_B} \right] \dot{T}_g = T_l - T_g. \tag{4.17}
\]

With \( V_B = \frac{4}{3} \pi a^3 \) and \( A_B = 4 \pi a^2 \), we can write

\[
\frac{V_B}{A_B} = \frac{a}{3} = \frac{D_B}{6}. \tag{4.18}
\]

Next, we introduce a new temperature variable,

\[
\theta \equiv T_l - T_g, \tag{4.19}
\]

so that \( \dot{T}_g = \dot{T}_l - \dot{\theta} \). Equation 4.17 becomes

\[
\tau \left( \dot{T}_l - \dot{\theta} \right) = \theta \tag{4.20}
\]

where the time constant for the bubble heat transfer process can be written

\[
\tau = \frac{\rho g D_B c_{v,g}}{6 h_B}. \tag{4.21}
\]

Rearranging, the equation becomes

\[
\dot{\theta} + \frac{\theta}{\tau} = \dot{T}_l. \tag{4.22}
\]

A simple Galilean transformation allows \( \dot{T}_l \) to be written as

\[
\dot{T}_l = \frac{dT_l}{dt} = u \frac{dT_l}{dr}, \tag{4.23}
\]
so that

\[ \dot{\theta} + \frac{\theta}{\tau} = u \frac{dT_i}{dr}. \] (4.24)

We assume for simplicity that the bubble is rising with constant velocity through a constant temperature gradient so that the right side of Eq. 4.24 is a constant, \( C_T \equiv u \frac{dT_i}{dr} \), and we have

\[ \dot{\theta} + \frac{\theta}{\tau} = C_T. \] (4.25)

The solution to this ODE can be divided up into a homogeneous solution and a particular solution,

\[ \theta = \theta_H + \theta_P. \] (4.26)

The particular solution is a constant chosen to remove the inhomogeneity in the equation so that

\[ \theta_P = \tau C_T. \] (4.27)

The particular solution, \( \theta_P \), is a constant so that \( \dot{\theta} = \dot{\theta}_H \), and

\[ \dot{\theta}_H + \frac{\theta_H + \theta_P}{\tau} = C_T. \] (4.28)

The homogeneous equation is then

\[ \dot{\theta}_H + \frac{\theta_H}{\tau} = 0 \] (4.29)

so that

\[ \theta_H = ce^{-\frac{t}{\tau}} \] (4.30)
And the full solution is of the form

\[ \theta = ce^{-\frac{t}{\tau}} + \tau C_T \]  

(4.31)

An initial condition based on the temperature offset between the gas and liquid when the bubble appears at the outer wall establishes the constant of integration, \( c \),

\[ c = \theta_0 - \tau C_T \]  

(4.32)

where

\[ \theta_0 \equiv T_{l,0} - T_{g,0} \]  

(4.33)

so that the final form of the analytical solution is

\[ \theta = (\theta_0 - \tau C_T)e^{-\frac{t}{\tau}} + \tau C_T \]  

(4.34)

Let us evaluate Eq. 4.34 with the average values taken from a typical run of the MATLAB model, and we will assume a linear temperature profile for the liquid from 1500 \( K \) at the outer wall to 4000 \( K \) at the core across an annulus of 15 \( mm \). The selected values are \( \rho_g = 1.0 \ kg/m^3 \), \( d_B = 0.8 \ mm \), \( c_{v,g} = 22,800 \ J/kg\,K \), \( h_B = 28,700 \ W/m^2K \), and \( u = 2.8 \ m/s \). These produce \( \tau = 0.106 \ ms \), and \( C_T = u\frac{dT_t}{dr} = 466.67 \ K/ms \).

The evolution of the gas temperature in the bubble across the annulus is shown in Figure 4.33 for a notional annulus extending from 4.0 cm to 5.5 cm and the linear liquid temperature profile as shown. Here we transform bubble time back into position within the annulus with \( r = \frac{t}{u} \). The graph assumes the gas temperature at bubble formation is 500 \( K \) so that the initial offset between liquid and gas is 1000 \( K \).
The result shown in Figure 4.33 supports the finding from the MATLAB model that nearly all the temperature difference between the gas and liquid at injection is resolved very near the outer wall and a small (and in the case of a fixed liquid temperature gradient) constant temperature offset between the liquid and gas obtains across the remainder of the annulus. The steady temperature offset between the liquid and gas temperatures, $\theta_p = 49.4 \text{ K}$ is on the order of the results from the MATLAB model. The small time constant, $0.106 \text{ ms}$ for an annulus traverse time of $5.4 \text{ ms}$ allows the bubble to adjust quickly to the rising liquid temperature so that the temperature offset is maintained over almost the entire annulus.

Figure 4.33 An example result from the Lagrangian bubble model.
4.11. Potential Challenge – Bubble Shells

A challenge raised to the CNTP concept has been the idea that a thin solid uranium shell would form around the propellant bubbles as they are introduced into the annulus. This would be due to “cold” injected bubbles quickly cooling the uranium immediately around the bubble below the melting point of uranium, causing a thin solid shell to form. This would effectively result in a gas-filled metal sphere as in Figure 4.34.

![Figure 4.34 Propellant Bubble Surrounded by Uranium Shell](image)

The concern with this phenomenon is that if it were to occur and the shells become thick enough, these bubble shells could be thrown outward by centrifugal forces instead of passing through and exiting the uranium layer. This would result in propellant being trapped inside the CFE within these uranium shells. In order to assess the potential of forming such a shell we employ from Mills [74] a simple closed-form model of the steady-state interface temperature at the interface between two large and purely conductive media,
Rearranging Eq. 4.35 gives

\[
\frac{T_l - T_g}{T_l - T_{g,0}} = \frac{k_g}{k_l} \sqrt{\frac{\alpha_l}{\alpha_g}}.
\] (4.35)

The interface temperature, \(T_I\), is a function of the far-field temperatures of the liquid and gas along with the conductivities and diffusivities \((k\) and \(\alpha\), respectively) of the liquid and gas. The equation is the result of the coupling of two semi-infinite solids, and the solution gives a time-independent solution for the interface temperature. In using this equation as an estimator, we are neglecting the advection within and around the bubble, and we are assuming the average gas temperature within the bubble can be substituted for the far-field temperature in Eq. 4.36. This estimate of the interface temperature is plotted in Figure 4.35 for an example case within 0.2 mm away from the frit where the temperatures are closest to the solidification temperature of the uranium and the gas and liquid temperatures are the most disparate. The parameters for this case are those used in Table 4.1. The resulting interface temperature remains only a few Kelvins below the temperature of the uranium and is well above the solidification temperature despite the fact that the temperature of the propellant in the bubble is hundreds of Kelvins below the solidification temperature very near the frit. This result indicates that the conductivity of the uranium dominates, and the interface temperature is essentially the uranium temperature. When we consider the extremely small size and total heat capacity of these small bubbles (not accounted for in Eq. 4.36), it is likely that the interface temperature will be even closer to the uranium temperature as the heat transfer process would quickly raise
the temperature throughout the bubble. Therefore, it seems unlikely that the formation of a uranium shell around a bubble would occur.

Figure 4.35 Plot of Bubble Interface Temperature as Estimated by Equation 4.36

In addition, even if the formation of bubble shells did occur, the total weight of the bubble shell must be greater than that of the molten uranium displaced by the bubble and the shell in order for the encapsulated bubble to be thrown outward toward the frit by centrifugal forces. If the mass of the encapsulated bubble is lower than the displaced liquid, the bubble and shell would still be pushed inward by buoyancy. As the shell moves radially inward it would experience temperatures well in excess of the melting point of uranium, causing the shell to melt and allowing the engine to still effectively operate as envisioned.
To further investigate this possibility, the mass of a bubble shell was calculated and compared to the mass of an equivalent volume sphere of molten uranium. The physical properties used correspond to the properties at the outermost surface of the uranium annulus for the baseline run from Table 4.1. The mass of a bubble with a surrounding shell is given in Eq. 4.37, and the mass of an equivalent volume of molten uranium is given in Eq. 4.38.

\[ m_{sphe} = m_B + \rho_s \pi \frac{4}{3} \left( (t_s + a)^3 - a^3 \right). \]  

\[ m_t = \rho_l \pi \frac{4}{3} (t_s + a)^3. \]  

In these equations, \( t_s \) is the shell thickness, \( m_B \) is the mass of a bubble at injection previously given by Eq. 3.77, and \( \rho_s \) is the density of solid uranium. Using the values from the run described in Table 4.1 evaluated at the outer surface of the fuel annulus, along with a solid uranium density at the melting point of 17721 kg/m³ (from Kirillov [49]), the mass of the bubble shell and the mass of an equivalent uranium volume are calculated and plotted in Figure 4.36 as a function of the shell thickness divided by the equivalent bubble radius, \( t_s/a \). The analysis indicates that the mass of the encapsulated bubble will be lower than the mass of an equivalent sphere of molten uranium until the shell thickness becomes roughly 1.74 times the equivalent radius of the propellant bubble. Therefore, even if a shell were able to form around a bubble it would have to be very thick relative to the size of the bubble before the phenomenon became a problem affecting engine performance. Based on the results of these two approaches to analyzing the question of bubble shells, it seems extremely unlikely that the problem will occur.
Figure 4.36 Comparison of Bubble Shell Mass Versus Equivalent Molten Uranium Sphere Mass
CHAPTER 5. STUDY SUMMARY, FUTURE WORK, AND FINAL CONSIDERATIONS

5.1. Summary

An engineering model of a conceptual nuclear thermal propulsion system with molten uranium fuel has been created using a simple finite-difference approach to analyze the temperatures within the centrifugal reactor. This model was developed and run within MATLAB R2020a. The model analyzed a single centrifugal fuel element, including the annular fuel region and the surrounding porous frit in the analysis, as well as modeling the convective heat transfer to the propellant inside of the clearance gap around the fuel element. This model treats the heat transfer in the uranium fuel as solid conduction for the sake of simplicity. The purpose of this study was to understand the maximum propellant temperatures which may be attained in a CNTP system for a given frit temperature, as well as whether or not adequate heat transfer to the bubbles could be attained.

The model relied heavily on thermophysical property data of hydrogen, liquid uranium, silicon carbide and zirconium carbide which were sourced from the literature and integrated into the current model. It also employed models of supporting phenomena such as:

- Bubble formation.
- Bubble velocity.
- Bubble heat transfer.
- Taylor-Couette flow.
• Laminar developing flow in a round duct.
• Energy generation from nuclear decay.

Because this model assumes the fuel annulus is stationary, mixing which would likely result from the high-velocity hydrogen bubbles moving through the liquid uranium was neglected. As a result, the performance predictions can be viewed as best-case outcomes, as they establish an upper performance boundary for the engine, since incorporating the effect of mixing will lower the core temperature.

5.2. Observations

A number of key observations can be made which are useful for guiding future investigations and designs into CNTP systems:

• The temperature of the propellant bubbles rises to meet the local uranium temperature very quickly, such that by the time the bubbles move approximately 1.5 mm into the fuel annulus they are at approximately the same temperature as the fuel.
• The desire to keep the maximum void fraction to a reasonable value (40% in this study) introduces a significant constraint on the mass flow rate.
• A major constraint on the core temperature is the strongly nonuniform nuclear energy generation presently predicted for these annular geometries.
• High core pressure and high rotational speeds are required to achieve core temperatures of 4000 K while maintaining a containing-wall temperature of 1500 K. These requirements introduce additional constraints on engine performance and additional design challenges that are beyond the scope of this study.
Based on this study, a maximum temperature in the range of 5000 to 5500 $K$ is not achievable while maintaining a 1500 $K$ wall temperature. Either a lower core temperature must be used, or the wall must be designed such that it can withstand temperatures in the 2500 – 3000 $K$ range.

5.3. Future Work

Although the maximum propellant temperatures attained in the CNTP reactor (with a 1500 $K$ wall temperature) are lower than what is desired, it should be noted that from the study by Barrett [16] the $I_{sp}$ of a uranium-fueled system would degrade rapidly beyond about 3300 $K$ due to uranium vaporization. If the uranium is hot enough, a significant quantity of uranium fuel is vaporized, increasing the average molecular weight of the exhaust gases. The specific impulse would then be reduced. A more detailed study looking at mass transfer in a CNTP system is needed to verify some of the assumptions used in the study by Barrett and the similar results from Nelson et al. However, if Barrett’s analysis was correct, one may not wish to get fuel temperatures hotter than 3300 $K$ if a metallic uranium fuel is used.

This study has focused on developing an understanding of the thermal processes within a CNTP reactor. However, there are a number of other research areas which will need to be seriously investigated.

This model used a Taylor-Couette flow model to calculate the heat transfer to the propellant in the clearance gap. However, it is acknowledged that there are some significant differences between textbook Taylor-Couette flow and the flow situation which would be present in the clearance gap of a CFE. In particular, the gases in the CFE
clearance gap are being ingested into the CFE itself instead of simply circulating around the CFE. Because of this, a CFD simulation using Fluent or some other software to investigate this unique flow phenomenon could be useful in further CNTP investigations.

The present model assumes bubble velocities computed from the terminal velocity of a rising cap-shaped bubble at the bubble sizes computed from thermodynamic considerations. This construction is consistent with past studies and avoids the solution of the momentum field in a high-void-fraction two-phase flow with internal energy generation. A computational fluid dynamics study of a more realistic treatment of this problem would pose a research problem that may be well beyond present and reasonable computing limits.

Another area of further research is in the field of neutronics modeling and optimization. As mentioned previously, the highly asymmetric power generation distribution of the CFE results in thermal gradients which make it difficult to maintain a 1500 K wall temperature and a high core temperature. If the CNTP reactor geometry and/or materials could be reconfigured to provide a more uniform power distribution, the performance of the reactor would be significantly enhanced.
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