

Sensitivity Analysis of Thermophysical Properties of Molten Salts using a Molten Salt Demonstration Reactor Model in TRANSFORM

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Sarah Elizabeth Creasman

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One never notices what has been done; one can only see what remains to be done.

-Marie Curie, Letter to her brother (1894)

I have no dress except the one I wear every day. If you are going to be kind enough to give me one, please let it be practical and dark so that I can put it on afterwards to go to the laboratory.

-Instructions regarding a proposed gift of a wedding dress for her marriage to Pierre in July 1895, as quoted in “Madame Curie: A Biography” by Eve Curie Labouisse, as translated by Vincent Sheean, p. 137

Abstract

Molten Salt Reactors (MSRs) are currently of interest due to the push for smaller reactors that are easier to deploy and the need for sustainable energy around the world. Nuclear energy can play an important role in addressing the issue of energy inequality and climate change. One of the main obstacles to deploying MSRs is licensing. An important aspect to understand in terms of licensing is the uncertainty of the thermophysical properties of the molten salt at the beginning of the cycle and during normal operations and transients. MSRs have already been proven as a viable concept; two research reactors—The Aircraft Reactor Experiment and the Molten Salt Reactor Experiment—have been successfully built and operated at Oak Ridge National Laboratory (ORNL) in 1954 and from 1965-1969, respectively. In this research, an MSR design similar to the proposed Molten Salt Demonstration Reactor design from ORNL in the 1970s was modeled using the Modelica programming language-based TRANSFORM library. Ultimately, this work’s analysis addresses the impact thermophysical property uncertainty has on reactor behavior during steady-state and transient conditions. To explore the reactor behavior, a sensitivity analysis is performed of density, viscosity, thermal conductivity, and heat capacity through the parameter space. This was performed for steady state conditions and transient conditions including a reactivity insertion and partial flow blockage. This sensitivity analysis facilitates the study of the effect that uncertainty has on operation. From this analysis, it was found that varying the heat capacity had the most effect on the temperature by a wide margin, but even so no property was found to have a significant

change to temperature when it was perturbed during both steady state and transient conditions. Based on these conclusions, molten salt developers and researchers should be reassured that the current uncertainty of the four thermophysical properties investigated here, density, thermal conductivity, heat capacity, and viscosity, are well within the bounds of safe operation.

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List of Acronyms

ANL	Argonne National Laboratory
ARE	Aircraft Reactor Experiment
BOP	Balance of Plant
CIET	Compact Integral Effects Test
CMSR	Compact Molten Salt Reactor
DSC	Differential Scanning Calorimetry
Dymola	Dynamic Modeling Laboratory
FLiBe	LiF-BeF ₂ (67-33 mole %)
HALEU	High Assay Low Enriched Uranium
IMSR	Integral Molten Salt Reactor
INL	Idaho National Laboratory
LEU	Low Enriched Uranium
LFTR	Liquid Fluoride Thorium Reactor
LWR	Light Water Reactor
MCFR	Molten Chloride Fast Reactor

MSBE Molten Salt Breeder Experiment

MSBR Molten Salt Breeder Reactor

MSDR Molten Salt Demonstration Reactor

MSR Molten Salt Reactor

MSRE Molten Salt Reactor Experiment

MSRR Molten Salt Research Reactor

MSTDB-TP Molten Salt Thermal Properties Database-Thermophysical

NEUP Nuclear Energy University Program

NRC Nuclear Regulatory Commission

ORNL Oak Ridge National Laboratory

PCL Primary Coolant Loop

PFL Primary Fuel Loop

PHX Primary Heat Exchanger

RAVEN Risk Analysis and Virtual Control Environment

SHX Secondary Heat Exchanger

SMR Small Modular Reactor

SNF Spent Nuclear Fuel

TRANSFORM Transient System Framework of Reconfigurable Models

Chapter 1

Introduction

1.1 Dissertation Goals

The following are goals for this dissertation:

- Investigate four thermophysical properties: density, thermal conductivity, heat capacity, and viscosity
- Investigate uncertainties in molten salt thermophysical properties that could be a risk to licensing
- Investigate steady state and transient scenarios
- Provide a review of measurement techniques
- Determine uncertainty values for all four thermophysical properties
- Determine if measurements need to be refined
- Determine if thermophysical properties need to be known with less uncertainty

1.2 Overview

One of the aims of the Paris Agreement, the international treaty on climate change, is to hold the increase in the global average temperature to well below 2°C above pre-industrial levels since this would significantly reduce the impacts and risks of climate change. To achieve this, coal power plants need to be phased out and replaced with clean energy sources, such as nuclear, wind, or solar. Currently, there is an increase in energy consumption in the developing world with over 100 million more people connected to the power grid every year since 2010 [1]. Since the developing world cannot afford more climate friendly energy sources, such as nuclear, wind, or solar, they have predominately been using fossil fuels since they are cheap. Introducing an alternative that is cheaper than fossil fuels is fundamental to continuing the decrease in global poverty and reducing greenhouse gas emissions that must be curbed to mitigate climate change. Nuclear energy will play a critical role in this.

In 2001, the Gen IV International Forum was established and chose six types of advanced reactors to pursue. Molten Salt Reactors (MSRs) were included as one of these six reactor types; renewing interest in the technology originally explored in the 1940s-1970s. Since then, more and more interest has been sparked for MSRs with both public and private funding being allocated.

There are 2 different types of MSRs: salt-cooled and salt-fueled. The salt-cooled MSRs use molten salt as the coolant only and use solid fuel. In a molten salt-fueled reactor, the fuel itself is a molten salt fluid. In this dissertation, molten salt-fueled reactors are the subject and MSR will refer to only the salt-fueled ones.

In a Light Water Reactor (LWR), the fuel is contained in solid fuel rods with water flowing through the core and acting as both moderator and coolant. Conversely, MSRs have liquid fuel that flows around the primary loop through the reactor core to the Primary Heat Exchanger (PHX) and then back to the core. Unlike LWRs, MSRs operate at high temperature and low pressure, eliminating the need for large reactor vessels and thick containment buildings. MSRs also have a high thermal efficiency

of around 44% versus a thermal efficiency of 33% for the typical turbines in current nuclear power plants, allowing MSRs to produce the same amount of electricity as LWRs using less fissile material than LWRs [2]. The high operating temperature of MSRs opens up the possibility of economical hydrogen production, grid storage facilities, and opportunities to be used as process heat, in addition to the better efficiency for generating electricity.

MSRs could eventually make beneficial use of Spent Nuclear Fuel (SNF), minimize the need for high level waste repositories, minimize weapons-usable material in storage, and increase proliferation resistance of nuclear power [3]. In addition to these benefits, it would also reduce the cost of fuel fabrication and handling since the fuel needs less processing due to being a liquid.

1.3 History

The bulk of MSR research took place between the 1940s and the 1970s. During that time, two research reactors were built and operated. The first of these was the Aircraft Reactor Experiment (ARE), which was part of the Aircraft Nuclear Propulsion program at Oak Ridge National Laboratory (ORNL) which investigated MSRs to develop a nuclear powered airplane [2]. In the 1950s, the ARE was built to investigate fluoride molten salts for aircraft propulsion reactors and to study the nuclear stability of circulating fuel systems. ARE was successfully operated between November 8-12, 1954 at ORNL and had steady state outlet temperatures up to 860°C and a maximum sustained power of 2.5 MW. In total, it generated 96 MW-hours of energy [2], [4]. ARE's fuel salt was NaF-ZrF₄-UF₄ (53.09-40.73-6.18 mole %) with highly enriched uranium of 93.4% ²³⁵U. The moderator was beryllium oxide and all the piping was made of Inconel. The neutron spectrum was thermal and epithermal. During the operation, it was both stable and self-regulating and there were no chemical or mechanical problems found.

The second research reactor was the Molten Salt Reactor Experiment (MSRE), which ran from 1960-1969. The purpose of this project was to demonstrate MSR technology gleaned from ARE and extend that technology to an MSR power reactor. The MSRE was a 7.4 MW_{th} test reactor that operated between 1964 and 1969 [5]. The fuel salt for the MSRE was LiF-BeF₂-ZrF₄-UF₄ (65-29.1-5-0.9 mole %) and the coolant salt was LiF-BeF₂ (67-33 mole %) (FLiBe). The lithium had to be enriched to 99.99% ⁷Li, and the uranium enrichment was 33% ²³⁵U. It was moderated using graphite, and Hastelloy-N was used for the structural components and piping. The layout of the MSRE reactor can be seen in Figure 1.1, and a schematic of the reactor vessel can be seen in Figure 1.2. It was determined the salt chemistry behaved well at the high temperatures seen in the reactor and in the high radiation environment of the reactor. The reactor's dynamic behavior correlated well with predictions as reported by Kerlin et al. [6]. The MSRE had several achievements, including the first reactor to use mixed U/Pu fuel salt, the first reactor to use U-233 fuel, online refueling, and over 13,000 fuel power hours [7].

1.4 Design

The design space for MSRs is vast. The fuel salt can be made up of fluorides, chlorides, or even nitrates, and the neutron spectrum can be thermal, epithermal, or fast. The reactor can be a breeder or a burner. There are also a plethora of fuel options including Low Enriched Uranium (LEU), High Assay Low Enriched Uranium (HALEU), thorium, plutonium, and SNF. There are several companies and governments working on designs, including the USA, China, India, Copenhagen Atomics, and Thorcon Power. A list of these with some design choices can be seen in Table 1.1. All the reactor designs in Table 1.1 have a thermal neutron spectrum and all have forced circulation. Copenhagen Atomic's MSR design is heavy water moderated, but all the others are moderated with graphite.

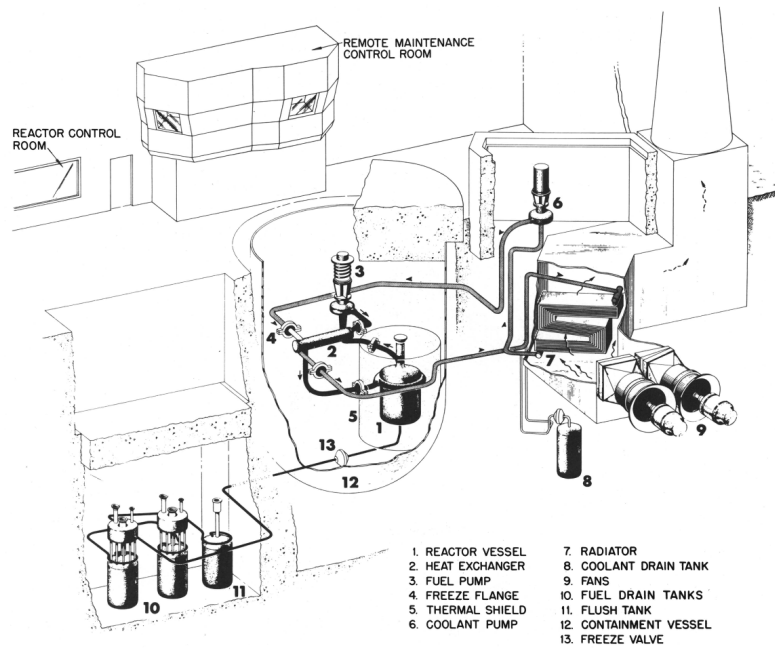


Figure 1.1: Layout of MSRE from [8]

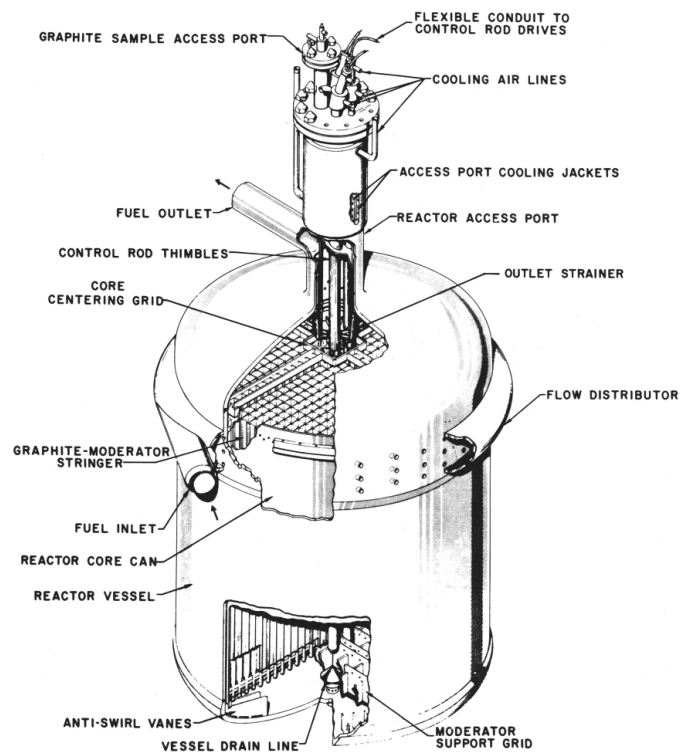


Figure 1.2: Reactor Vessel from [8]

Table 1.1: MSR concepts and their specifications

Company	Concept	Power ($\text{MW}_{th}/\text{MW}_e$)	Country	Fuel	Core Inlet/Outlet Temperature ($^{\circ}\text{C}$)
Japan	FUJI	450/200	Japan	$\text{ThF}_4 + \text{UF}_4 + \text{carrier salt}$	565/704
CAS-SINAP	smTMSR-400	400/168	China	$\text{FLiBe} + \text{Th-U}$ (19.75% U-235)	650/700
Copenhagen Atomics	Waste Burner 0.2.5	100/(not defined)	Denmark	LiF-ThF_4	600/650-700
ThorCon Power	ThorCon TMSR-500	557/250	US	$\text{UF}_4 + \text{ThF}_4 + \text{carrier salt}$	565/704
Flibe Energy	LFTR	600/250	US	$\text{LiF-BeF}_2 + \text{UF}_4\text{-ThF}_4$	500/650
Terrestrial Energy	IMSR	440/195	Canada	5% U-235 LEU	620/700

The Fuji design is a 200 MW_e Liquid Fluoride Thorium Reactor (LFTR) that has a thermal power of 350 MW_{th} [9]. Copenhagen Atomics, a company in Denmark, is developing a design for MSRs that will fit in a shipping container in order to make them easily mass manufactured. It is planned to be a single-fluid, waste burner, fluoride-based reactor that is autonomously controlled. Terrestrial energy uses a denatured MSR design that is currently undergoing licensing. It uses LEU fuel and has a compact, replaceable core unit. The Integral Molten Salt Reactor (IMSR) finished the first stage of pre-licensing review by the Canadian Nuclear Safety Commission in 2017.

In addition to those listed in Table 1.1, there are other MSR designs; Terrapower, Abilene Christian University, and Seaborg Technologies are a few. The Molten Chloride Fast Reactor (MCFR) designed by Terrapower in collaboration with Idaho National Laboratory (INL) is a 30 MW_{th} fast research reactor. Abilene Christian University has applied for a construction license with the Nuclear Regulatory Commission (NRC) for their 1 MW_{th} Molten Salt Research Reactor (MSRR); they currently have plans to achieve criticality by December of 2025. Seaborg Technologies in Denmark is developing the core for a compact MSR aptly named Compact Molten Salt Reactor (CMSR); the first version of their core design is expected to produce 250 MW_{th} and 100 MW_e. It is expected to be a high temperature, thermal neutron spectrum, single salt design that uses LEU fuel. It will use a proprietary NaOH moderator. The core is estimated to be replaced every 12 years, and the fuel is not replaced during operation.

1.5 Licensing

The main challenge to proving the MSR design concept and obtaining NRC licensing is the intrinsic difference between liquid fuel and solid fuel. For LWRs, an accident scenario is significant if there is fuel failure or fission product release into the coolant.

For an MSR, the fission products are already in the coolant, making the solid-fueled reactor accident discussion irrelevant to MSRs. Due to this difference, the current standard, NRC-approved modeling and simulation tools for LWRs will not suffice for MSRs due to the neutron precursor drift and the evolution of the molten salt properties. Additionally, data on thermophysical properties for molten salts is lacking, especially for chloride molten salts. Uncertainty quantification and sensitivity quantification are very important when considering licensing. Licensing will consider reactor operations under molten salt conditions bounded by the uncertainties in their physical and chemical properties. This research sets out to provide insight into which molten salt properties have the most effect on the reactor in terms of safety to allow for a smaller, more focused experimental envelope for molten salt measurements. If there is a better understanding of uncertainty, the variability goes down, therefore the cost goes down. The primary goal of this research is to gain a greater understanding of how uncertainty in the thermophysical properties impacts reactor operation and safety to help accelerate licensing of MSRs and propel their deployment.

It is important to point out the differences between LWRs and MSRs since most of today's regulatory and licensing experience is with LWRs. MSRs operate at near atmospheric pressure and in a temperature range of 500-1400°C, whereas LWRs operate at a pressure of approximately 150 atm and at a temperature around 315°C for Pressurized Water Reactors and at a pressure of 75 atm and a temperature of 285°C for Boiling Water Reactors. This results in MSRs having better thermodynamic efficiency than LWRs due to their ability to maintain low vapor pressure at high temperature. The fraction of delayed neutrons versus prompt neutrons is an important regulatory aspect in all nuclear reactors. MSRs introduce a new challenge into the mix, since the amount of delayed neutrons happening inside the core versus outside the core must be taken into account, whereas in LWRs all the delayed neutrons happen inside the core. MSRs need less fissile material than LWRs since the fuel salt can be reprocessed and fuel can be added while the MSR is in operation. Even with no reprocessing,

the xenon and krypton gases will escape via the off-gas system. For reactors with solid oxide fuel, the fuel must never reach a molten state to ensure safety; whereas to ensure safety for MSRs, the solutions must be in a molten state to keep the fission products and actinides in solution [3], [7].

1.6 Thermophysical Properties

There are four thermophysical properties investigated in this thesis: density, viscosity, thermal conductivity, and heat capacity. The thermophysical properties of molten salts are not well characterized for several reasons. For one, multi-component mixtures rely on extrapolation of simpler phase diagrams for prediction of even the simplest properties such as freezing/melting point if no direct experimental data is present. There is limited experimental data for several salt mixtures, irradiated salt mixtures in particular. For some measurements, such as thermal conductivity, reported values are drastically different for the same salt mixture. Others, such as thermal conductivity and heat capacity in particular, are hard to measure. Significant uncertainty in experimental values can also be caused by instrumental limitations. Another issue is even if good data exists for the clean (beginning of cycle) molten salt with no impurities, the fuel salt quickly evolves due to corrosion and burnup causing fission products and corrosion products to become part of the salt. There is significant uncertainty about the effects contaminants have on salt behavior. There is uncertainty in the experimental values, as well as the salt composition itself. Properties within the reactor could and most likely will change throughout operation due mostly to burnup and how they change during operation are subject to the uncertainties in their properties. Significant uncertainty in the properties exists, as well as significant uncertainty in how the properties affect reactor behavior. Property uncertainty could influence reactor behavior in ways that affect the safe, efficient, and economical operation of MSRs. The impact this uncertainty in basic thermophysical property

data has on modeling predictions of both normal operations and during transient scenarios will need to be understood by MSR researchers and developers alike.

1.7 Thesis Synopsis

This research uses modern system computational tools to investigate the impact of thermophysical property uncertainty under normal and transient conditions. This area of interest has been explored in Robertson and Short [10], Williams et al. [11], and Abou-Jaoude et al. [12]; this study will go more in depth and explore the effect uncertainty has on reactor performance, as well as safety. In addition, another objective of this study compiles data on molten salt thermophysical property values and explores the methods used to obtain these experimental and analytical values. Ultimately, the analysis in this work addresses the impact uncertainty in the four thermophysical properties has on reactor behavior during steady-state and transient conditions. To do this, a sensitivity analysis is performed of density, viscosity, thermal conductivity, and heat capacity through the parameter space. This facilitates the study of the effect uncertainty bounds have on operation. The coolant salt used for this study is LiF-BeF₂ (67-33 mol%) with 99.995% enrichment for Li-7 and the fuel salt used is LiF-Be₂-ThF₄-UF₄ (71.5-16-12-0.5 mol%).

Chapter 2 provides an overview of the thermophysical properties and their measurement techniques. Chapter 3 includes the methodology used in this analysis. Chapter 4 has the results of this study. Chapter 5 contains a discussion of these results. A summary and conclusion are included in Chapter 6.

1.8 Author's Contribution

The work presented in this dissertation explores historical knowledge and contributes new knowledge about molten salt thermophysical properties. This is important for

licensing, the safety envelop, and eventually MSR deployment. Several publications came out of this work; Creasman et al. 2023 [13] and Rose and Creasman 2022 [14]

- Comparison of thermophysical property values from literature
- Compilation of experimental methods
- Determination of uncertainties used in this sensitivity analysis
- Modified TRANSFORM models to change the thermophysical properties, pipe diameters, and reactor kinetics
- Ran simulations to perform a sensitivity study for steady state and transient events
- Analyzed and discussed the results of the sensitivity study

Chapter 2

Salt Properties

This dissertation will focus on the standard thermophysical properties that are related to performance of the molten salt as a reactor fuel salt. These properties are density, viscosity, thermal conductivity, and heat capacity. This is not meant to be a complete list of properties important to the reactor performance or other parts of the reactor. These four thermophysical properties are currently being investigated at national laboratories: ORNL [15] and Argonne National Laboratory (ANL) [16]. They are included in several molten salt property compilations. Magnusson et al. [17] covered these four plus electrical conductivity in their 2020 report. Sohal et al. [18] included these four properties plus surface tension in their 2013 INL report. A panel of experts identified the thermophysical properties of primary interest in terms of modeling and simulation to be viscosity, thermal conductivity, heat capacity, and coefficient of thermal expansion [19]. These four thermophysical properties along with surface tension were included as the thermal-hydraulic properties of interest in their report since they are important to transport phenomena, as well as important in evaluating the momentum and energy balance of the molten salt. They are also the four thermophysical properties included in the Molten Salt Thermal Properties Database-Thermophysical (MSTDB-TP) [20]. It is a collection of empirical models

for the thermophysical properties, ρ , ν , κ , and C_p , as a function of both temperature and composition.

These four thermophysical properties (density, viscosity, thermal conductivity, and heat capacity) investigated here are used as inputs to reactor system models. There are other thermophysical properties in these models such as heat transfer radiation, optical properties, and surface tension. In these models, if heat transfer from radiation is included, it is simplified by the assumption that it is black body radiation. Optical properties are not being used in these models since they are not available. The reason that optical properties are not available for fluoride salts is that they must be heated in a transport cell to measure the properties; the fact that fluoride eats through sapphire and even scuffs diamond makes these measurements difficult. As for interfacial properties, like surface tension and wetting properties, reactor system models do not take them into account.

2.1 Density

Density is important to the heat transfer capabilities of the molten salt. The fact that density decreases linearly with increasing temperature is true for molten salts and can be seen in Eq. 2.1. This equation is recommended for use to predict the density of salt mixtures [21]

$$\rho_{mix}(T) = \frac{\sum_{i=1}^n N_i M_i}{\sum_{i=1}^n N_i V_i(T)}, \quad (2.1)$$

where N_i is the mole fraction of component i, M_i is the molecular weight of component i, and V_i is the molar volume of component i at temperature T. This equation along with the molar volumes of the single compounds from Table 2.1 allow for estimation of the densities of molten salt mixtures [21].

Table 2.1: The empirical molar volumes of fluorides from [21]

Component fluoride	Molecular weight (g/mole)	Molar volume (cm ³ /mole)	
		600°C	800°C
⁷ LiF	26.0	13.46	14.19
NaF	42.0	19.08	20.20
KF	58.1	28.1	30.0
RbF	104.5	33.9	36.1
CsF	151.9	40.2	43.1
BeF ₂	47.0	23.6	24.4
MgF ₂	62.3	22.4	23.3
CaF ₂	78.1	27.5	28.3
AlF ₃	86.7	26.9	30.7
YF ₃	145.9	34.6	35.5
LaF ₃	195.9	37.7	38.7
CeF ₃	197.1	36.3	37.6
PrF ₃	197.9	36.6	37.6
SmF ₃	207.36	39.0	39.8
ZrF ₄	167.2	47.0	50.0
ThF ₄	308.0	46.6	47.7
UF ₄	314.0	45.5	46.7

Another method for prediction of molten salt density is the Redlich-Kister expansion; this method accounts for non-ideal mixing, as well as ideal mixing. It has been used in several studies to estimate the density of pseudo-ternary fluoride salts [22], [23].

According to Magnusson et al. [17], the sole author of experimental density data for LiF-BeF₂-ThF₄ fuel salt is Cantor [24] and the sole publisher of experimental density data for LiF-BeF₂-UF₄ fuel salt is Blanke [25]. There is no known experimental density data for LiF-BeF₂-ThF₄-UF₄.

Blanke et al. [25] presents raw data for compositions of LiF-BeF₂-UF₄ and FLiBe which can be seen in Table 2.2. This set of data was obtained using buoyancy to measure the change in weight of a solid of known volume, in their case a platinum cylinder, immersed in the solution of molten salt. The apparatus can be seen in Figure 2.1. The overall experimental error cited for this method was $\pm 1\%$ [25].

In 1973, Cantor’s experiments to measure the densities as a function of temperature for FLiBe and LiF-BeF₂-ThF₄ were conducted using a nickel dilatometer [24]. In this method, changes in liquid level are detected by a metal probe in the neck of a volume-calibrated metal vessel. The results for FLiBe are in Table 2.3, along with those calculated using an equation determined by the least squares evaluation of the data, which can be seen in Equation 2.2. The apparatus can be seen in Figure 2.2.

$$\rho(g/cm^3) = 2.2797 - 4.884 \times 10^{-4}T(^{\circ}C) \quad (2.2)$$

An equation with an unspecified temperature range was given by Cohen et al. [26] for a composition of LiF-BeF₂-ThF₄-UF₄ (71-16-12-1 mol%), where they assigned a 5% uncertainty, and seen in Equation 2.3.

$$\rho(g/cm^3) = 3.82 - 8.2 \times 10^{-4}T(^{\circ}C) \quad (2.3)$$

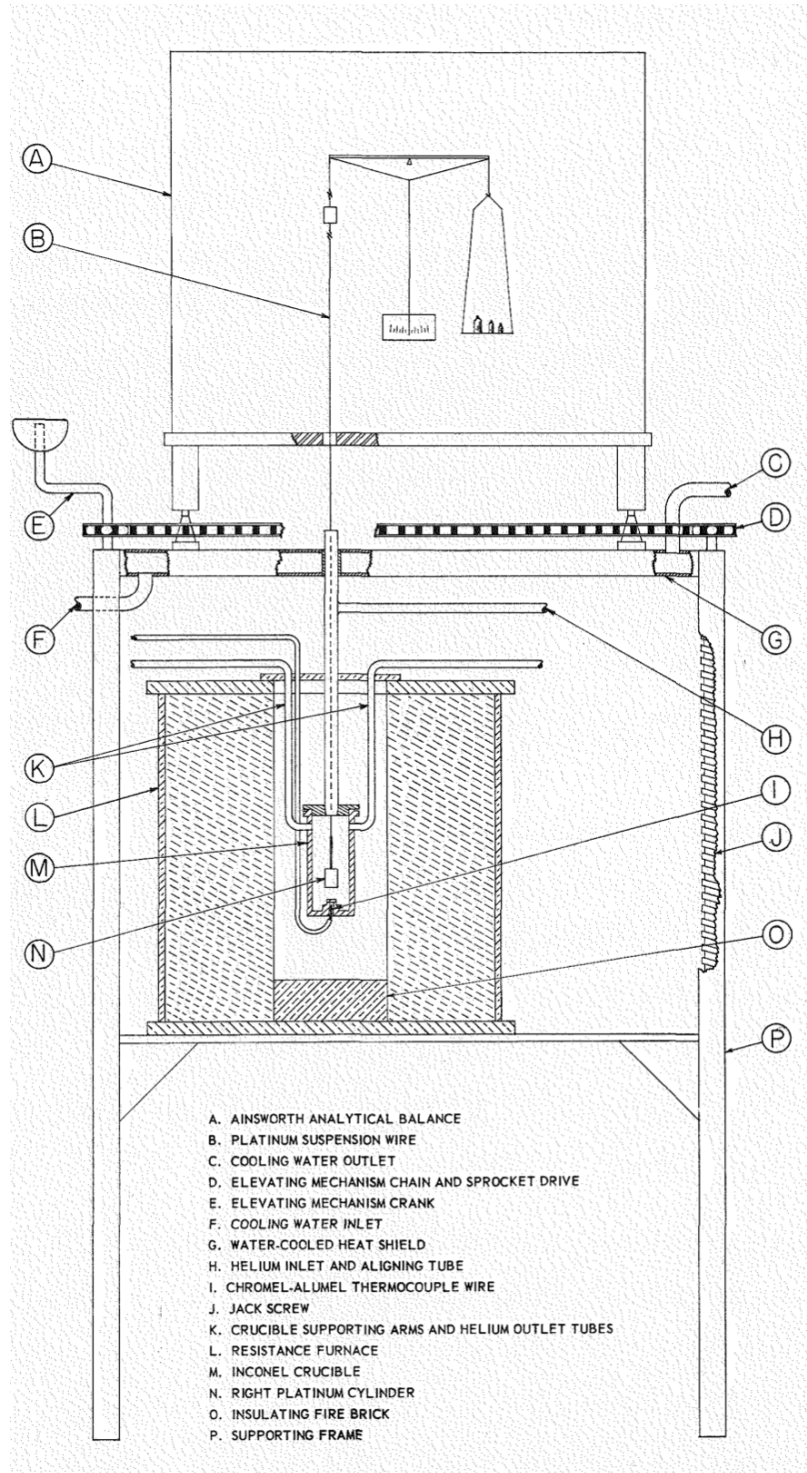


Figure 2.1: Schematic Diagram of the Density Apparatus used by Blanke et al. in the 1950s [25]

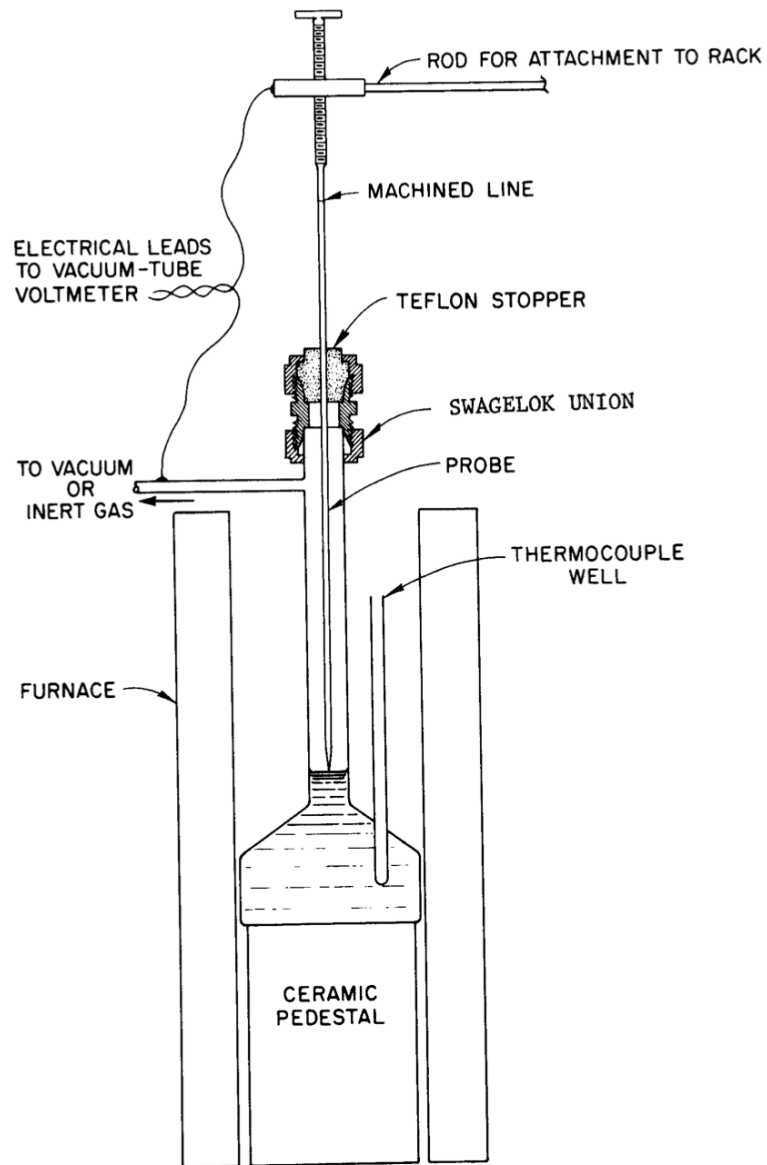


Figure 2.2: The nickle dilatometer used by Cantor [24]

Table 2.2: Raw density data from [25] (Units of g/ml)

Salt & Composition	600°C	700°C	800°C
LiF-BeF ₂ (66.67-33.33 mol%)	1.941	1.905	1.866
LiF-BeF ₂ -UF ₄ (70-22-8 mol%)	2.825	2.772	2.725
LiF-BeF ₂ -UF ₄ (70-18-12 mol%)	3.208	3.154	3.134

Table 2.3: Raw density data from [24] (Units of g/cm³)

Salt & Composition	590.5°C	614.6°C	667.1°C	719.5°C	794.7°C	820.3°C
LiF-BeF ₂ (66-34 mol%)	1.991	1.979	1.954	1.928	1.891	1.879
Calculated from Equation 2.2	1.9913	1.9795	1.9539	1.9283	1.8915	1.8790

More recently, Gallagher et al. built a custom system to measure the density of molten salts [27]. Their method was based on the Archimedes principle and used a mass/volume calibrated high purity platinum plummet, which is suspended by a thin wire from a precision balance. The weight of the immersed sinker is measured using the balance. This technique can not be used for volatile salts due to its open top. A schematic of this can be seen in Figure 2.3. The maximum relative error is less than 6%, with the largest uncertainty happening at low temperatures [28]. “The source of this error is expected to be due to a non-uniformly melted specimen during measurement” [27].

Alternatively, sealed-vessel dilatometry is a more appropriate measurement method for volatile or hazardous salts. Sealed-vessel dilatometry measures a salt of known mass that is contained in a tube that has been volume calibrated; from this, the changes in fluid height are measured and used to determine the change in density with respect to temperature. Currently, the change in height is typically performed visually with the salt sample in a glass container, which is possible for chloride molten salts, but not for fluoride salts. According to Gallagher et al., there is a x-ray-based image system currently under development that may look something like Figure 2.4 that will be able to measure non-transparent crucibles for fluoride salts [27].

2.2 Viscosity

The viscosity is important for both fluid dynamics and heat transfer performance, and affects several important aspects of the reactor including the flow velocity, the total power and power distribution, and the distribution of salt temperatures throughout the core and flow loops. It is important in terms of natural circulation, more specifically the timing of the transition from forced circulation to natural circulation. In addition, fluid viscosity sees a significant impact from compositional changes.

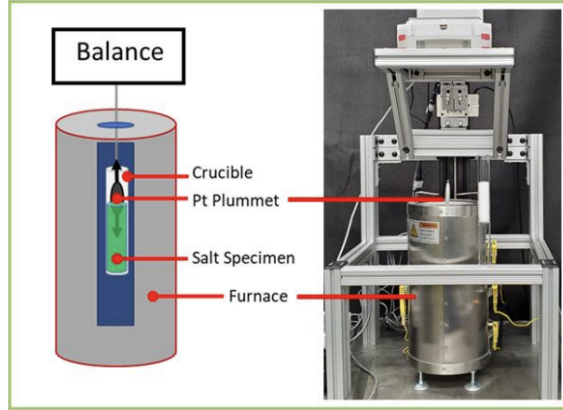


Figure 2.3: The Archimedes-bob density system using by Gallagher et al. [27]

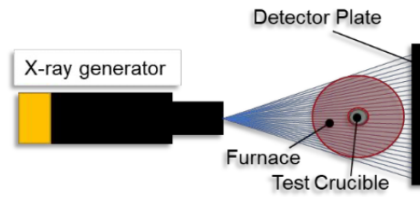


Figure 2.4: An illustration by Gallagher et al. for measuring the density and viscosity by x-ray imaging for non-transparent fluids [27].

Assuming liquid molten salts have normal fluid behavior and are Newtonian fluids, Equation 2.4 can be used to determine the viscosity.

$$\mu(cP) = A \times \exp(-B/T(K)) \quad (2.4)$$

where μ is the viscosity, T is the temperature in Kelvin, and A and B are coefficients obtained from goodness of fit for an exponential least squares analysis.

Blanke et al. [25] presents raw viscosity data for compositions of LiF-BeF₂-UF₄ and FLiBe. Raw viscosity is not given for LiF-BeF₂-ThF₄-UF₄, but is given for 2 different compositions of LiF-BeF₂-ThF₄ in Cantor [24]. These values can be seen in Figure 2.5 and Table 2.4. Measurements in both of these works were obtained for a temperature range up to 900°C using a concentric cylinder viscometer. This apparatus can be seen in Figure 2.6. The overall experimental error, including the error for the density measurement, was estimated at $\pm 5\%$ [25].

In MacPherson [29], there were three different viscometer cups used to measure viscosity and all three are plotted in Figure 2.7; the fit line from least squares analysis is also plotted and yielded Equation 2.5. These were found using a skirted capillary efflux viscometer. No error was given.

$$\mu(cP) = 0.0812 \times \exp(-4422/T(K)) \quad (2.5)$$

Cohen et al. references their own unpublished work and presents 3 viscosity values (seen below) each at a different temperature for a fuel salt composition of LiF-BeF₂-ThF₄-UF₄ (71-16-12-1 mol%) and the exponential form of the viscosity equation seen in Eq. 2.6 [26]; these values are also seen in Cohen and Jones [30]. This data set has 10% uncertainty [30].

Table 5. Viscosity of $\text{LiF-BeF}_2\text{-ThF}_4$

(72.7-15.7-11.6 mole %)

Least-squares fit: $\eta(\text{cP}) = 0.1094 \exp (4092/T(^{\circ}\text{K}))$

T($^{\circ}\text{C}$)	Experimental $\eta(\text{cP})$	Calculated $\eta(\text{cP})$
553	14.1, 14.3, 14.1 ₅	15.5
582	12.4, 13.4, 13.0	13.1
613	11.4, 11.2, 11.1	11.1
638	9.74, 9.56, 9.47	9.76
622	11.5, 11.5, 11.4	10.6
588	13.4, 13.5, 13.4	12.7
555	15.5, 16.5, 16.1	15.3
572	13.4 ₅ , 13.3, 14.1 ₅	13.9
649	9.21, 9.79, 9.22	9.25
673	7.74, 7.75, 7.74	8.27

Figure 2.5: Viscosity Values from Cantor [24]

Table 2.4: Viscosity in centipoise (cP) for fluoride mixtures containing LiF, BeF₂, and UF₄ [25]

Composition Mole Percent			Temperature		
LiF	BeF ₂	UF ₄	600°C	700°C	800°C
69	31	0	7.25	4.54	3.10
62.67	37.33	0	7.98	5.29	3.46
70	28	2	7.49	4.92	3.48
70	26	4	9.08	5.58	3.78
70	22	8	11.6	7.34	5.06
70	18	12	12.3	7.30	4.82

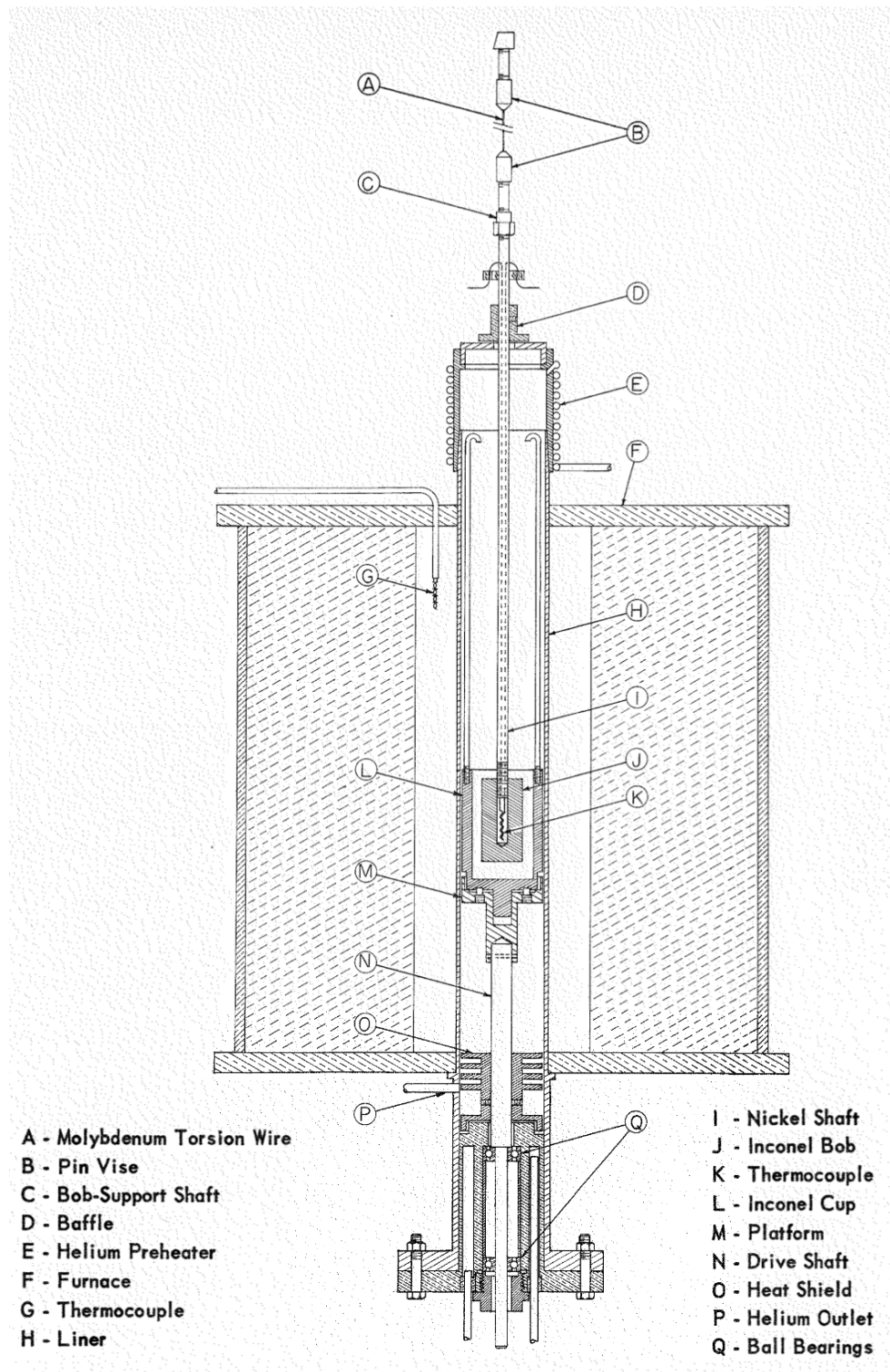


Figure 2.6: Schematic Diagram of the Viscosity Apparatus used by Blanke et al. in the 1950s [25]

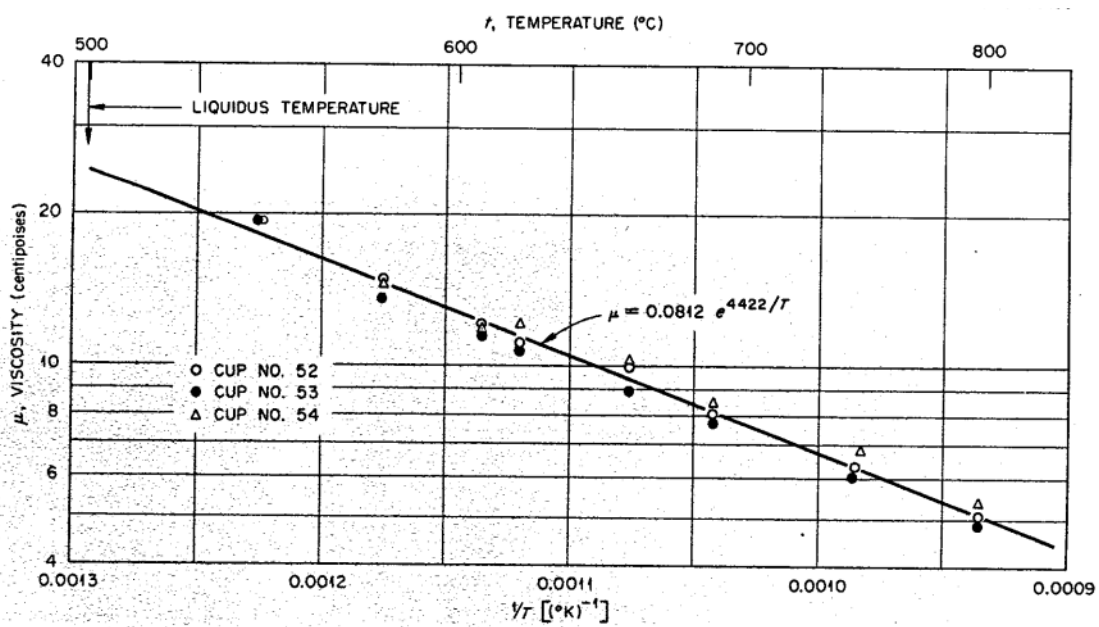


Figure 2.7: Viscosity Values for $\text{LiF}-\text{BeF}_2-\text{ThF}_4-\text{UF}_4$ (67-18.5-14-0.5 mole%) from [29]

- $600^{\circ}\text{C} = 13.0 \pm 1.3$ centipoises
- $700^{\circ}\text{C} = 7.1 \pm 0.71$ centipoises
- $800^{\circ}\text{C} = 4.8 \pm 0.48$ centipoises

$$\mu(cP) = 0.0620 \times \exp(4666/T(K)) \quad (2.6)$$

Cohen and Jones compared experimental viscosity values to those predicted by Equation 2.7 in their paper [30]. These can be seen in Table 2.5 for FLiBe. The percent deviation was calculated as $(\text{difference}/\text{experimental}) \times 100$. They used both a rotational and capillary viscometer apparatus; both a photo and diagram of their apparatus can be seen in Figure 2.8 and 2.9. They used Equation 2.7 to predict the viscosity of molten salt mixtures.

$$\mu = \mu_1 x + \mu_2 (1 - x) \quad (2.7)$$

where μ is the viscosity of the mixture, μ_1 and μ_2 are the viscosities of the components, and x is the mole fraction of one of the components.

The mixture shown in Table 2.5 has the largest percent deviation out of all the salts investigated by Cohen and Jones. There were three more salts that differed by more than 20%, and the average deviation of all studied mixtures was 10% [30]. This leads to the conclusion that the correlation from Equation 2.7 should not be trusted to predict the viscosity of new salt mixtures. This leads to the thought that maybe the experimental values had more error than expected; although, it could just be that the correlation does not work due to non-ideal mixing.

Abe et al. [31] is the most reliable source for viscosity data on FLiBe according to Magnusson et al. [17]. They used a high temperature oscillating cup viscometer, which yielded 1.3% uncertainty.

Table 2.5: The comparison of experimental and predicted viscosities in units of cP at 700°C from [30]

Mixture	Experimental	Predicted	Percent Deviation
LiF-BeF ₂ (69-31 mol%)	4.9	7.80	59%

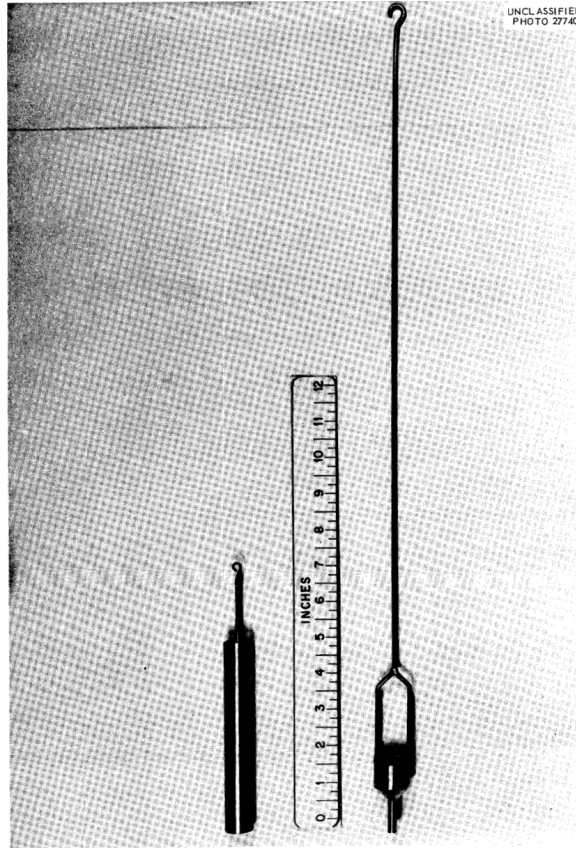


Figure 2.8: Photo of the capillary viscometer or efflux cup and the spindle for the Brookfield viscometer taken from [30]

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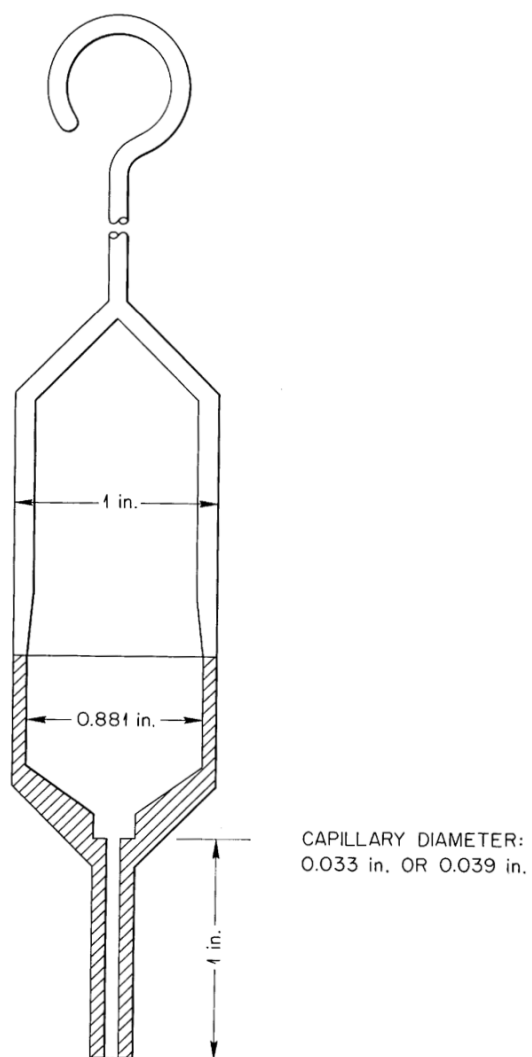


Figure 2.9: Diagram of the capillary or efflux cup viscometer taken from [30]

According to Gallagher et al., another method for measuring viscosity is under development: a high temperature falling ball viscometer [27]. As long as the salt and container are transparent, an optical camera can be used to track the ball's velocity. If either the salt or container is opaque, an x-ray generator like that in Figure 2.4 could be used. Ultimately, Stoke's law is used to calculate viscosity from the experimentally measured terminal velocity of the ball which is used to calculate the drag force. This technique is similar to those seen to calculate density in Figures 2.3 and 2.4. ANL's viscosity measurements are being obtained by using a rotating spindle viscometer.

2.3 Heat Capacity

It can be assumed that C_p is independent of temperature due to a very small variation in C_p across the temperature range of interest. The heat capacity affects the temperature distribution of the salt throughout the core and flow loops.

The Dulong and Petit method is the best way to estimate the heat capacity of salt mixtures,

$$C_p = 8 \times \frac{\sum_{i=1}^n N_i p_i}{\sum_{i=1}^n N_i M_i} \quad (2.8)$$

where the assumed contribution is 8 cal/Kelvin (33.47 J/K), N_i is the mole fraction of component i, p_i is the number of atoms in a molecule of component i, and M_i is the molecular weight of component i. For example, LiF-BeF₂ (66-34 mol%) would be calculated as seen below:

$$\begin{aligned} \sum_{i=1}^n (N_i p_i) &= 0.66(2) + 0.34(3) = 2.34 \\ \sum_{i=1}^n (N_i M_i) &= 0.66(26) + 0.34(47) \\ C_p &= \frac{8(2.34)}{33.1} = 0.57 \text{ cal/K} - g \end{aligned}$$

The validity of using additive contributions for estimating heat capacities was explored by comparing them with the measured values; this can be seen in Table 2.6. The level of agreement between the predictions and measurements is excellent.

Rosenthal [33] tested two samples of FLiBe in Inconel capsules using separate copper-block drop calorimeters [17]. The value of 0.577 cal/g·K (2.414 J/g·K) yielded an error of 1.4% after sixteen enthalpy measurements. This value matched the value by Cantor [32]. Douglas and Payne [34] got a value of 0.561 cal/g·K (2.347 J/g·K) with an ice Bunsen calorimeter, but they were working with a different compound, which was Li₂BeF₄.

The experimental results from Rosenthal [33] yielded Equation 2.9 as the relation for enthalpy in a temperature range of 500-720°C for LiF-BeF₂ (66-34 mole %). This was found by doing the least squares fit to the data and can be seen in Figure 2.10.

$$H_t - H_{30} = 33.62 + 0.577(T - 30) \quad (2.9)$$

According to Rosenthal [33], the total uncertainty was on the order of 1% with a standard error of $\pm 0.6\%$ that is associated with Equation 2.9 and an error of $\pm 0.5\%$ associated with calorimeter calibration. The derived heat capacity for their experiments was 0.577 ± 0.008 cal/g·°C (2.414 ± 0.033 J/g·°C); the uncertainty here is $\pm 1.4\%$.

In Russia, Redkin et al. used Differential Scanning Calorimetry (DSC) to measure heat capacity of the FLiBe system; a STA 449F1 Jupiter thermal analyzer (NETZSCH, Germany) was used to record the change in the mass of the sample and the DSC curve synchronously [35]. The standard error was taken to be 5% for their test measurements, but for molten salts, due to their complexity where significant changes in shape occur after melting, the measurement error was estimated at 10% [35]. In another paper by Redkin, the experimental C_p and C_p calculated from Eq. 2.10

Table 2.6: All C_p values are in cal/(g·°C) with J/(g·°C) in parentheses. All measurements are from unpublished measurements references in [32]

Salt Mixture	Estimated C_p	Measured C_p
LiF-BeF ₂ (66-34 mole %)	0.57 (2.38)	0.57 (2.38)
LiF-BeF ₂ -ThF ₄ (72-16-12 mole %)	0.32 (1.34)	0.324 (1.356)
LiF-ThF ₄ (75-25 mole %)	0.24 (1.00)	0.25 (1.05)

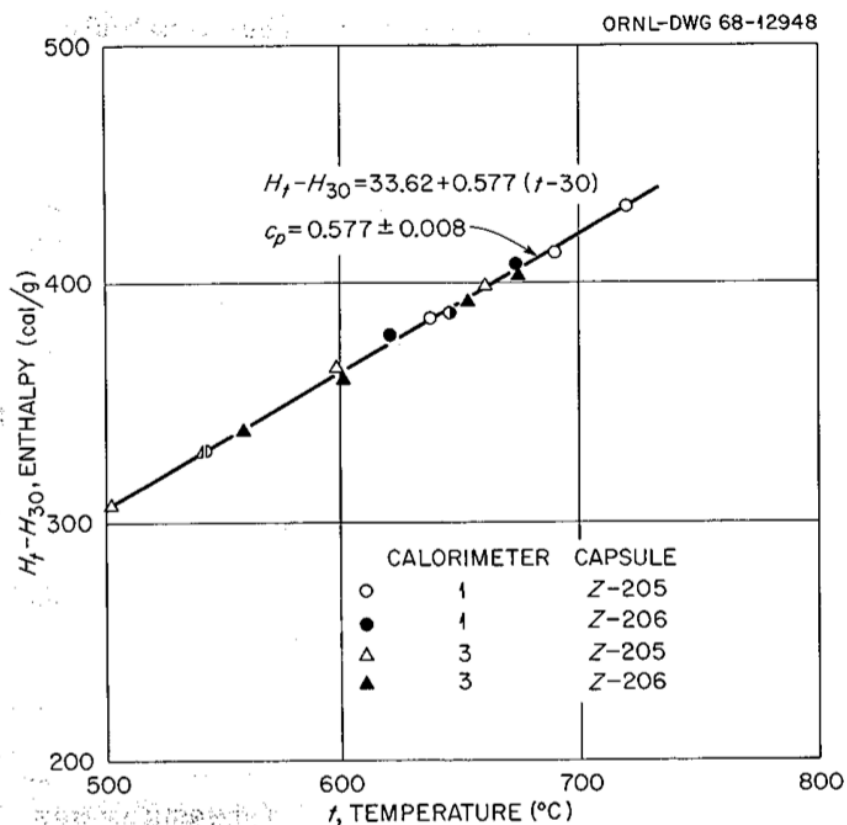


Figure 2.10: Enthalpy of LiF-BeF₂ (66-34 mole %) from [33]

were given, these can be seen in Table 2.7 [36].

$$C_p = X \times 63.8 + Y \times 103.5 + Z \times 167 \quad (2.10)$$

where C_p is the heat capacity in J/mol·K, X is the molar fraction of LiF, Y is the molar fraction of BeF₂, and Z is the molar fraction of UF₄. It is seen in Table 2.7 that the calculated values show excellent results when compared to the experimental values. ANL's heat capacity measurements use DSC as well.

2.4 Thermal Conductivity

Thermal conductivity is important to the temperature distribution of the salt and the power distribution of the salt including peak power since thermal conductivity is fundamental to the simulation of thermal hydraulic conditions. According to Diamond et al. [37], thermal conductivity has a greater uncertainty than heat capacity with fluoride fuel salt thermal conductivity being known to within 10-15%. An equation for estimating thermal conductivity by using a theoretical expression can be seen in Equation 2.11. The equation was originally proposed by Rao and refined for molten salts by Turnbull [38]; it is also found in [32].

$$k(\text{watt/cm} \cdot ^\circ\text{C}) = 11.9 \times 10^{-3} \frac{T_m^{1/2} \times \rho_M^{2/3}}{(M/n)^{7/6}} \quad (2.11)$$

where k is the thermal conductivity, T_m is the melting point in Kelvin, ρ_M is the liquid density in g/cm³, M is the average molar weight of the salt, and n is the average number of discrete ions per molecule.

Alternatively, Equation 2.12 is recommended by [39], [40].

$$k(\text{watt/m} \cdot \text{K}) = 0.0005 \times T(\text{K}) + \frac{32.0}{M} - 0.34 \quad (2.12)$$

Table 2.7: Heat capacity data taken from [36]

Composition	Experimental	Calculated
LiF-BeF ₂ (66.67-33.33 mol %)	2.34	2.34
LiF-BeF ₂ (73-27 mol %)	2.38	2.36
LiF-BeF ₂ (66-34 mol %)	2.30	2.34
LiF-BeF ₂ -UF ₄ (72.3-26.7-1 mol %)	2.15	2.19
LiF-BeF ₂ -UF ₄ (71.5-26.5-2 mol %)	1.95	2.05

where k is the thermal conductivity in watt/m·K, T is the temperature in K, and M is the molecular mass in g/mole.

According to Rosenthal [33], they recommend using a value of 0.010 W/cm·°C at melting temperature for LiF-BeF₂ (65.8-34.2 mol%). The results from their experiments can be seen in Table 2.8. They used an absolute, variable gap apparatus, noting corrections to be made for radial heat transfer, natural circulation, and radiation; uncertainty estimates were 15-35%. The description of this method can be seen in [33].

Rosenthal et al. [41] provided some preliminary results for thermal conductivity during the MSRE in 1969; these can be seen in Figure 2.11. This included results for the MSRE fuel salt, MSRE coolant salt, proposed MSBR fuel salt, and proposed MSBR coolant salt.

Cooke [42] later determined that the main cause of historic error for thermal conductivity measurements was heat shunting. This heat shunting comes from some of the heat being diverted around the thermal conductivity cells and is unavoidable. To account for this, they modified the technique using fluids to minimize thermal resistance in the measured temperature range for the apparatus, with a maximum error of 15% for FLiBe.

Gallagher et al. designed and built a variable gap system that is a modified version of the previous systems that were developed for the MSRE; an illustration of this can be seen in Figure 2.12 [27]. 1-D approximations of Fourier's Law were used in this technique that measure the temperature difference across a thin layer of salt, which is heated on the top and cooled on the bottom of the apparatus, which can be seen in Figure 2.12. This system has several improvements such as using Computational Fluid Dynamics codes and modern Finite Element Analysis to reduce uncertainty that is caused by convection. In addition, the uncertainty associated with radiative heat transfer was reduced by minimizing the emissivity of internal components by

Table 2.8: Thermal Conductivity in W/cm·°C of LiF-BeF₂ (65.8-34.2 mol%) from [33]

Salt Composition	500°C	600°C	700°C	800°C	900°C
LiF-BeF ₂ (65.8-34.2 mol%)	0.010	0.011	0.011	0.011	0.011

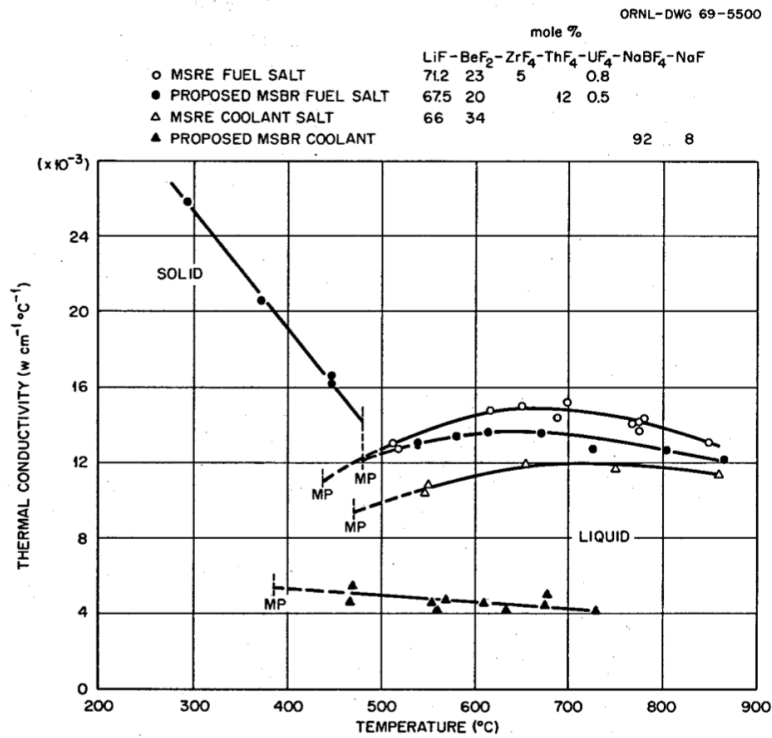


Figure 2.11: Preliminary results for salt mixtures of interest to the MSRE and MSBR programs [41]

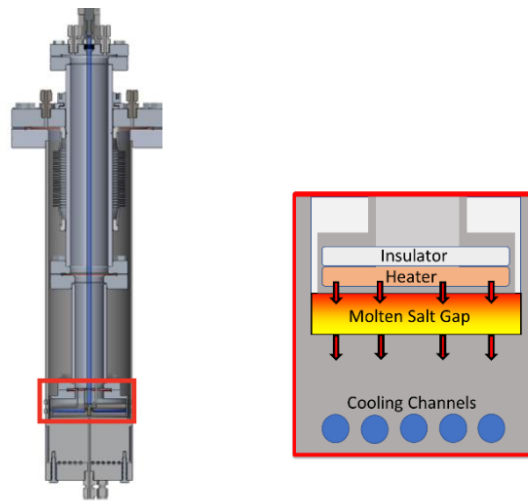


Figure 2.12: Modified variable gap system [27]

mechanical polishing. The variable gap technique is a sealed system, so it can be used for measuring both irradiated and unirradiated salts.

ANL's thermal conductivity measurements use a laser flash analysis system. An et al. measured thermal conductivity using a laser flash technique as well [43]. An et al.'s apparatus can be seen in Figure 2.13. In this method, the sample is shot with a single pulse from a laser that starts at the bottom of the crucible through the top of the crucible. The temperature of the crucible lid is detected using an infrared sensor, as can be seen in Figure 2.13.

2.5 Uncertainty

For the values obtained from Cantor [32], the uncertainty is considered to be the largest probable combination of random and systematic errors that are associated with the value. The salt mixtures studied in [32] are

- LiF-BeF₂-ThF₄-UF₄ (73-16-10.7-0.3 mole%)
- LiF-BeF₂-ThF₄-UF₄ (72-21-6.7-0.3 mole%)
- LiF-BeF₂-ThF₄-UF₄ (68-20-11.7-0.3 mole%)
- LiF-BeF₂-ThF₄-UF₄ (63-25-11.7-0.3 mole%)
- LiF-Be₂ (66-34 mole%)

These salt compositions will be referred to throughout this section and are relatively close to the fuel composition used in the model of LiF-BeF₂-ThF₄-UF₄ (71.5-16.0-12.0-0.5 mole%). The uncertainties in viscosities for these 4 fuel compositions were all estimated to be 25% with FLiBe being estimated at 15% by Cantor [32]. The fuel salts were estimated empirically from viscosities in the system LiF-BeF₂-UF₄ [25] and measurements of LiF-BeF₂-ThF₄ (71-16-13 mole%) [29]. In Cantor's [32] discussion on viscosity for the LiF-BeF₂-UF₄ system, for LiF concentrations at

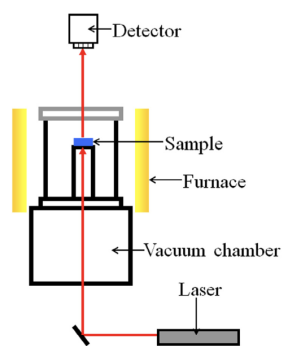


Figure 2.13: Laser flash analysis system [43]

or above 60%, an increase in viscosity happens when UF_4 is substituted for BeF_2 . Using these data and trends for the $\text{LiF-BeF}_2\text{-UF}_4$ system, the viscosities can be predicted to within 25% with several assumptions about the composition values: 62-73 mole% LiF , 15-30 mole% BeF_2 , and 6-16 mole% of MF_4 , where M is equal to U, Th, and/or Pu. This leads to viscosities in a range of 9-16 centipoise at 600°C and 5-9 centipoise at 700°C . In this study, the uncertainty was set at 30% for viscosity.

For thermal conductivity, the uncertainty was more than 25% for the 4 fuel salt compositions and 10% for FLiBe by Cantor [32]. For the fuel salts, thermal conductivity was estimated using the theoretical expression mentioned earlier that was derived by Rao [44] and adapted to molten salts by Turnbull [38]. This expression can be seen in Equation 2.11. On average, it agreed with experimental results for eleven molten mixtures of nitrates and chlorides to within 15%. Although the expression yielded values that were approximately 25% less than the experimental values for FLiBe and $\text{LiF-BeF}_2\text{-ThF}_4\text{-UF}_4$ (71.2-23-5-0.8 mole%), the theoretical equation was greatly extended to apply to the fuel salt mixtures seen here. For FLiBe , the thermal conductivity value was measured. The uncertainty value was set to 30% for thermal conductivity in this study.

For heat capacity, a different value was given for the liquid compared to the equation given for the solid. For the 4 fuel salt compositions, the uncertainties were 4% for the liquid and 10% for the solid by Cantor [32]. For FLiBe , the uncertainty was 3% for both states [32]. The contribution to heat capacity from LiF and BeF_2 was chosen as $8 \text{ cal}/(\text{g}\cdot\text{atom})\cdot^\circ\text{C}$ since it is the average observed value for alkali and alkaline earth halides and $44 \text{ cal}/(\text{mole}\cdot^\circ\text{C})$ was chosen for ThF_4 's contribution, which was assumed from the average value of $8.8 \text{ (cal}/(\text{g}\cdot\text{atom})\cdot^\circ\text{C})$ for the lanthanide halides [32]. For FLiBe , the liquid heat capacity is the average of two independent sets of measurements performed by Hoffman that went unpublished and Douglas and Payne [45], these are $0.577 \text{ cal}/\text{g}\cdot^\circ\text{C}$ and $0.56 \text{ cal}/\text{g}\cdot^\circ\text{C}$ respectively. The solid heat capacity equation, for heat capacity in units of $\text{cal}/\text{g}\cdot^\circ\text{C}$, of $0.317+3.61\text{e-}4\times T(^\circ\text{C})$ was taken

from Douglas and Payne. The results from using additive contributions for heat capacity estimation was compared with measured values and showed good agreement, which can be seen in Table 2.6. The uncertainty value was set to 25% for heat capacity in this study.

The uncertainty for density was given as 3% for the fuel salts and 2% for FLiBe by Cantor [32]. For the fuel salts, density was estimated by addition of molar volumes [21]. For FLiBe, 3 experimental determinations were reported with those by Grimes [21] averaging 3% higher than Blanke et al. [25]. Briggs [46] reported densities measured at 649°C that vary from 1.87 to 2.02 g/cm³ for FLiBe. The density-temperature equation given in [32] and seen in Equation 2.13 was derived from molar volume addition.

$$\rho(g/cm^3) = 2.27 - 7.4 \times 10^{-4}T(^{\circ}C) \quad (2.13)$$

It is approximately the average of the densities in [21] and [25]. In this study, the uncertainty was set at 10% for density.

A compiled list of all the values and equations that influenced the uncertainty of the four thermophysical properties can be seen in Tables 2.9-2.14.

Table 2.9: Density Measurements

Units	Value	Uncertainty	Salt	Composition (mol%)	Temperature	References
lb/ft ³	190	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	67-23-9-1	1200°F	[47]
lb/ft ³	120	not given	LiF-BeF ₂ -UF ₄	63-36-1	1200°F	[47]
kg/m ³	3250	not given	LiF-BeF ₂ -ThF ₄	72-16-12	700°C	[48]
g/ml	2.825	±1%	LiF-BeF ₂ -UF ₄	70-22-8	600°C	[25]
g/ml	2.772	±1%	LiF-BeF ₂ -UF ₄	70-22-8	700°C	[25]
g/ml	2.725	±1%	LiF-BeF ₂ -UF ₄	70-22-8	800°C	[25]
g/ml	3.208	±1%	LiF-BeF ₂ -UF ₄	70-18-12	600°C	[25]
g/ml	3.154	±1%	LiF-BeF ₂ -UF ₄	70-18-12	700°C	[25]
g/ml	3.134	±1%	LiF-BeF ₂ -UF ₄	70-18-12	800°C	[25]
g/cm ³	2.034±0.096	±4.7%	LiF-BeF ₂ -UF ₄	68.5-31.3-0.2	not given	[49]
g/cm ³	4.437±0.224	± 5%	LiF-BeF ₂ -ThF ₄	71-27-2	not given	[49]
g/cm ³	3.2839	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	71.7-16.0-12.0-0.3	not given	[49]

Table 2.10: Density Equations

Units	Equation	Uncertainty	Salt	Composition (mol%)	Temperature	References
lb/ft ³	$236.3-2.33 \times 10^{-2} \times T(^{\circ}\text{F})$	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	71.5-16.0-12.0-0.5	not given	[50]
g/cm ³	$3.82-8.2 \times 10^{-4} \times T(^{\circ})$	$\pm 5\%$	LiF-BeF ₂ -ThF ₄ -UF ₄	71-16-12-1	not given	[51]
g/cm ³	$2.38-4 \times 10^{-4} \times T(^{\circ})$	$\pm 5\%$	LiF-BeF ₂ -UF ₄	67-30.5-2.5	not given	[51]
g/cm ³	$3.82-8.2 \times 10^{-4} \times T(^{\circ}\text{C})$	$\pm 5\%$	LiF-BeF ₂ -ThF ₄ -UF ₄	71-16-12-1	not given	[26]
g/cm ³	$3.628-6.6 \times 10^{-4} \times T(^{\circ}\text{C})$	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	73-16-10.7-0.3	not given	[16], [52]
g/cm ³	$3.153-5.8 \times 10^{-4} \times T(^{\circ}\text{C})$	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	72-21-6.7-0.3	not given	[16], [52]
g/cm ³	$3.644-6.3 \times 10^{-4} \times T(^{\circ}\text{C})$	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	68-20-11.7-0.3	not given	[16], [52]
g/cm ³	$3.628-6.6 \times 10^{-4} \times T(^{\circ}\text{C})$	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	63-25-11.7-0.3	not given	[16], [52]
g/cm ³	$3.752-6.68 \times 10^{-4} \times T$	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	71.7-16.0-12.0-0.3	not given	[49]
lb/ft ³	$236.3-2.33 \times 10^{-2} \times T(^{\circ}\text{F})$	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	68-22-9-1	not given	[49]
lb/ft ³	$236.3-2.33 \times 10^{-2} \times T(^{\circ}\text{F})$	not given	LiF-BeF ₂ -ThF ₄	68-23-9	not given	[49]
lb/ft ³	$236.3-2.33 \times 10^{-2} \times T(^{\circ}\text{F})$	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	71.5-16.0-12.0-0.5	not given	[49]
g/cm ³	$3.752-6.68 \times 10^{-4} \times T(^{\circ}\text{C})$	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	71.7-16.0-12.0-0.3	not given	[49]

Table 2.11: Viscosity Values

Units	Value	Uncertainty	Salt	Composition (mol%)	Temperature	References
lb/ft-hr	21	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	67-23-9-1	1200°F	[47]
lb/ft-hr	21	not given	LiF-BeF ₂ -UF ₄	63-36-1	1200°F	[47]
m ² /s	2.21e-6	not given	LiF-BeF ₂ -ThF ₄	72-16-12	700°C	[48]
cP	13.0±1.3	±10%	LiF-BeF ₂ -ThF ₄ -UF ₄	71-16-12-1	600°C	[30]
cP	7.1±0.71	±10%	LiF-BeF ₂ -ThF ₄ -UF ₄	71-16-12-1	700°C	[30]
cP	4.8±0.48	±10%	LiF-BeF ₂ -ThF ₄ -UF ₄	71-16-12-1	800°C	[30]
cP	11.161±1.24	±11%	LiF-BeF ₂ -UF ₄	68.5-31.3-0.2	not given	[49]
cP	15.708±7.854	±50%	LiF-BeF ₂ -ThF ₄	71-27-2	not given	[49]
cP	7.1515	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	71.7-16.0-12.0-0.3	not given	[49]

Table 2.12: Viscosity Equations

Units	Equation	Uncertainty	Salt	Composition (mol%)	Temperature	References
lb/ft-hr	$0.2637 \times \exp(7362/(459.7+T(^{\circ}\text{F})))$	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	71.5-16.0-12.0-0.5	not given	[50]
cP	$0.062 \times \exp(4666/(T(\text{K})))$	$\pm 10\%$	LiF-BeF ₂ -ThF ₄ -UF ₄	71-16-12-1	700°C	[51]
cP	$0.128 \times \exp(3650/(T(\text{K})))$	$\pm 20\%$	LiF-BeF ₂ -UF ₄	67-30.5-2.5	not given	[51]
cP	$0.0620 \times \exp(4666/(T(\text{K})))$	$\pm 20\%$	LiF-BeF ₂ -ThF ₄ -UF ₄	71-16-12-1	600-800°C	[26]
cP	$0.0812 \times \exp(-4422/(T(\text{K})))$	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	67-18.5-14-0.5	550-800°C	[29]
cP	$0.084 \times \exp(4340/(T(\text{K})))$	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	73-16-10.7-0.3	700°C	[16], [52]
cP	$0.072 \times \exp(4370/(T(\text{K})))$	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	72-21-6.7-0.3	700°C	[16], [52]
cP	$0.044 \times \exp(5030/(T(\text{K})))$	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	68-20-11.7-0.3	700°C	[16], [52]
cP	$0.084 \times \exp(4340/(T(\text{K})))$	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	63-25-11.7-0.3	700°C	[16], [52]
lb/ft-hr	$0.2637 \times \exp(7362/(459.7+T(^{\circ}\text{F})))$	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	68-22-9-1	not given	[49]
lb/ft-hr	$0.2637 \times \exp(7362/459.7+(T(^{\circ}\text{F})))$	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	71.5-16.0-12.0-0.5	not given	[49]
cP	$0.109 \times \exp(4090/(T(\text{K})))$	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	71.7-16.0-12.0-0.3	not given	[49]

Table 2.13: Thermal Conductivity Values

Units	Value	Uncertainty	Salt	Composition (mol%)	Temperature	References
Btu/hr-ft-°F	2.9	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	67-23-9-1	1200 °F	[47]
Btu/hr-ft-°F	3.5	not given	LiF-BeF ₂ -UF ₄	63-36-1	1200 °F	[47]
Btu/hr-ft-°F	0.75	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	71.5-16.0-12.0-0.5	not given	[50]
W/m-°C	1.2	not given	LiF-BeF ₂ -ThF ₄	72-16-12	700 °C	[48]
W/m-K	0.01	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	73-16-10.7-0.3	700°C	[16], [52]
W/m-K	0.01	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	72-21-6.7-0.3	700°C	[16], [52]
W/m-K	0.007	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	68-20-11.7-0.3	700°C	[16], [52]
W/m-K	0.01	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	63-25-11.7-0.3	700°C	[16], [52]
Btu/hr-ft-°F	0.8	not given	LiF-BeF ₂ -UF ₄	68.5-31.3-0.2	not given	[49]
Btu/hr-ft-°F	0.6	not given	LiF-BeF ₂ -ThF ₄	71-27-2	not given	[49]
Btu/hr-ft-°F	0.72	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	68-22-9-1	922 K	[49]
Btu/hr-ft-°F	0.75	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	71.5-16.0-12.0-0.5	not given	[49]
W/m-K	1.19	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	71.7-16.0-12.0-0.3	978 K	[49]

Table 2.14: Heat Capacity Values

Units	Value	Uncertainty	Salt	Composition (mol%)	Temperature	References
Btu/lb-°F	0.4	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	67-23-9-1	1200°F	[47]
Btu/lb-°F	0.5	not given	LiF-BeF ₂ -UF ₄	63-36-1	1200°F	[47]
Btu/hr-ft-°F	0.32	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	71.5-16.0-12.0-0.5	not given	[50]
cal/g-°C	0.37	±10%	LiF-BeF ₂ -ThF ₄ -UF ₄	71-16-12-1	700°C	[51]
cal/g-°C	0.57	±20%	LiF-BeF ₂ -UF ₄	67-30.5-2.5	700°C	[51]
kJ/kg-°C	1.34	not given	LiF-BeF ₂ -ThF ₄	72-16-12	700°C	[48]
cal/g-°C (J/g-°C)	0.32 (1.34)	±4%	LiF-BeF ₂ -ThF ₄	72-16-12	not given	[32]
cal/g-°C (J/g-°C)	0.324 (1.356)	±4%	LiF-BeF ₂ -ThF ₄	72-16-12	not given	[32]
(J/g-K)	2.15	±10%	LiF-BeF ₂ -UF ₄	72.3-26.7-1	not given	[36]
(J/g-K)	2.19	±10%	LiF-BeF ₂ -UF ₄	72.3-26.7-1	not given	[36]
(J/g-K)	1.95	±10%	LiF-BeF ₂ -UF ₄	71.5-26.5-2	not given	[36]
(J/g-K)	2.05	±10%	LiF-BeF ₂ -UF ₄	71.5-26.5-2	not given	[36]
cal/g-°C	0.34	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	73-16-10.7-0.3	700°C	[16], [52]
cal/g-°C	0.39	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	72-21-6.7-0.3	700°C	[16], [52]
cal/g-°C	0.33	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	68-20-11.7-0.3	700°C	[16], [52]
cal/g-°C	0.34	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	63-25-11.7-0.3	700°C	[16], [52]
Btu/lb-°F	0.55±0.14	±25%	LiF-BeF ₂ -UF ₄	68.5-31.3-0.2	not given	[49]
Btu/lb-°F	0.22±0.06	±27%	LiF-BeF ₂ -ThF ₄	71-27-2	not given	[49]

Table 2.14: *(Continued)*

Units	Value	Uncertainty	Salt	Composition (mol%)	Temperature	References
Btu/lb-°F	0.32	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	68-22-9-1	922 K	[49]
Btu/hr-ft-°F	0.32	not given	LiF-BeF ₂ -ThF ₄ -UF ₄	71.5-16.0-12.0-0.5	not given	[49]
J/g-K	1.357	±4%	LiF-BeF ₂ -ThF ₄ -UF ₄	71.7-16.0-12.0-0.3	978 K	[49]

Chapter 3

Methodology

This study focuses on studying the effect that perturbations of the four thermophysical properties have on reactor behavior, such as temperature, during steady state and transient progression. Two transient conditions are simulated for purposes of this study. The first simulated transient is a reactivity insertion that simulates an external reactivity insertion that progresses on the order of several hundred seconds; this type of transient could occur in the event of a control rod withdrawal. The second simulated transient explores the effects of the reduction of the pipe cross sectional area possibly due to fission product buildup from phenomena such as fouling. These simulations are performed using Transient System Framework of Reconfigurable Models (TRANSFORM) and Modelica in the Dynamic Modeling Laboratory (Dymola) proprietary compiler.

3.1 Modelica

Modelica is a multi-domain, equation-based, declarative, object-oriented programming language [53]. It was first created back in 1997 by Hilding Elmqvist with the goal of developing an object oriented language to model technical systems in a standardized format. In 2000, Modelica started being used for industrial applications

and the Modelica Association was formed to manage the Modelica language and the Modelica Standard Library. The Modelica Standard Library is developed by the Modelica Association and is freely available. It has components to model electrical, mechanical, thermal, magnetic, and control systems. Dr. Tiller, the author of Modelica by Example, describes Modelica as “a high-level declarative language for describing mathematical behavior” [54]. It was designed to be a modeling language that supports multi-physical systems, library development, and model exchange [55]. Modelica provides a way to holistically model complex systems by describing their behavior and characteristics in the form of algebraic and differential equations.

Modelica was purposely built for dynamic system modeling, therefore it uses an acausal approach allowing equation rearrangement during model compilation to optimize computing performance. Considering that Modelica is an equation-based language, differential and algebraic equations describe the system’s dynamic behavior. An example of an appropriate equation to be implemented in Modelica can be seen in Equation 3.1.

$$x + y = z + yz \tag{3.1}$$

There are many other appropriate equation forms. During model development, rearrangement of the equations is not required, and the inputs and outputs do not need to be specified. The compiler itself performs the equation rearrangement to optimize the problem.

An object oriented approach allows systems to be expressed in comprehensible mathematical expressions. Using inheritance, complex systems can be modeled through vertical stacking to create a hierarchy of complexity in models. This allows reuse of existing models and their attributes within another model. Modelica utilizes a class system to organize modeling packages. Classes have their own attributes which allow clear organization to achieve inheritance. A class can include variables and equations that define the behavior. These classes and individual components can be individually diagnosed and validated. Another advantage to using Modelica

is the models and their solvers are separate, which allows the user to focus on component behavior without requiring a lot of knowledge about numeric solvers, symbolic manipulation, code generation, or post-processing.

3.2 TRANSFORM

TRANSFORM was originally created as a high level approach for advanced reactor modeling. Modelica was chosen as the modeling language since it is flexible, capable of creating complex models, and has acausal capabilities. Back in the early 2010s, Modelica had no standard heat transfer or fluid libraries; this made the task of developing a high level interface for use with nuclear reactors much harder. Thus, in 2017, TRANSFORM was born and provided a library of components that made modeling thermal hydraulic and multi-physics systems easier.

TRANSFORM is a component library written in the Modelica programming language for the simulation tool Dymola. It was made to fill the gap between existing Modelica libraries and the needs for advanced reactor modeling. TRANSFORM allows the user to modify components to fit their needs. It includes components for heat exchangers, mass and heat transfer, media, reactor kinetics, reactor core, pipes, volumes, and more.

Some capabilities of TRANSFORM include components needed to model nuclear energy and auxiliary systems. It also includes components to model heat transfer, thermal hydraulics, and control systems. TRANSFORM has been used to model LWRs, sodium gas reactors, MSRs, solar salts, integrated energy systems, and nuclear space reactors. It has been used for several projects including integrated energy systems, which created physics based models of nuclear reactors that were coupled with energy storage and energy generation [56]; radionuclide mass accountancy, which explored radionuclide transport in MSRs [57]; nuclear thermal propulsion modeling, where a nuclear thermal rocket was modeled [58]; primary flow stability for Small

Modular Reactor (SMR)-160, which performed linear stability studies of a pressurized SMR [59]; accident analysis for the Transformational Challenge Reactor, which is a helium-cooled, yttrium-hydride moderated reactor [60]; an investigation for siting an Integrated Energy System for the Eastman Chemical Company, which looked at the ability of advanced reactors to deliver steam [61]; demonstration of tritium transport to demonstrate an extension for generic trace substance transport [62]; and dynamic mass accountancy using equilibrium thermodynamics [63]. TRANSFORM was also used for an experimental benchmark of UC Berkeley’s Compact Integral Effects Test (CIET) facility [64]. CIET was built to verify modeling tools for the Fluoride High Temperature Reactor. The simulant fluid, Dowtherm A, was benchmarked, which is the fluid used at CIET.

3.3 Dymola

“Dymola is a Modelica compliant solution that efficiently models and simulates multi-physic dynamic systems” [65]. Dymola features several advantages, one is its cross discipline support, which allows for components from different engineering domains. It is most popular in the automotive industry and is also used in aerospace, architecture, and energy as well as many others. These components are described by algebraic equations and ordinary differential equations, which result in reusable models of complete systems. “Dymola has unique and outstanding performance for solving systems of differential algebraic equations. The key to this high performance and robustness is symbolic manipulation that optimizes and solves the systems of equations that define the system.” [65]. Another advantage is Dymola’s graphical editor. The graphical editor along with the libraries allow components to easily be dragged and dropped to build a system model. Connections that couple the components and model their physical coupling make building a system model even

easier. This allows a more visual representation over other languages since it is not just block text; this allows for more intuitive modeling.

3.4 Modeling Overview

An Molten Salt Demonstration Reactor (MSDR) model, with nominal thermal output of 750 MW_{th} , was simulated in this analysis using the TRANSFORM library and the Modelica Standard Library [66], [67]. A schematic of the MSDR design can be seen in Figures 3.1 and 3.2. The MSDR design has a Primary Fuel Loop (PFL), Primary Coolant Loop (PCL), and Balance of Plant (BOP). The model used here also has a PFL, PCL, and BOP as seen in Figure 3.2. This model uses $\text{LiF-BeF}_2\text{-ThF}_4\text{-UF}_4$ (71.5-16.0-12.0-0.5 mole %) fuel salt and FLiBe coolant salt. In the PFL, the fuel salt circulates through the reactor into the primary fuel pump, where it then circulates into the primary heat exchanger and then back into the reactor. The reactor consists of the core, axial reflectors, a radial reflector, and the inlet and outlet plenum. The heat exchanger is a simple shell-and-tube heat exchanger. The PFL will be explained in more detail later and even more information about this model and TRANSFORM can be found in [68]. The simulations were all run for $1.5768\text{e}8$ seconds, which is 5 years. The chosen integrator was `Esdirk45a`, which is a single step, Runge Kutta method of the 5th order. Runge-Kutta methods are designed to start fresh on every step; this reduces the cost of restarting after an event. `Esdirk45a` is a stiff solver, meaning that it is suited for stiff systems; these are systems where the fastest time-scale in the model is substantially faster than the interesting dynamics [69]. It is also A-stable, which means that for all linear systems, it is stable. `Esdirk45a` starts with a higher order, making it more suited for systems with events or discontinuities. The number of intervals was set to 1825 and the tolerance allowed between steps in the values calculated for the loop was set to 0.0001. The settings for the simulation can

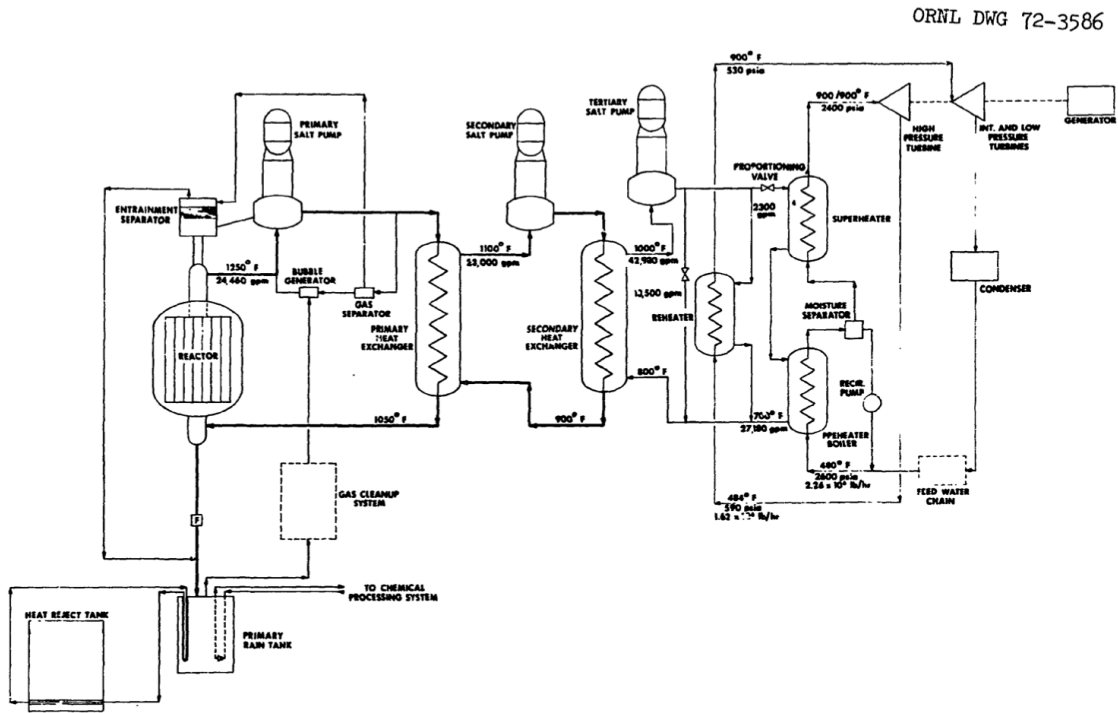


Figure 3.1: Flowsheet for the MSDR taken from Bettis et al. [50]

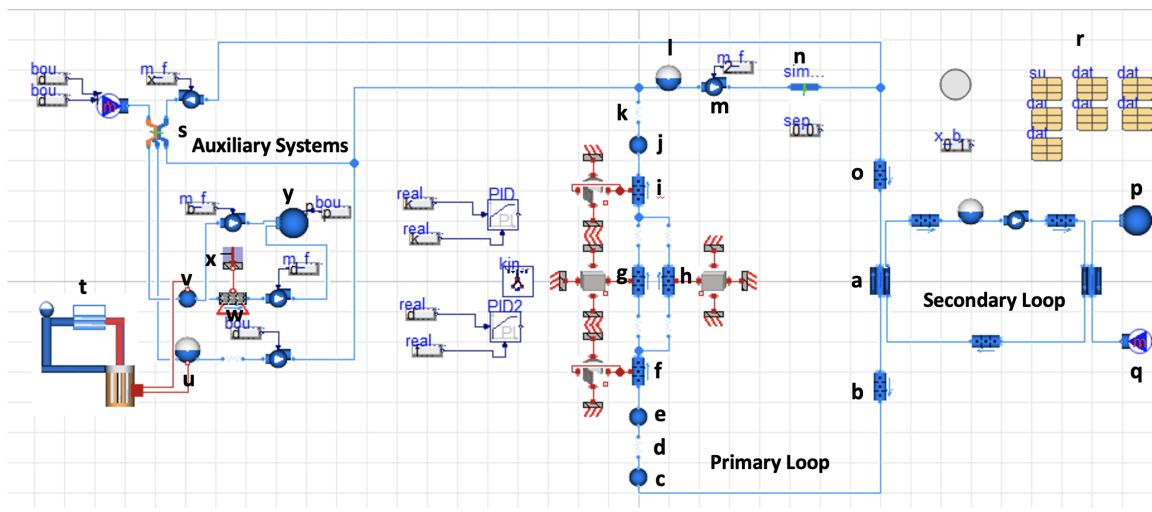


Figure 3.2: The MSDR model used in TRANSFORM with several important components labeled.

be seen in Table 3.1. Components in Figure 3.2 are listed along with their labels in Table 3.2.

3.5 Perturbation Approach

To explore how sensitive the reactor behavior is to the four thermophysical properties, the code was modified with each simulation in order to change the values of the fluid properties by a set percentage from nominal. The four thermophysical properties being assessed were varied using multiplication factors to simulate changes to the nominal baseline value. They were perturbed by adding four variables to the medium part of the code (`d_multi`, `lambda_multi`, `cp_multi`, and `eta_multi`). At nominal all these multipliers were set equal to 1. For perturbations, the relevant multiplier was changed a specified amount. For example, for density, the uncertainties explored were $\pm 5\%$ and $\pm 10\%$ so the density multiplier (`d_multi`) was changed from a value of 1 to 0.9, 0.95, 1.05, and 1.1. This process was repeated for the other three properties, changing their multiplier by the maximum perturbation as seen in Table 3.3 as well as intermediate percentage values. The ranges of uncertainty for the four properties were determined back in chapter 2. Values for density and viscosity are temperature dependent and were modeled using the functions in Table 3.4 taken from Bettis et al. [50]. The values for the four properties can also be seen in Table 3.5 where the values are in metric units. In this analysis, a one at a time approach was performed first where properties were varied one at a time to examine their individual effects. Then, a grid approach was performed varying two properties at a time for density, thermal conductivity, and heat capacity. This was done to explore any correlation between properties and any possible adverse effects from these correlations. No changes to the temperature dependencies of these properties were evaluated in these simulations.

Table 3.1: Simulation Settings

Parameter	Value
Simulation Time (s)	1.5768e8
Solver	Esdirk45a
Tolerance	1e-4
Number of Intervals	1825

Table 3.2: Labels corresponding to important components to be used with Figure 3.2.

Label	Component
a	Heat Exchanger
b	Pipe
c	Tee Inlet
d	Resistance at Tee to Plenum
e	Lower Plenum
f	Lower Axial Reflector
g	Fuel Cell
h	Radial Reflector
i	Upper Axial Reflector
j	Upper Plenum
k	Resistance to Pump
l	Pump Bowl
m	pump
n	Simple Separator
o	Pipe
p	Boundary to Steam Loop
q	Ideal Flow Source
r	Data Tables
s	Trace Separator
t	DRACS
u	Drain Tank for Liquid
v	Drain Tank for Gas
w	Absorber Bed
x	Temperature Boundary Condition for Absorber Bed
y	Boundary for Off-gas Sink

Table 3.3: Uncertainties chosen for the four thermophysical properties

Property	Nominal Value/Equation	Uncertainty	Intermediate Perturbations
Density (kg/m ³)	$3785-0.373 \times T(K)$	10%	5%
Viscosity (kg/(s·m))	$1.09e^{-4} \times \exp(4090/T(K))$	30%	20%, 10%
Heat Capacity (J/(kg·K))	1340	25%	15%, 5%
Thermal Conductivity (W/(m ² ·K))	1.3	30%	20%, 10%

Table 3.4: Nominal values for the MSDR fuel salt taken from Bettis [50]

Property	Nominal Value/Equation
Density (lb/ft ³)	$236.3-0.0233 \times T(^{\circ}F)$
Thermal Conductivity (Btu/hr·ft·(°F))	0.75
Specific Heat Capacity (Btu/lb·(°F))	0.32
Viscosity (lb/hr·ft)	$0.2637 \times \exp(7362/(459.7+T(^{\circ}F)))$

Table 3.5: Nominal values for the MSDR fuel salt taken from Greenwood [68]

Property	Nominal Value/Equation
Density (kg/m ³)	$3785-0.373 \times T(K)$
Thermal Conductivity (W/(m ² ·K))	1.3
Specific Heat Capacity (J/(kg·K))	1340
Viscosity (kg/(s·m))	$1.09 \times 10^{-4} \times \exp(4090/T(K))$

The outputs that were examined in this preliminary investigation were temperatures at the inlet and outlet of the core and the inlet and outlet of the PHX. The location of these can be better visualized in Figure 3.3. The difference between the output of the perturbation of the thermophysical property and the output for the nominal thermophysical property value provides quantification of the effect of uncertainty.

3.6 Primary Fuel Loop

The PFL is a forced flow loop type system. The components contained in the primary loop are the reactor, pump bowl, pump, piping, and the PHXs. There are three heat exchanger loops. Each loop has two heat exchangers in parallel and one pump for a total of six heat exchangers and three pumps in the whole PFL. The pumps are sump-type centrifugal pumps with a capacity of 8,100 gpm, which are described in more detail in [70]. The PHXs are shell-and-tube heat exchangers and reject heat to the PCL. A shell-in-tube heat exchanger was chosen since it is the most widely used heat exchanger type in the nuclear industry and it allows for maximum heat transfer area resulting in more power being generated. The PHXs each have a nominal capacity of 125 MW and are constructed of Alloy-N. Several thermophysical properties of Alloy-N can be seen in Table 3.6. The vessel and piping material are also made of Alloy-N. Some more information on the PHXs can be seen in Table 3.7.

The reactor consists of the core, axial reflectors, a radial reflector, and the inlet and outlet plenum. A schematic of the core can be seen in Figure 3.4. The inlet and outlet plenums are assumed to be uniformly mixed volumes. The reflectors are made of graphite; some physical properties can be seen in Table 3.8. The radial reflector is made up of stacked rectangular slabs and modeled using a two-dimensional conduction model with second-order finite difference using slab (x-z) geometry. Only half the slab is modeled since the slabs are assumed to have an adiabatic centerline.

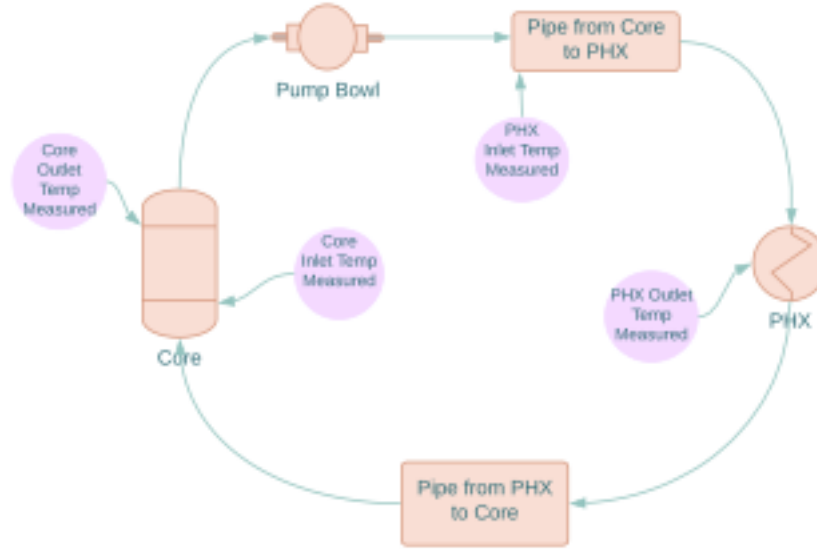


Figure 3.3: A simplified schematic of the temperature locations in the model

Table 3.6: Thermophysical properties of Alloy-N (Temperature is in K) [68]

Parameter	Value	Unit
Density (at room temperature)	8,860	kg/m ³
Thermal conductivity	$9.77 - (3.2e^{-4} \times T) + (1.46e^{-5} \times T^2)$	W/(m ² ·K)
Specific heat capacity	$489 - (0.34 \times T) + (4.6e^{-4} \times T^2)$	J/(kg·K)

Table 3.7: Nominal operating conditions of the PHXs

Parameter	Value	Unit
Tube Side Conditions		
Fluid	Fuel Salt	
Inlet Temperature	1250 (677)	°F (°C)
Outlet Temperature	1050 (566)	°F (°C)
Pressure Drop	127 (0.876)	psi (MPa)
Mass Flow Rate	6.6e6 (832)	lb/hr (kg/s)
Shell Side Conditions		
Fluid	Coolant Salt	
Inlet Temperature	900 (482)	°F (°C)
Outlet Temperature	1100 (593)	°F (°C)
Pressure Drop	115 (0.793)	psi (MPa)
Mass Flow Rate	3.7e6 (466)	lb/hr (kg/s)

Table 3.8: Thermophysical properties of Graphite (Temperature is in K) [68]

Parameter	Value	Unit
Density	1776.66	kg/m ³
Thermal conductivity	$169 - (0.125 \times T) + (3.28e^{-5} \times T^2)$	W/(m ² ·K)
Specific heat capacity	$-144 - (3.67 \times T) + (2.2e^{-3} \times T^2) + (4.63e^{-7} \times T^3)$	J/(kg·K)

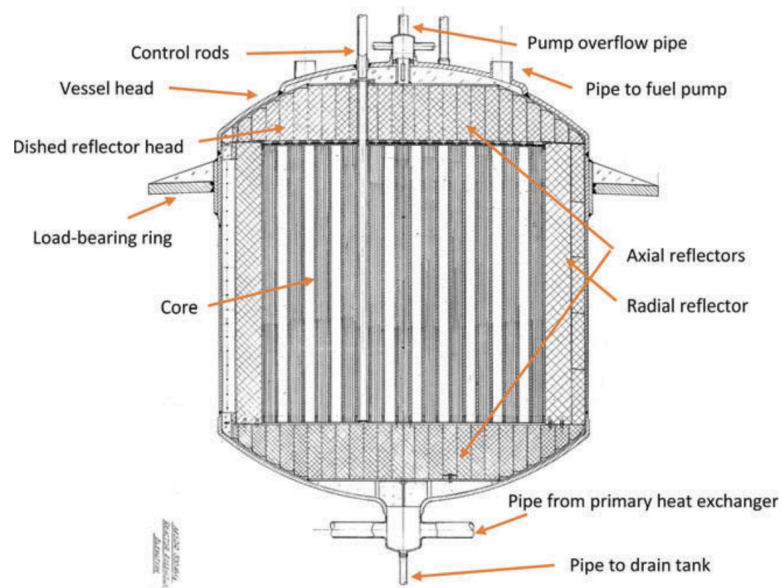


Figure 3.4: Reactor Core from [57], originally from [50]

This is accounted for by increasing the number of parallel characteristic slabs by a factor of two. The axial reflectors, both inlet and outlet, are radial rings of graphite with each ring being made up of smaller sections of graphite. The graphite is modeled using a two dimensional conduction model, as was used before for the radial reflector, but radial (r-z) geometry is used here. The core region is also modeled using a two dimensional conduction model with second order finite difference and slab geometry. In terms of heat and mass transfer, for axial reflectors, it is modeled on the inner and outer radial surface. For the radial reflectors, it is only modeled on the main, large edge of the slab. The edges that were not modeled are so small that including them would be negligible for the results, but would increase simulation time.

3.7 Primary Coolant Loop

The salt mixture in the PCL is FLiBe. The PCL includes the shell side of the PHX, the tube side of the Secondary Heat Exchanger (SHX), and the coolant pump. There are three PCLs, corresponding to the three PFLs, that all reject heat to the BOP. In this model, the PCL interacts directly with the power cycle and is connected to the OTSG. This is different than the original MSDR design, which had a secondary coolant loop. Each loop has a sump-type pump to circulate the flow around the loop to the PHX and SHX. The material and nominal capacity of the SHXs are the same as for the PHXs.

3.8 Power Cycle

The proposed MSDR design used a secondary coolant loop containing nitrate-nitrate working fluid for the power cycle. In this model, the secondary loop was not considered. The selected power cycle is a supercritical steam Rankine cycle. When the water leaves the secondary heat exchanger, it has a temperature of 838.71 K (1050°F)

and a pressure of 24132 kPa (3500 psi). The BOP is simplified using boundary conditions of a supercritical water cycle. This is not relevant to a parameter sensitivity study but can effect reactor dynamics.

3.9 Pressure Loss and Heat Transfer Correlation

3.9.1 Pressure Loss

Bernoulli's principle relates the speed of a fluid to static pressure. It states that the potential energy of the fluid will decrease as the speed of the fluid increases. Bernoulli's principle gives Eq. 3.2

$$P_1 + \frac{1}{2}\rho v_1^2 + \rho g h_1 = P_2 + \frac{1}{2}\rho v_2^2 + \rho g h_2 + H, \quad (3.2)$$

where P_1 is the pressure at elevation 1, ρ is the fluid density, v_1 is the velocity at elevation 1, g is the acceleration due to gravity, h_1 is the height at elevation 1, P_2 is the pressure at elevation 2, v_2 is the velocity at elevation 2, h_2 is the height at elevation 2, and H is the head loss due to friction.

The head loss is the energy used to overcome the friction caused by the piping walls. It is dependent on the pipe diameter, pipe length, flow velocity, and friction factor. There is an increase in the fluid's temperature equivalent to the head loss.

The Darcy-Weisbach Equation relates head loss due to friction across a length of pipe to the average velocity of the flow of the fluid for an incompressible fluid. This makes up the H value in the Bernoulli equation if there are no pumps. The Darcy-Weisbach equation can be seen in Eq. 3.3

$$\frac{\Delta h}{L} = f \times \frac{1}{2g} \times \frac{v^2}{D}, \quad (3.3)$$

where Δh is the head loss due to friction, L is the length of the pipe, f is the Darcy friction factor, g is the acceleration due to gravity, D is the hydraulic diameter of the pipe, and v is the mean velocity.

For turbulent flow in smooth and rough pipes, the Darcy friction factor is expressed by the Colebrook-White equation, which can be seen in Equation 3.4. It can be used to solve iteratively for the Darcy friction factor

$$\frac{1}{\sqrt{f}} = -2\log\left(\frac{\varepsilon}{3.7D} + \frac{2.51}{Re\sqrt{f}}\right), \quad (3.4)$$

where ε is the effective roughness height for the pipe and Re is the Reynolds number.

The Swamee-Jain equation, which is an approximation of the implicit Colebrook-White equation above, can be seen in Eq. 3.5. It can be used to solve for the friction factor directly for a full-flowing circular pipe and is often used as a way to directly solve for the Darcy friction factor.

$$f = \frac{0.25}{\left[\log\left(\frac{\varepsilon/D}{3.7} + \frac{5.74}{Re^{0.9}}\right)\right]^2} \quad (3.5)$$

For laminar flow, the below equation is used to calculate the Darcy friction factor through a circular pipe.

$$f = 64/Re \quad (3.6)$$

3.9.2 Heat Transfer Correlations

The Nusselt number is the ratio of convective heat transfer to conductive heat transfer at a boundary in a fluid. The Dittus-Boelter equation, seen in Eq. 3.7, was used for all the single-phase fluids under turbulent conditions.

$$Nu = 0.023 \times Re^{0.8} Pr^{0.4} \quad (3.7)$$

where Nu is the Nusselt number, Re is the Reynolds number for the hydraulic diameter, and Pr is the Prandtl number. This correlation is valid for a Pr number between 0.6 and 160, a Re number greater than 10,000.

For laminar flow, the solution for circular pipes was used as seen in Eq. 3.8. From this equation, it was determined that Nu is equal to 4.36.

$$Nu = \frac{hL}{\lambda} \quad (3.8)$$

where h is the convective heat transfer coefficients in $W/m^2 \cdot K$, L is the characteristic length in m , and the λ is the thermal conductivity of the fluid in $W/m \cdot K$.

The Sieder-Tate equation should be considered if there are large property variations; this equation adds a viscosity correction factor and can be seen below in Equation 3.9

$$Nu = 0.027 \times Re^{0.8} Pr^{0.33} \left(\frac{\mu}{\mu_s} \right)^{0.14}, \quad (3.9)$$

where μ is the viscosity of the fluid at the bulk fluid temperature and μ_s is the viscosity of the fluid at the heat transfer boundary surface temperature. This correlation is valid for a Pr number between 0.7 and 16700, and a Re number over 10,000.

The Gnielinski equation is much more complex, but can reduce the error that comes from using the Dittus-Boelter and Sieder-Tate. This equation can be seen in Equation 3.10.

$$Nu = \frac{(f/8)(Re - 1000)Pr}{1 + 12.7(f/8)^{1/2}(Pr^{2/3} - 1)} \quad (3.10)$$

This equation is valid for Pr numbers between 0.5 and 2000 and Re numbers between 3000 and $5e6$.

The Dittus-Boelter equation was chosen here since it is the least complex and avoids iterative solving. This allowed the model to have a faster run time.

3.10 Reactor Kinetics

The reactor kinetics are based on a modified form of the traditional point reactor kinetics equations. Terms to account for fission product decay and generation outside the core were added. The fission products are treated as trace substances that are transported around the loop at the same rate as the fuel salt. The parameters for the point kinetics model can be seen in Table 3.9 where λ_i is the decay constant for the precursor group i , α_i is the normalized precursor fraction used to calculate β_i , which is the delayed neutron fraction for that precursor group i ($\beta_i = \alpha_i \beta$), β is the effective delayed neutron fraction, and Λ is the generation time for the prompt neutrons.

For the reactivity coefficients, the salt temperature feedback is equal to $-3.22\text{e-}5$ and the graphite temperature feedback is $+2.35\text{e-}5$ taken from [70]. In this study, it was assumed that each reactivity coefficient contributed equally. These reactivity coefficients can be seen in Table 3.10. The Doppler coefficient is the same as the fuel temperature coefficient and is the change in reactivity per degree change in the fuel temperature. Thorium is the main contributor to the Doppler coefficient. The thermal base coefficients of both the fuel salt and the graphite are positive. All effects of salt expansion are included in the salt density component. Displacement of graphite surfaces and changing graphite density is included in the graphite density component. The total salt coefficient is a relatively large negative coefficient; this is very important since it is prompt and largely controls the fast transient response [70]. This gives adequate reactor stability and controllability. In this model, the power is based on feedback of temperature.

3.11 Closure Relations

The thermophysical properties of both the fuel and coolant salt are modeled as linear compressible fluid. “The linear compressible fluid model indicates that the density is a linear function of temperature and pressure and assumes the following” [57]:

Table 3.9: Parameters for point kinetics model from Betzler, Powers, and Worrall [71]

Parameter	Value
λ_i (s^{-1})	0.0125, 0.0318, 0.109, 0.317, 1.35, 8.64
α_i	0.0320, 0.1664, 0.1613, 0.4596, 0.1335, 0.0472
β	0.0065
Λ (s)	1e-5

Table 3.10: The isothermal reactivity coefficients of the reference reactor used for MSBR [70]

Component	Reactivity Coefficient, $\frac{1}{k} \frac{\partial k}{\partial T}$ (per °C) $\times 10^{-5}$
Doppler	-4.37
Salt thermal base	+0.27
Salt density	+0.82
Total salt	-3.22
Graphite thermal base	+2.47
Graphite density	-0.12
Total graphite	+2.35
Total core	-0.87

1. The specific heat capacity at constant pressure (C_p) is constant.
2. The isobaric expansion coefficient (β) is constant.
3. The isothermal compressibility (κ) is constant.
4. Pressure and temperature are used as states.
5. The influence of density on specific enthalpy (h), entropy (s), internal energy (u), and heat capacity (C_v) at constant volume is neglected.

At this point in time, changing fuel composition due to burnup is not taken into account for the fuel salt. There are plans to add accountancy for time dependent fluid property changes in the future.

3.12 Validation

“Historically, nuclear technology has followed a path to product maturation that involves continuous prototyping and measurement that has provided the software validation data needed for nuclear regulatory licensing” [72]. Data from these prototypes are used to establish uncertainties for the safety parameters. MSRs have a lack of data to use in establishing these uncertainties, therefore, modeling and simulation are more important than ever before.

The typical ways of validating a model are done versus existing benchmarks, simple experiments, or against simulations with another code that are both published and credible. In this realm, there is a benchmark for the MSRE that was first published in 2019, but there is no benchmark for the MSDR. This is because the MSDR was a paper design and was never built let alone operated, therefore there are no experimental data available.

The MSRE benchmark [73] is a reactor physics benchmark that was based on the MSRE zero-power experiments. The benchmark investigated the criticality and

reactivity effects, and was not focused on temperature or thermophysical properties. In this benchmark, an operating core temperature of 638°C (911.15 K) was used for the criticality models and an operating core temperature of 649°C (922.15 K) was used for reactivity effect models. These values are directly from the initial zero-power criticality experiment back in 1965 during the MSRE program. During the zero power experiments, the initial estimate for the core temperature was 649°C (922.15 K) at the time of criticality, but the core temperature at the time of criticality was actually measured to be 638°C (911.15 K). Design criteria for MSDR were not exact due to these temperatures being roughly calculated and not simulation based.

Table 3.11 shows the temperatures for the reactor vessel inlet and outlet in Kelvin for four different reactor designs: MSRE, Molten Salt Breeder Experiment (MSBE), Molten Salt Breeder Reactor (MSBR), and MSDR. Figure 3.5 shows the temperatures used in the MSDR design in green and the temperatures from the TRANSFORM model in black. They agree pretty closely, but there are deviations between the paper design and the TRANSFORM model. Table 3.12 shows the temperatures at nominal for the TRANSFORM model at the four locations, the MSDR design document [50] values at the inlet and outlet of the core extended to the PHX inlet and outlet, the ΔT between the TRANSFORM model and MSDR design, and the percent change between the two. At this stage of understanding, it is concluded that the percent change values of <5% are not significant since there are simplifying assumptions in the MSDR design parameters. Further, the property uncertainties are up to 30% uncertainty, which surpasses any model assumptions.

Table 3.11: The temperatures in Kelvin at the reactor vessel inlet and outlet for four different MSR designs. [74]

	MSRE	MSBE	MSBR	MSDR
Temperature Inlet of Reactor Vessel	905.37	838.7	838.7	838.7
Temperature Outlet of Reactor Vessel	927.6	977.6	977.6	949.8

Table 3.12: Temperature difference between model and design document

Location	Model	MSDR	ΔT	Percent Change (%)
PHX Inlet	954.27 K	949.82 K	4.47 K	0.47%
PHX Outlet	863.37 K	838.71 K	24.67 K	2.94%
Core Inlet	863.42 K	838.71 K	24.72 K	2.95%
Core Outlet	954.82 K	949.82 K	5.02 K	0.53%

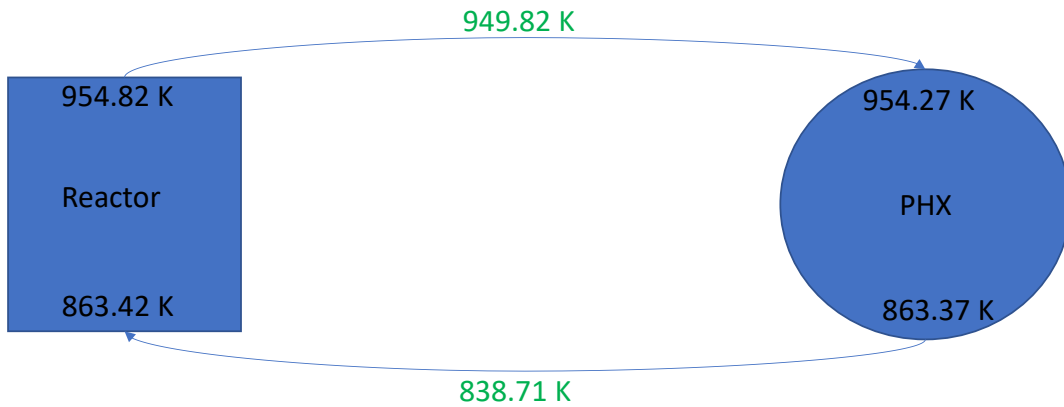


Figure 3.5: A schematic showing the temperatures from the paper MSDR design in green and the temperatures from the TRANSFORM model in black.

Chapter 4

Results

In this chapter, the temperature values at several locations for all the different perturbations are presented to understand how uncertainty in the thermophysical properties affects reactor behavior at steady state operations. Next, a reactivity insertion scenario is explored to understand how temperature reacts during a reactivity insertion of 200 pcm. Next, temperature behavior during a buildup transient is explored by reducing the diameter of the piping. Lastly, the effects of perturbing two properties at the same time is explored. These scenarios were chosen to see if there is a justification to perform better measurements for the four thermophysical properties to reduce their uncertainties.

4.1 Steady State

For steady state, 23 different simulations were conducted to obtain the temperature values at the core inlet, core outlet, PHX inlet, and PHX outlet for each run. In this section, those results are presented along with the ΔT between the inlet and outlet of the core and the ΔT between the inlet and outlet of the PHX. The four output temperatures of the core inlet and outlet and the PHX inlet and outlet were calculated for separate simulations that were run for each property value perturbation. In this

effort, properties were varied one at a time to examine their effect on the temperatures individually. The results of this are seen in Figure 4.1. All temperatures are in Kelvin. The PHX inlet and core outlet are plotted on the primary axis and the core inlet and PHX outlet are plotted on the secondary axis. The percent variation of the property is on the x-axis, with 0% corresponding to the nominal value; the nominal value for the four thermophysical properties can be seen in Table 3.4 in Chapter 3. The nominal values for the PHX inlet and PHX outlet temperatures are 954.27 K and 863.37 K, respectively, and the ΔT for the PHX is 90.91 K. The nominal temperature for the core inlet and core outlet temperatures are 863.42 K and 954.82 K, respectively, and the ΔT for the core is 91.39 K. It is apparent in Figure 4.1 that the PHX inlet and core outlet temperatures are almost identical for all the explored perturbations; the same is seen for the PHX outlet and core inlet temperatures. This is as expected since no significant heat generation or heat loss should happen in the piping. The majority of heat loss happens in the PHX, and the majority of heat generation happens in the core region. This gives us confidence that the model is functioning as expected.

The first set of perturbations were for density at steady state. Examining Figure 4.1a, it can be seen that for all the locations, a smaller density value resulted in a higher temperature. The -10% density perturbation had the highest temperatures at 954.60, 863.58, 863.64, and 955.15 K for the PHX inlet, PHX outlet, core inlet, and core outlet, respectively. The lowest temperatures happen at the +10% perturbation for all four locations; those temperatures are 953.95, 863.16, 863.21, and 954.49 K for the PHX inlet, PHX outlet, core inlet, and core outlet, respectively. These are considered safe conditions with nothing indicating these temperatures are critical. Figure 4.2a shows these data as a percent difference compared to nominal; the percent difference is used to highlight the differences in the data obtained from each set of property perturbations. The highest percent difference from nominal is seen for the maximum or minimum property value for all four properties. The range of percent

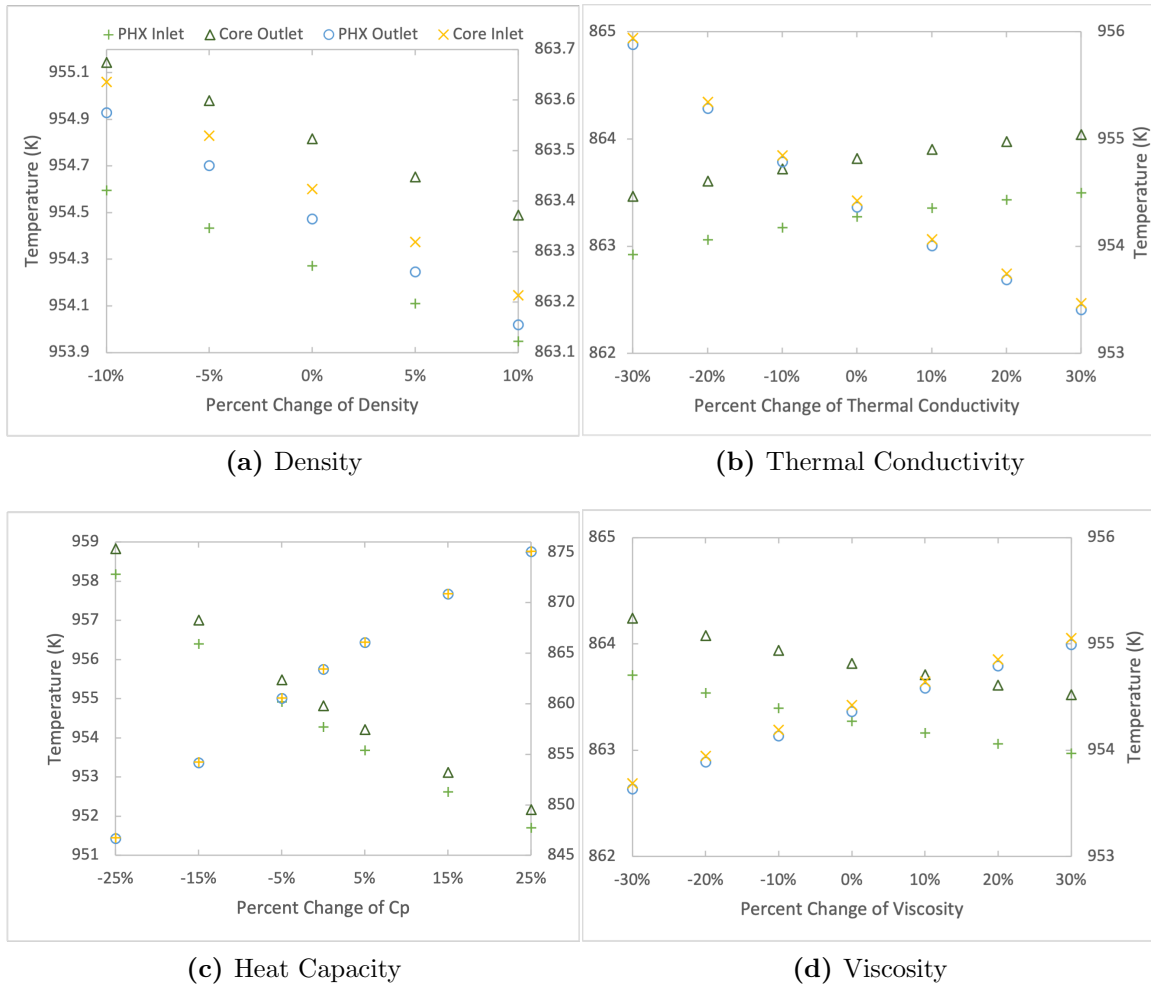


Figure 4.1: Temperatures for the loop at steady state. The core outlet and PHX inlet temperatures are plotted on the primary axis, while the PHX outlet and the core inlet temperatures are plotted on the secondary axis.

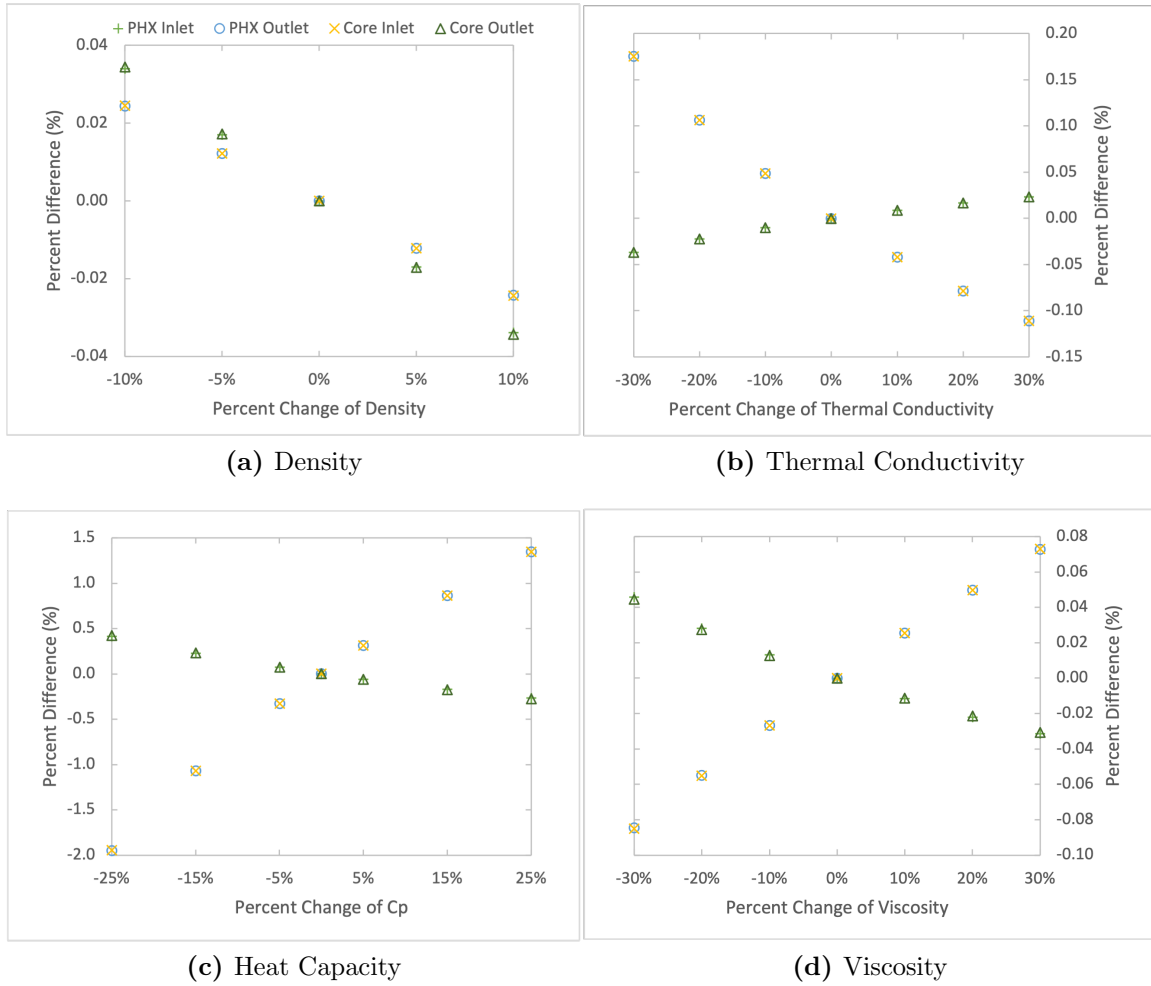


Figure 4.2: Comparison of results to nominal for steady state. The core outlet and PHX inlet temperatures are plotted on the primary axis, while the PHX outlet and the core inlet temperatures are plotted on the secondary axis.

difference values is between -0.0343% and 0.0344% when accounting for all four locations. Both of these values actually occur at the core outlet signaling to us that the maximum difference between the minimum perturbation of -10% density and maximum perturbation of +10% density occurs at the core outlet location, but only by a small margin. Tables 4.1-4.4 show the ΔT across the PHX and core for all four properties; ΔT was found by subtracting the difference between the outlet and inlet temperatures of the two components, the core and the PHX, individually. The ΔT values can be seen in Table 4.1 for perturbations of density. Closer inspection of the table shows that a decrease was seen in ΔT for both components when the density increased. The ΔT values for the PHX were between -90.79 K and -91.02 K and the core ΔT values were between 91.28 K and 91.51 K.

Density and temperature are inversely related, so these temperature trends are consistent. The somewhat basic statement “as temperature increases, the kinetic energy increases, as this happens the particles in the substance move faster, which results in density decreasing” is true for an inert gas, but not necessarily true when dealing with a liquid. The particles move faster in a gas than a liquid for all kinetic energy sources including vibration, rotation, and translation. One example where the statement does not hold true is for water (H_2O) where the temperature also increases when the density increases, but water is an anomaly among substances. This anomaly for water is primarily due to hydrogen bonding. This approach of assuming only kinetic energy matters and nothing else is too categorical here. The other sources of energy, such as electrostatic forces, do not matter as much for a gas as they do for a liquid. Hydrogen bonding is an intermolecular force of attraction along with dipole-dipole interactions and van der Waal forces. There are also intramolecular forces at play, which include ionic bonds, covalent bonds, and metallic bonding. The intermolecular forces are generally much weaker than the intramolecular ones.

Table 4.1: The change in temperature across the PHX and core during steady state conditions for perturbations of density

Density	ΔT PHX	ΔT Core
-10%	-91.02	91.51
-5%	-90.96	91.45
0	-90.91	91.39
5%	-90.85	91.34
10%	-90.79	91.28

Table 4.2: The change in temperature across the PHX and core during steady state conditions for perturbations of thermal conductivity

Lambda	ΔT PHX	ΔT Core
-30%	-89.04	89.53
-20%	-89.78	90.26
-10%	-90.39	90.87
0	-90.91	91.39
10%	-91.35	91.84
20%	-91.74	92.23
30%	-92.09	92.58

Table 4.3: The change in temperature across the PHX and core during steady state conditions for perturbations of heat capacity

Heat Capacity	ΔT PHX	ΔT Core
-25%	-111.52	112.09
-15%	-102.27	102.80
-5%	-94.41	94.91
0	-90.91	91.39
5%	-87.65	88.13
15%	-81.79	82.24
25%	-76.66	77.08

Table 4.4: The change in temperature across the PHX and core during steady state conditions for perturbations of viscosity

Viscosity	ΔT PHX	ΔT Core
-30%	-92.07	92.55
-20%	-91.65	92.13
-10%	-91.26	91.75
0	-90.91	91.39
10%	-90.58	91.07
20%	-90.27	90.76
30%	-89.98	90.47

Intramolecular forces occur within a molecule and refers to the chemical bonds that hold atoms together in those molecules. Intermolecular forces, also called electrostatic interactions, occur between molecules. Basically, as the temperature of the system increases, the ions get more excited and the structure of the salt loosens, reducing the density.

The next set of perturbations were for thermal conductivity at steady state. From examining Figure 4.1b, it is seen that unlike the density perturbation set, the highest temperatures do not happen for the same perturbation value of thermal conductivity with the maximum temperature happening at -30% for some and +30% for others. For the PHX inlet and core outlet, the maximum temperature of 954.50 and 955.04 K, respectively, happen at the largest thermal conductivity value, the +30% perturbation. For the core inlet and PHX outlet, the maximum temperatures of 864.94 and 864.88 K happen at the -30% perturbation. Upon examination of Figure 4.2b, it is seen that the range of percent difference values for all four locations is -0.1111% and 0.1755%. Both of these happened at the PHX outlet. The ΔT values for the thermal conductivity can be seen in Table 4.2. An increase in ΔT was seen for both components when the thermal conductivity increased. The ΔT values for the PHX were between -89.04 K and -92.09 K and the ΔT values for the core were between 89.53 K and 92.58 K. The thermal conductivity was the only perturbed property that saw an increase in ΔT as the property increased; the opposite was seen for the other three properties. A common equation relating ΔT and thermal conductivity is seen in Equation 4.1.

$$\lambda = \frac{Qd}{A\Delta T} \quad (4.1)$$

In this equation, Q is the amount of heat transferred, A is the cross sectional area of the material transferring heat, d is the thickness of the material, and ΔT is the difference in temperature between one side of the material and the other side.

At first glance, one would expect a decreasing ΔT with an increase in thermal conductivity, but the opposite was seen here in all four locations. The issue with using this equation is that, in Figure 4.1, ΔT is taken across a medium such as the wall of a heat exchanger, but in this study, the ΔT is the difference between the temperature of the molten salt fluid at the inlet and outlet of the component. The equation is ideal for heat conduction through a solid, but not for heat conduction through a liquid. In Figure 4.1, the fluid is not rejecting the heat, but rather the heat is rejected through the walls of the solid heat exchanger. In reality, a larger thermal conductivity will result in the heat flowing more quickly in the fluid which causes the whole system to cool more quickly due to the heat being able to flow better. Further, the temperature difference between the centerline of the fluid and the heat exchanger wall is smaller at larger thermal conductivity values. Further, more heat is being rejected through the PHX at a higher thermal conductivity. To sum this up, at a higher thermal conductivity, the system cools more effectively.

The next set of perturbations were for heat capacity at steady state. The data for perturbations of heat capacity can be seen visually in Figures 4.1c and 4.2c. For a positive perturbation of heat capacity to a larger value, the core inlet and PHX outlet saw a higher temperature, 875.09 and 875.04 K, respectively. The opposite was seen for the locations of the PHX inlet and core outlet. The maximum temperature value for the PHX inlet was 958.17 K, and the maximum temperature value at the core outlet was 958.83 K; both occurring at the smallest heat capacity value. Examining Figure 4.2c, we see that the range of percent difference values is -1.9539% to 1.3431%. Both of these values occur at the PHX outlet, telling us that the max difference happens between the -25% perturbation and the +25% perturbation at the location of the PHX outlet. The largest percent difference by far out of all the thermophysical properties is seen for the heat capacity. The ΔT values for perturbations of heat capacity can be seen in Table 4.3. A decrease was seen in ΔT for both components when the heat capacity increased. The ΔT values for the PHX ranged between -76.66

K all the way up to -111.52 K and the ΔT values were in a range between 77.08 K to 112.09 K for the core. The highest and lowest ΔT values out of all the studied properties happened for the heat capacity. The heat capacity data is consistent when looking at Equation 4.2 with a constant power and mass flow rate, an increasing C_p will result in a smaller ΔT . This also becomes clear when examining Table 4.3.

$$Q = \dot{m}C_p\Delta T \quad (4.2)$$

where Q is the heat, $\dot{m}$ is the mass flow rate, C_p is the heat capacity, and ΔT is the change in temperature.

The final set of perturbations in this section were for viscosity at steady state. The data for perturbations of viscosity are seen in Figures 4.1d and 4.2d. Similar trends are seen for viscosity as those trends seen for the heat capacity. Examining Figure 4.1d closer, a positive perturbation of the viscosity to a larger value results in a higher temperature for the core inlet and PHX outlet, 864.05 and 863.99 K respectively. Alternatively, for the PHX inlet and core outlet, the opposite is seen with the smallest viscosity value resulting in the highest temperature, 954.71 K for the PHX inlet and 955.24 K for the core outlet. By looking at Figure 4.2d, we see that the maximum range of the percent difference at all four locations is -0.0851% to 0.0728%. This happens at the core inlet. The ΔT values for perturbations of heat viscosity can be seen in Table 4.4. A decrease was seen in ΔT for both components when the viscosity increased. The ΔT values for the PHX were between -89.98 K up to -92.07 K and the ΔT values for the core were in a range between 90.47 K and 92.55 K.

With decreasing viscosity, there should be an increase in temperature; this is seen in Equation 4.3. This is true for PHX inlet and core outlet, but is false for PHX outlet and core inlet.

$$\eta = Ae^{b/T} \quad (4.3)$$

where T is the absolute temperature and A and b are constants [75].

4.2 Reactivity Insertion

For this scenario, the same 23 simulations were run with an added element of a reactivity insertion of 200 pcm at 7.776e6 seconds (approximately three months). 200 pcm was chosen since it is a little less than half of what the effective delayed neutron fraction, β_{eff} , is when corrected for circulation of the fuel salt. In this scenario, only one thermophysical property was varied at a time. The temperature values are in Kelvin and taken after the reactivity insertion initially occurs. The reactivity insertion was instantaneous with the feedback mechanisms following the dynamics of the kinetic model. The temperature results at all four locations can be seen in Figure 4.3, and the percent difference compared to nominal can be seen in Figure 4.4.

Tables 4.5-4.8 show the ΔT across the PHX and core for all four properties. To compare the difference between steady state and reactivity insertion temperatures, the mean temperature for both the steady state and reactivity insertion scenarios were calculated by averaging the temperatures at the PHX inlet, PHX outlet, core inlet, and core outlet. The increase in mean temperature for the reactivity insertion is highlighted in Table 4.9. The mean temperature for steady state was between 900-910 K for all the perturbations of all the properties and the mean temperature for the reactivity insertion is between 1090-1110 K. The temperatures are on average about 200 K more than the temperatures during steady state conditions with the average temperature for steady state conditions being 908.97 K and 1104.85 K for reactivity insertion conditions at nominal value.

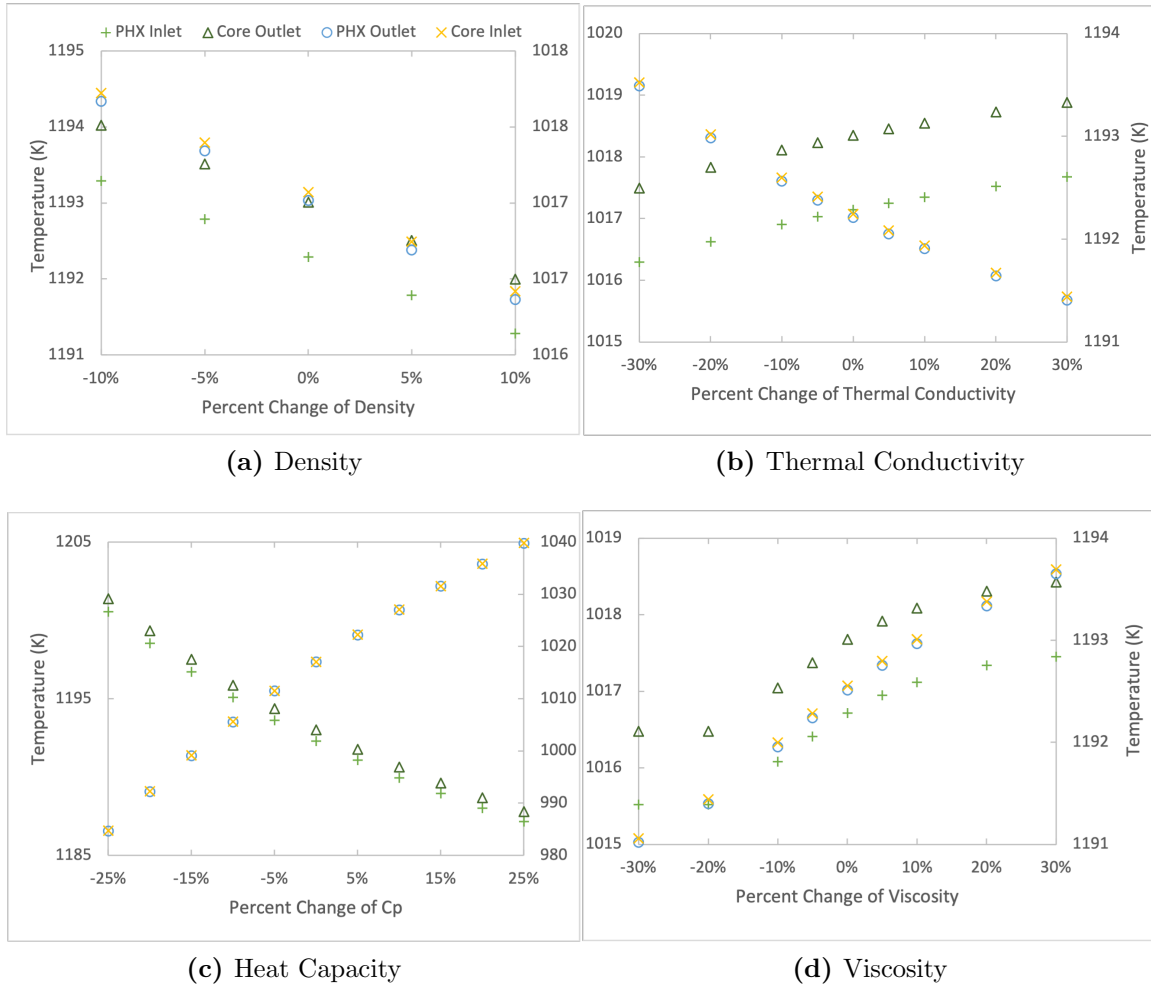


Figure 4.3: Temperatures for a reactivity insertion transient of 200 pcm. The core outlet and PHX inlet temperatures are plotted on the primary axis, while the PHX outlet and the core inlet temperatures are plotted on the secondary axis.

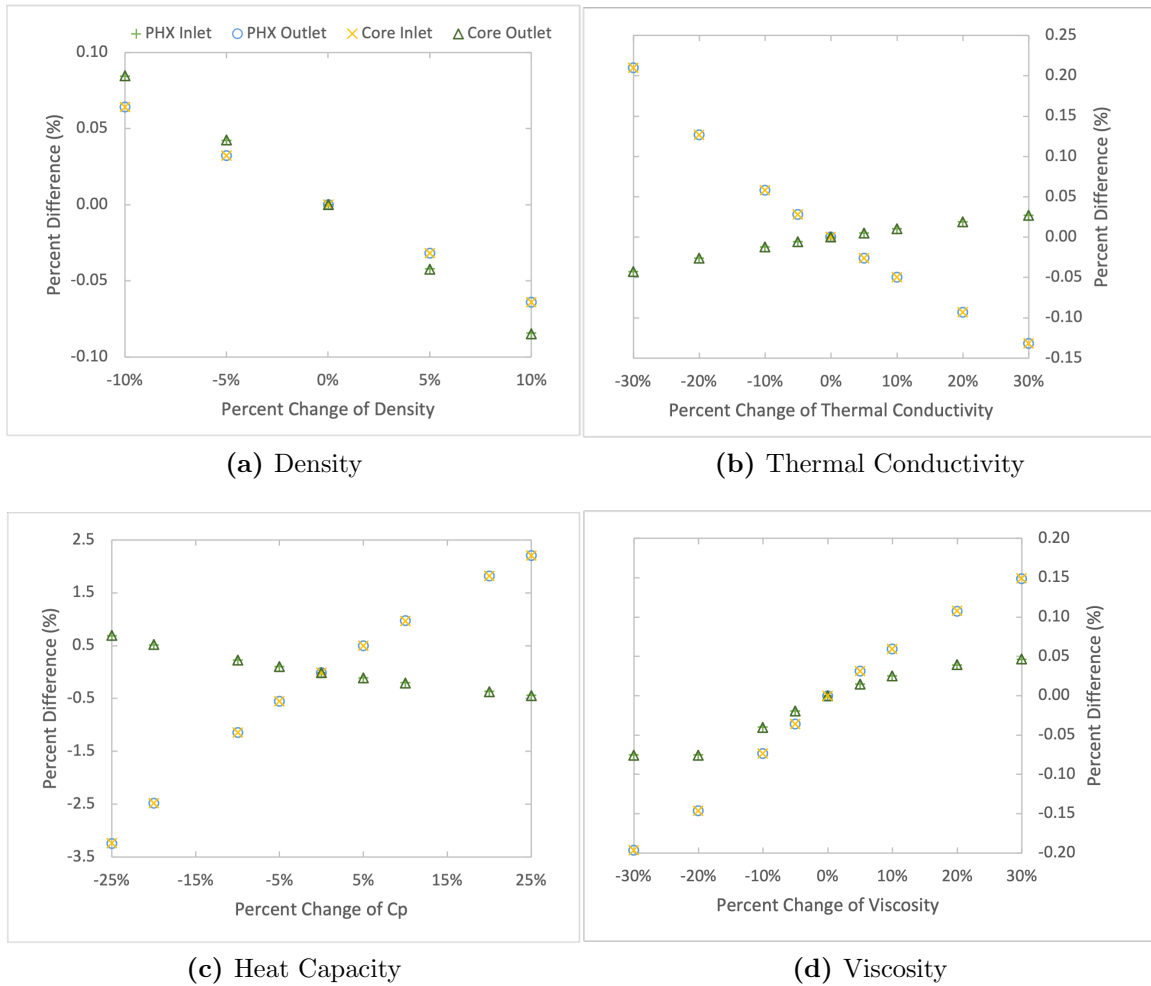


Figure 4.4: Comparison of results to nominal for a reactivity insertion event for 200 pcm. The core outlet and PHX inlet temperatures are plotted on the primary axis, while the PHX outlet and the core inlet temperatures are plotted on the secondary axis.

Table 4.5: The change in temperature across the PHX and core during a reactivity insertion of 200 pcm for perturbations of density

Density	ΔT PHX	ΔT Core
-10%	-175.62	176.30
-5%	-175.45	176.12
0	-175.27	175.94
5%	-175.09	175.76
10%	-174.92	175.58

Table 4.6: The change in temperature across the PHX and core during a reactivity insertion of 200 pcm for perturbations of thermal conductivity

Lambda	ΔT PHX	ΔT Core
-30%	-172.62	173.29
-20%	-173.67	174.34
-10%	-174.54	175.20
0%	-175.27	175.94
10%	-175.90	176.57
20%	-176.45	177.12
30%	-176.93	177.60

Table 4.7: The change in temperature across the PHX and core during a reactivity insertion of 200 pcm for perturbations of heat capacity

Heat Capacity	ΔT PHX	ΔT Core
-25%	-215.90	216.66
-15%	-197.61	198.34
-5%	-182.14	182.83
0%	-175.27	175.94
5%	-168.89	169.54
15%	-157.42	158.04
25%	-147.39	147.99

Table 4.8: The change in temperature across the PHX and core during a reactivity insertion of 200 pcm for perturbations of viscosity

Viscosity	ΔT PHX	ΔT Core
-30%	-176.37	177.03
-20%	-175.86	176.52
-10%	-175.54	176.20
0	-175.27	175.94
10%	-174.97	175.64
20%	-174.64	175.31
30%	-174.31	174.98

Table 4.9: Comparison of the mean temperature taken for all four locations and averaged for the steady state conditions and the reactivity insertion conditions

Property & Perturbation	Mean Temperature at Steady State (K)	Mean Temperature after Reactivity Insertion (K)
Density		
-10%	909.24	1105.68
-5%	909.10	1105.26
0	908.97	1104.85
5%	908.84	1104.43
10%	908.70	1104.01
Thermal Conductivity		
-30%	909.55	1105.66
-20%	909.32	1105.34
-10%	909.13	1105.07
0	908.97	1104.85
10%	908.83	1104.65
20%	908.71	1104.48
30%	908.60	1104.34
Heat Capacity		
-25%	902.60	1092.82
-15%	905.43	1098.13
-5%	907.87	1102.75
0	908.97	1104.85
5%	909.99	1106.81
15%	911.85	1110.42
25%	913.50	1113.64
Viscosity		
-30%	908.82	1103.40
-20%	908.86	1103.65
-10%	908.92	1104.23
0	908.97	1104.85
10%	909.03	1105.30
20%	909.08	1105.63
30%	909.14	1105.88

The first property perturbed under reactivity insertion conditions was density. Upon examining Figure 4.3a, it is seen that when the density is increased, the temperature increases at all four locations just like for the steady state scenario. The output temperatures were 1193.29, 1017.67, 1017.72, 1194.02 K for the PHX inlet, PHX outlet, core inlet, and core outlet, respectively. The percent differences for a reactivity insertion scenario can be seen in Figure 4.4a and are all between -1.013% and 1.011% with the minimum and maximum value occurring for the core outlet just like in steady state. The temperatures are on average about 200 K more than the temperatures during steady state conditions with the average temperature for steady state conditions being 909.24 K and at 1105.68 K for reactivity insertion conditions at a value of 10% less than the nominal density value, which can be seen in Table 4.9. Table 4.5 shows the change in temperature across the PHX and the core for perturbations of density. The ΔT between the PHX outlet and inlet ranges from -174.92 to -175.62 K, and the ΔT between the core outlet and inlet ranges from 175.58 to 176.30 K. The largest ΔT happens for the smallest density value for both components.

The second perturbed property was thermal conductivity. As can be seen in 4.4b, there was an increase in temperature for the largest thermal conductivity value for the PHX inlet and core outlet, which were 1192.61 and 1193.33 K, and the highest temperature for the core inlet and the PHX outlet happens at the smallest thermal conductivity value, which were 1019.21 and 1019.15 K. From looking at Figure 4.4, the range of percent differences for thermal conductivity were between -1.338 and 2.136 %; both of these happen at the core outlet. This is the same as what happened for steady state. The average temperatures are similar to the density here and show about a 200 K difference, which can be seen in Table 4.9. As seen in Table 4.6, the range of ΔT values for the PHX is between -174.92 and -175.62 K and for the core, it is between 175.58 and 176.30 K.

The third perturbed property was heat capacity. The heat capacity saw the inverse of what happened for the thermal conductivity. Examining Figure 4.3c, it can be seen that the heat capacity saw a decrease in temperature for increasing heat capacity for the PHX inlet and core outlet, 1200.54 and 1201.38 K. Meanwhile for an increasing heat capacity, an increase in temperature was seen for the core inlet and PHX outlet, 1039.81 and 1039.77 K, respectively. From Figure 4.4c, it is seen that the range of percent differences for heat capacity were between -32.373 and 22.752 %; both of these happen at the PHX outlet. This is by far the largest percent difference out of all the thermophysical properties. This is the same location as what happened for steady state. The average temperatures can be seen in Table 4.9 and are about a 200 degree difference between the steady state and reactivity insertion here as well. The ΔT values between the core inlet and outlet the core and PHX inlet and outlet can be seen in Table 4.7. The range of ΔT values for the PHX is between -147.39 and -215.90 K and for the core, it is between 147.99 and 216.66 K.

The last perturbed property was viscosity. Viscosity saw the opposite effect on temperature compared to the density. For viscosity, all four locations saw an increase in temperature for an increase in viscosity: 1192.84 K for PHX inlet, 1018.53 K for PHX outlet, 1018.59 K for core inlet, and 1193.57 K for core outlet. It is interesting to note that the reactivity insertion viscosity results follow a different pattern than the steady state viscosity results. The range of percent differences for viscosity were between -1.995 and 1.519%; both of these happen at the core inlet. This is the same location as steady state. The average temperatures are a little less than 200 K difference between the steady state and reactivity insertion as seen in Table 4.9. The ΔT values between the outlet and inlet of the core and PHX can be seen in Table 4.8. The range of ΔT values for the PHX is between -174.31 and -176.37 K and for the core, it is between 174.98 and 177.03 K.

4.3 Buildup Transient

The next scenario explored investigated a buildup transient where fission products, corrosion products, and other products build up on the hot leg and cold leg piping. This was simulated by shrinking the diameter of both the hot leg and cold leg piping from the original value of 12 inches down to 9 inches, 6 inches, and 3 inches. This was investigated by varying one thermophysical property at a time at steady state. This yielded some interesting results as can be seen in Figures 4.5 and 4.6. Figure 4.5 shows the temperature at all four locations for all four diameter values. From this figure, it can be seen that the PHX outlet temperature is lower than the core inlet temperature. This could make a bit of sense due to the possibility of heat gain in the salt from fissions, delayed neutrons, or the piping itself, but that theory does not seem to hold true since the opposite happens in the hot leg with heat being lost when the salt travels from the core outlet to the PHX inlet. Both should not be true. The 3 inch diameter result also has a much larger difference between the PHX inlet and core outlet than the other diameters, as well as a more pronounced difference between the core inlet and PHX outlet as well. Investigating Figure 4.6, which only has the PHX location plotted, it is seen that the 3 inch diameter deviated from the pattern seen between the 6, 9, and 12 inch results. The 3 inch result is unphysical and the code cannot handle such a small diameter for the piping.

The steady state results can be seen in Figure 4.7 for the temperatures of all the property perturbations at 6, 9, and 12 inches. As can be seen in Figure 4.7, the temperature increases for all the perturbations of all the properties when the diameter is decreased from 12 inches down to 6 inches. The 12 inch line on Figure 4.7 is exactly the same as the PHX inlet location of Figure 4.1 since it is at nominal diameter. Figures 4.7 and 4.8, make it clear that the 6 inch temperature is always highest and the 12 inch temperature is always lowest. Shrinking the diameter by 50% results in a temperature increase of 8.31 K at nominal property values, while shrinking

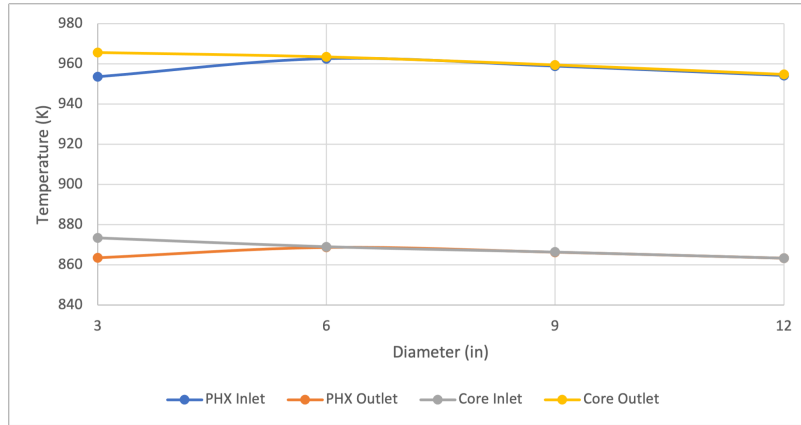


Figure 4.5: Temperatures for shrinking the diameter of the piping with no property perturbations

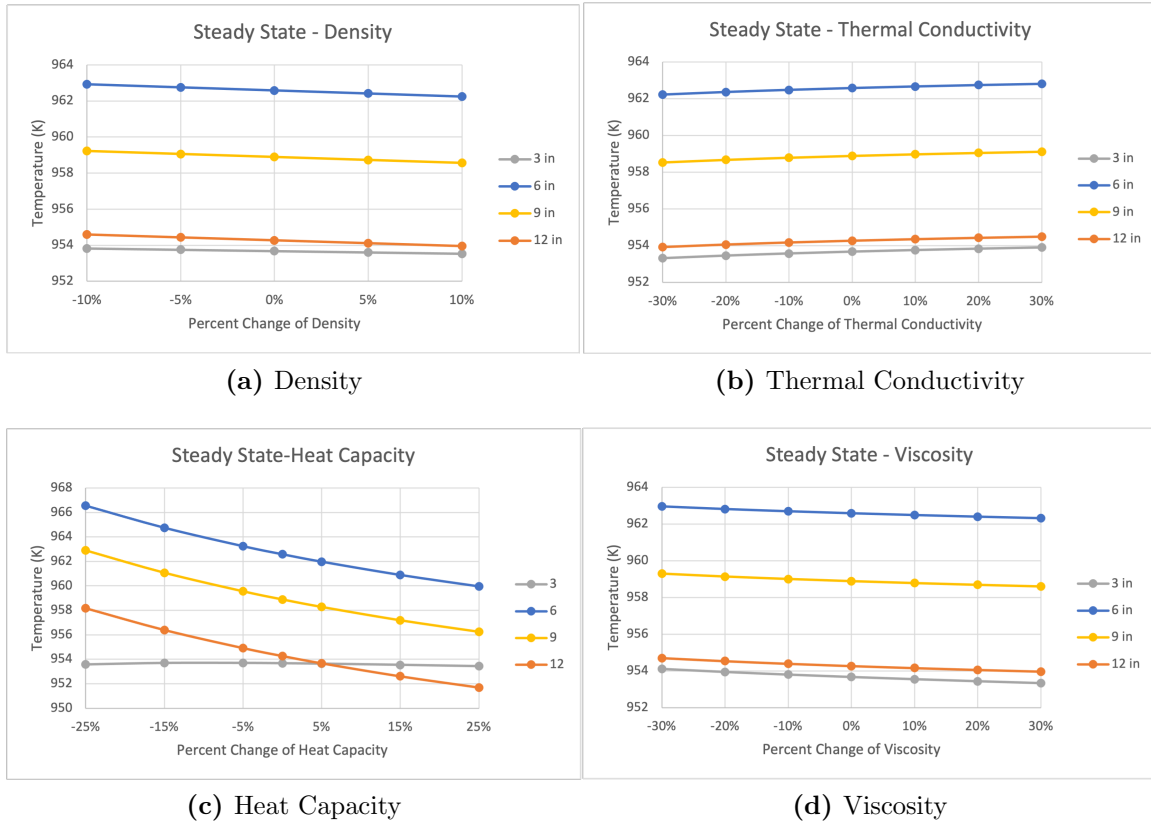


Figure 4.6: Temperatures for shrinking the diameter of the piping with perturbations of properties

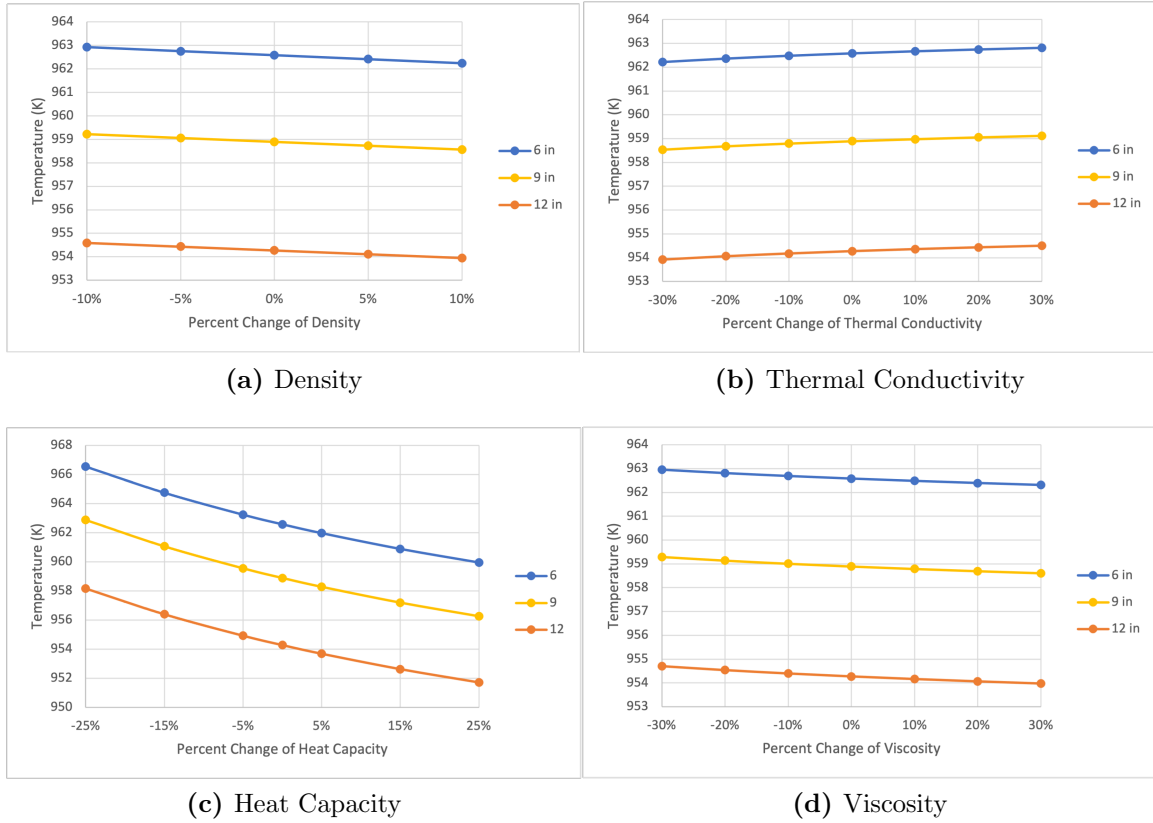


Figure 4.7: Temperatures for shrinking the diameter of the piping with perturbations of each property

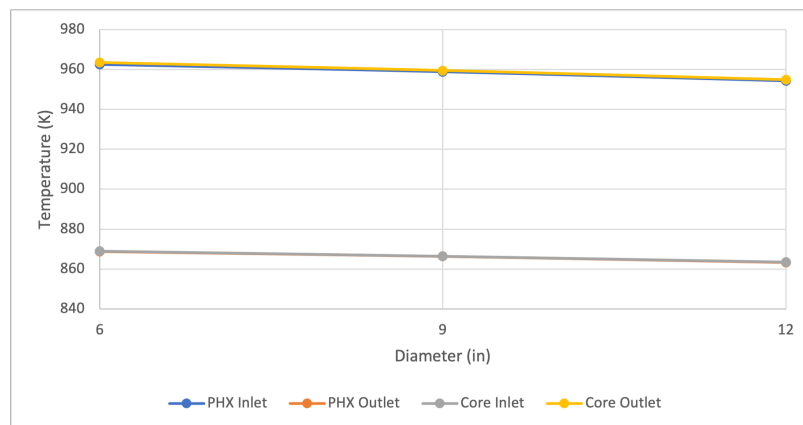


Figure 4.8: Temperatures for shrinking the diameter of the piping with no property perturbations without the 3 inch diameter

the diameter by 25% results in an increase in temperature of 4.62 K for nominal property values. This can be seen in Table 4.10.

The first property explored was density. The range of temperatures for the density perturbations are 962.24-962.92 K for the 6 inch scenario, 958.56-959.23 K for the 9 inch scenario, and 953.95-954.60 K for the 12 inch scenario as seen in Figure 4.7a. The 6 inch result has the highest percent difference for all perturbations of density; this can be seen in Figure 4.9a.

The second property explored was thermal conductivity. The range of temperatures for the density perturbations are 962.22-962.81 K for the 6 inch scenario, 958.53-959.12 K for the 9 inch scenario, and 953.92-954.50 K for the 12 inch scenario as seen in Figure 4.7. Upon examination of Figure 4.9b, it is seen that much like density, the 6 inch result has the highest percent difference for all perturbations of thermal conductivity.

The third property explored was heat capacity. Examining Figure 4.7c, the range of temperatures for the heat capacity perturbations are 959.95-966.56 K for the 6 inch scenario, 956.25-962.89 K for the 9 inch scenario, and 951.70-958.17 K for the 12 inch scenario. When examining Figure 4.9c, it can be seen that the 9 inch result has the highest percent difference for all perturbations of heat capacity.

The last property explored was viscosity. The range of temperatures for the viscosity perturbations are 962.31-962.96 K for the 6 inch scenario, 958.61-959.29 K for the 9 inch scenario, and 953.97-954.71 K for the 12 inch scenario as seen in Figure 4.7d. Upon examination of Figure 4.9d, it is easily seen that the 12 inch result has the highest percent difference for all perturbations of viscosity.

What is interesting and can be seen in Figure 4.9 is that the lines almost fully overlap for the density, thermal conductivity, and heat capacity, but they are a little more spread out for the viscosity. Viscosity sees the greatest spread for the 3 diameters studied.

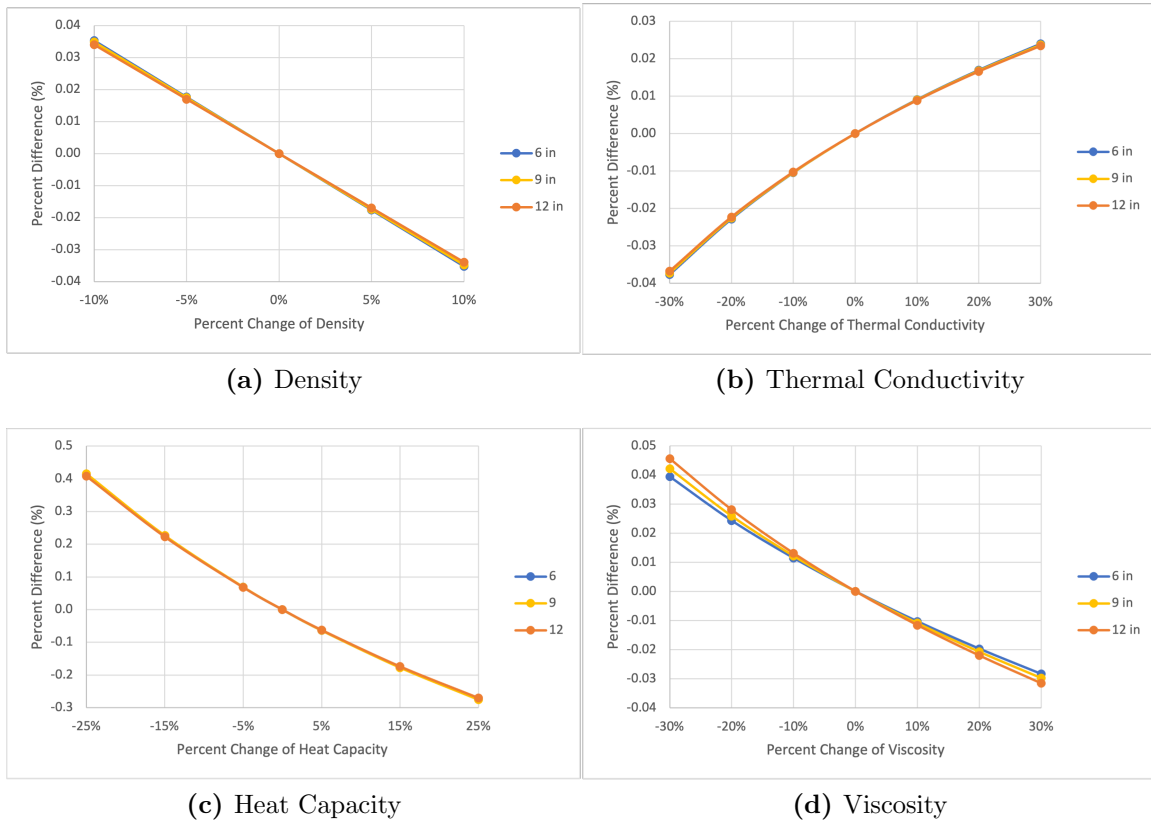


Figure 4.9: Comparison of temperatures to nominal for perturbations of each property with changing diameter

Table 4.10: The difference between the temperatures at different diameters

Property & Perturbation	Difference between 6in and 9in	Difference between 9in and 12in	Difference between 6in and 12in
Density			
-10%	3.70	4.63	8.33
-5%	3.69	4.62	8.32
0	3.69	4.62	8.31
5%	3.69	4.61	8.30
10%	3.69	4.61	8.29
Thermal Conductivity			
-30%	3.69	4.61	8.30
-20%	3.69	4.61	8.30
-10%	3.69	4.62	8.31
0	3.69	4.62	8.31
10%	3.69	4.62	8.31
20%	3.69	4.62	8.31
30%	3.70	4.62	8.32
Heat Capacity			
-25%	3.68	4.71	8.39
-15%	3.69	4.67	8.36
-5%	3.69	4.63	8.32
0	3.69	4.62	8.31
5%	3.69	4.60	8.30
15%	3.69	4.58	8.27
25%	3.69	4.56	8.25
Viscosity			
-30%	3.67	4.59	8.25
-20%	3.68	4.60	8.28
-10%	3.69	4.61	8.30
0	3.69	4.62	8.31
10%	3.70	4.62	8.32
20%	3.70	4.63	8.33
30%	3.70	4.63	8.34

As expected, the largest ΔT between both the 6 inch and 9 inch diameters compared with the 12 inch diameter occurs for heat capacity, then viscosity, then density, and lastly thermal conductivity. As can be seen in Table 4.10, these are all in the range of 4.68-4.71 K for reducing the diameter by 25% from 12 inches to 9 inches and 8.25-8.39 K for reducing the diameter by 25% from 12 inches to 6 inches.

4.4 Varying Two Parameters At A Time

In this scenario, two thermophysical properties were varied at the same time at steady state conditions. This was done to investigate whether there were adverse correlation effects and whether those might make the reactor not operational. The temperatures were taken at the PHX inlet only. A matrix was made of all possible combinations of thermophysical properties excluding viscosity since it is unrelated to the other properties. From this matrix, MATLAB was used to generate 3-D plots and contour plots. 3-D plots and contour plots allow one to visualize the effects of the perturbations of two parameters easier. The temperature profile for all of these plots go from blue as the lowest temperature up to yellow as the highest temperature. The two perturbations are on the x and y axis for both types of plots.

It can be seen in both Figure 4.10 and 4.11 that the heat capacity dominates the effect on temperature since it is almost the same as the heat capacity perturbations alone. For the perturbation of heat capacity alone, the maximum temperature for the PHX inlet happens at -25% and is 958.2 K. The maximum temperature for density alone is 954.6 K. When perturbing both the density and the heat capacity, the maximum temperature value is 958.5 K, only 0.3 K more than heat capacity alone. The maximum temperature value for perturbing both density and heat capacity occurs at a perturbation of -10% density and -25% heat capacity. The maximum temperature for thermal conductivity alone is 954.5 K. When perturbing both the

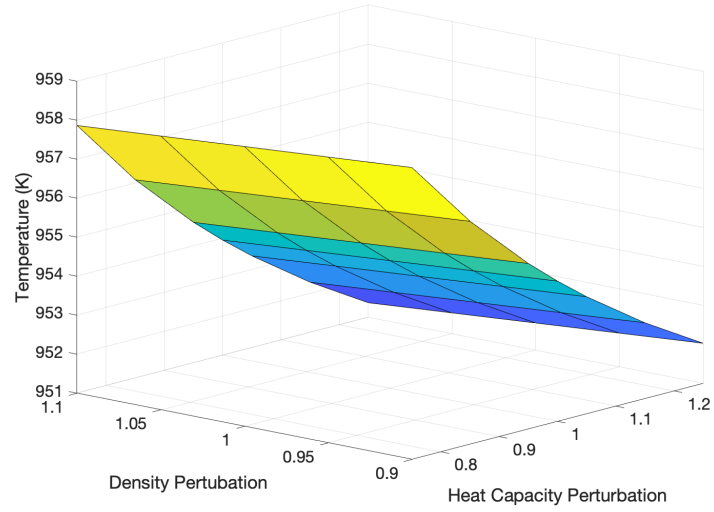


Figure 4.10: 3-D plot of the change in temperature in relation to perturbing both density and heat capacity at steady state

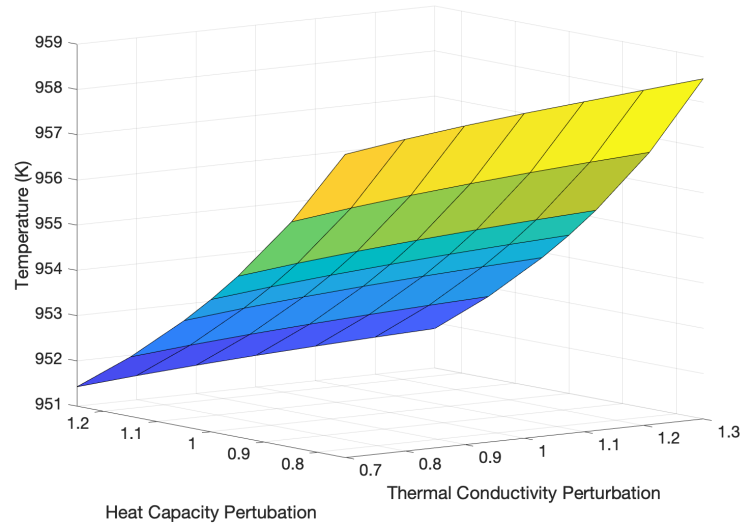


Figure 4.11: 3-D plot of the change in temperature in relation to perturbing both heat capacity and thermal conductivity at steady state

thermal conductivity and the heat capacity, the maximum temperature value is 958.5°K, which occurs at a perturbation of -25% for the heat capacity and +30% for the thermal conductivity. This is summed up in Table 4.11. The contour plots for both of these can be seen in Figures 4.12 and 4.13.

Figure 4.14 shows a much smaller range of temperatures showing that when both the thermal conductivity and density are perturbed, it results in a much lower temperature difference than the perturbations that include heat capacity. The maximum temperature during a perturbation of density alone is 954.6°K; the maximum temperature of thermal conductivity alone is 954.5°K. When both of them are perturbed together, the maximum temperature happens at -10% density and +30% thermal conductivity and is slightly higher at 954.8°K. This can also be seen by way of contour plot in Figure 4.15.

If these properties were not correlated, one would expect a straight line in the contour plots and a plane in the 3D plots if there is no curvature in the single property results. Some curvature is seen in all three 3D plots here and the lines in the contour plots are not completely straight. The individual contribution of heat capacity and thermal conductivity have a slight curvature, while density is linear with no curvature. The best fit line for density is linear, while the best fit line for heat capacity and thermal conductivity individually are third order polynomials. A further way to investigate whether properties are correlated or not is using the expression, $\Sigma \Delta T_i = \Delta T_{total}$, where ΔT_i is the individual contribution to temperature and ΔT_{total} is the combined change in temperature. This expression is true if it is uncorrelated. Since ΔT_{total} using the expression is different than the ΔT_{total} for the simulation for all property combinations, they are all correlated. There are no sudden spikes or anything of the sort, so this is a smooth correlation.

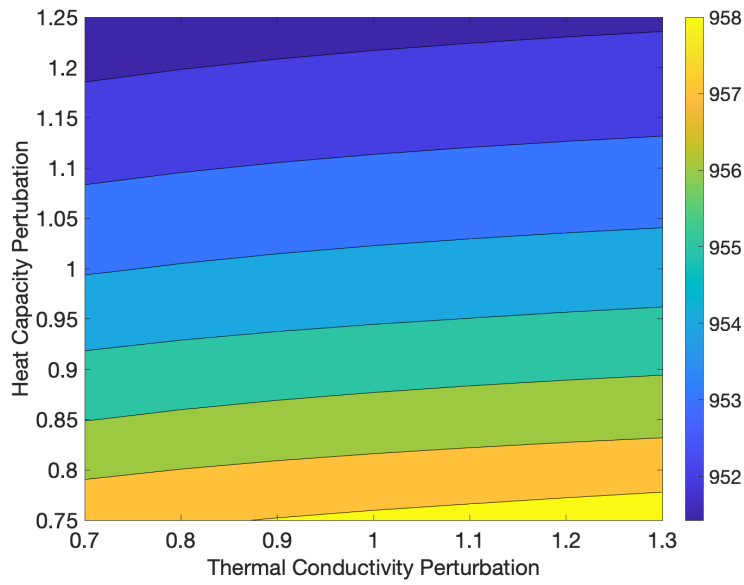


Figure 4.12: Contour plot of the change in temperature in relation to perturbing both heat capacity and thermal conductivity at steady state

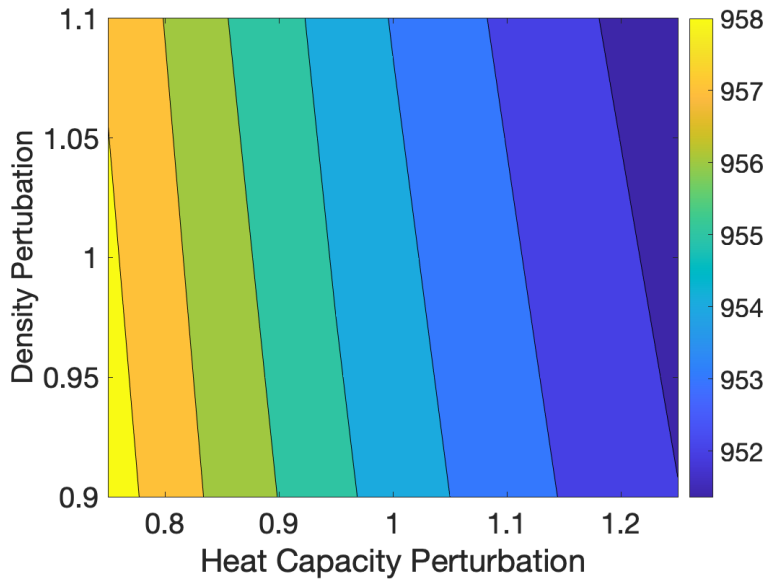


Figure 4.13: Contour plot of the change in temperature in relation to perturbing both heat capacity and density at steady state

Table 4.11: The largest temperature for each property and the varying two at a time runs and the perturbation value where the largest temperature occurs.

Property	Largest Temperature (K)	Perturbation Value
Density	954.6	-10%
Thermal Conductivity	954.5	+30%
Heat Capacity	958.2	-25%
Density and Thermal Conductivity	954.8	-10%/+30%
Density and Heat Capacity	958.5	-10%/-25%
Heat Capacity and Thermal Conductivity	958.5	-25%/+30%

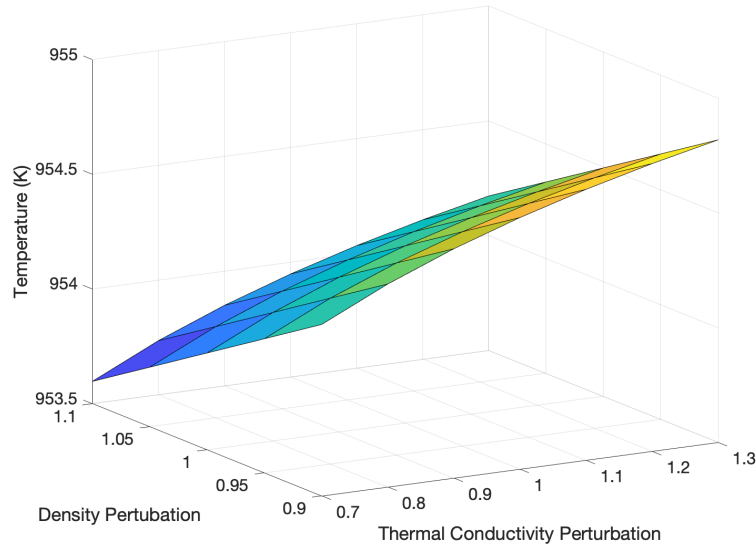


Figure 4.14: 3-D plot of the change in temperature in relation to perturbing both density and thermal conductivity at steady state

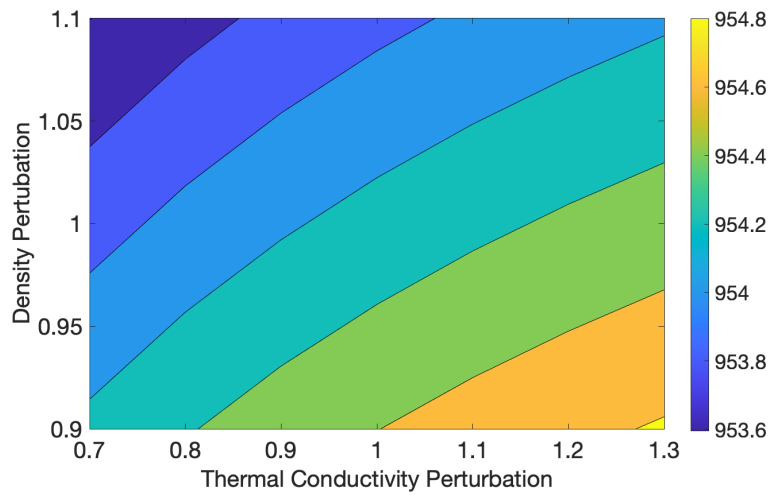


Figure 4.15: Contour plot of the change in temperature in relation to perturbing both thermal conductivity and density at steady state

Chapter 5

Discussion

The central purpose of this study was to use modern simulation tools to investigate the impact of thermophysical property uncertainty under normal and transient scenarios. This study examined perturbations of density, thermal conductivity, viscosity, and heat capacity under steady state conditions as well as during a reactivity insertion and a buildup transient. It also investigated perturbing two thermophysical properties at a time.

5.1 Results

The current study found clear support for the hypothesis that the current uncertainties in the four thermophysical properties examined do not have significant impact on the temperature of the reactor during steady state and transients. A significant impact on temperature would be if the salt freezes or reaches the maximum temperature of the structural material and interacts negatively with the pipes/pumps/other materials. Some variance in temperature was observed, but the variance was within the operating limits of the MSR design.

5.1.1 Steady State

A steady state analysis was performed to investigate the role thermophysical property uncertainty has on changing the reactor temperature at the PHX inlet, PHX outlet, core inlet, and core outlet and whether those changes in temperature are significant. The viscosity and heat capacity had similar trends with the PHX inlet and core outlet temperature decreasing as the property value increases and the core inlet and PHX outlet temperature increasing as the property value increases. The other two properties saw different trends in their temperature results. The density saw all four locations decrease in temperature as the density increases. The thermal conductivity saw the opposite of the heat capacity and viscosity with the PHX inlet and core outlet temperatures increasing as the thermal conductivity increases and the core inlet and PHX outlet temperatures decreasing as the thermal conductivity increases. The density results are consistent with the fact that density and temperature are inversely related since as the temperatures decrease, the density increases. The largest variations in temperature are seen for heat capacity; this makes sense due to the fact that heat capacity is the salt's capacity to hold the heat generated in the core and give it up in the PHX. This is better illustrated by looking at the ΔT between the PHX outlet and inlet and the ΔT between the core outlet and inlet. The lowest heat capacity has the highest ΔT and the largest heat capacity has the lowest ΔT out of all the properties. Heat capacity and ΔT are inversely related according to the equation below.

$$C_p = \frac{Q}{\dot{m}\Delta T} \quad (5.1)$$

where C_p is the heat capacity, Q is the heat, $\dot{m}$ is the mass flow rate, and ΔT is the change in temperature. The specific heat capacity is the quantity of heat absorbed per unit mass of the material when its temperature increases by 1 K. From this, it makes sense that the lowest heat capacity value would need the smallest amount of heat absorbed per unit mass to raise the salt temperature by 1 K.

Overall, the largest to smallest percent difference in ΔT is $C_p \rightarrow \lambda \rightarrow \nu \rightarrow \rho$. The PHX outlet and core inlet percent differences are much higher (at least 1.5x) than those for PHX inlet and core outlet except for density, which is all between 0.244% and 0.344% for all four locations. The properties ordered from largest to smallest ΔT between the PHX outlet and PHX inlet are C_p (111.52 K) $\rightarrow \lambda$ (92.09 K) $\rightarrow \nu$ (92.07 K) $\rightarrow \rho$ (91.02 K). An increase in the thermophysical property results in an increase of ΔT for thermal conductivity and a decrease of ΔT for density, heat capacity, and viscosity. The properties ordered from largest to smallest ΔT between the core outlet and core inlet are C_p (112.09 K) $\rightarrow \lambda$ (92.58 K) $\rightarrow \nu$ (92.55 K) $\rightarrow \rho$ (91.51 K). An increase in the thermophysical property results in an increase of ΔT for thermal conductivity and a decrease of ΔT for density, heat capacity, and viscosity. ΔT across the PHX and the core are approximately equal to each other for each individual property. The temperature values seen here will not cause the salt to freeze or boil, but they could have an effect on the stability of the reactor materials, such as Alloy-N or graphite.

For thermal conductivity, it makes more sense to look at the ΔT values rather than just the temperatures since thermal conductivity is related to heat transfer and thermal conductivity is the measure of a material's ability to conduct heat. Both the ΔT of the PHX and core are directly related to thermal conductivity, seeing an increase when there is an increase in thermal conductivity.

All of these results give a higher core inlet temperature than the PHX outlet temperature. This would typically be the other way around since heat is generated in the core and lost in the PHX and there should not be significant heat loss or gain in the piping, but I believe this is from a small amount of heat generation in the molten salt due to fissions and delayed neutrons happening outside of the core. The opposite happens in the hot leg with the PHX inlet having a lower temperature than the core outlet, which intuitively makes more sense since most of the heat is generated in the core and lost in the PHX.

5.1.2 Reactivity Insertion

During a reactivity insertion event, all the same patterns of temperature and ΔT either increasing or decreasing with an increase in the thermophysical property are seen for the density, thermal conductivity, and heat capacity. Viscosity sees a different result here with temperatures at all locations increasing with increasing viscosity during a reactivity insertion event; this is different than the behavior during steady state conditions. Viscosity behaves differently for reactivity insertion. This is due to the reactivity insertion overriding the difference that would be seen for perturbing viscosity and how that viscosity perturbation would affect temperature. Viscosity on its own affects temperature by decreasing at the PHX inlet and core outlet and increasing at the core inlet and PHX outlet for steady state conditions. The reactivity insertion raises the temperature everywhere in the loop. When the two effects on temperature are combined, an increase in temperature at all four locations is seen for an increase in viscosity values during a reactivity insertion incident. Changing the viscosity for a reactivity insertion follows the same trend for the cold leg as it did for steady state conditions; an increase in viscosity resulted in an increase in temperature. For the hot leg during steady state conditions, the temperature was found to decrease with increasing viscosity, but for a reactivity insertion transient, the opposite happened with a temperature increase for an increase in the viscosity value. This would indicate that something unexpected is happening to the temperature in the core during a reactivity insertion. One speculates that this might be due to changes in the amount of energy lost to conduction, convection, and radiation. At steady state, heat loss effects remove more energy from the molten salt than the core adds as viscosity increases. Alternatively, during a reactivity insertion, the increased viscosity allows for more energy absorption to occur in the molten salt than the energy that is lost due to conduction, convection and radiation; this explains the increase in temperature with increasing viscosity in the hot leg.

All the temperatures of all perturbations of all four properties are between 984.64-1201.38 K. Both of these extremes happen for heat capacity with both happening for a perturbation of -25% and 984.64 K happening at the PHX outlet and 1201.38 K happening at the core outlet. The largest percent difference by far was for heat capacity with a range of -32.373-22.752%. These percentages are rather large at first glance, but the temperatures seen here are still well within those needed for safe operating conditions for an MSR. Overall, the largest to smallest percent difference for the properties is $C_p \rightarrow \lambda \rightarrow \nu \rightarrow \rho$. This is the same order at steady state. Just like in the steady state, the temperature decreased with increasing density at all four locations. For the -10% perturbation of density, the mean temperature after the reactivity insertion was 1105.68 K and for steady state was 909.24 K, which is a difference of 196.44 K. For all the property perturbations, the difference between the mean temperatures was a little less than 200 K.

ΔT for the PHX and the core follow the same pattern for both the reactivity insertion and steady state for the four thermophysical properties with the ΔT decreasing as the viscosity increases. The ΔT s were much larger for reactivity insertion than steady state.

When comparing the maximum percent difference of the percent difference between the perturbation and nominal for the reactivity insertion and the steady state simulations, the reactivity insertion results show a larger percent difference. This can be seen in Table 5.1. Heat capacity sees the largest percent difference for both steady state and reactivity insertion conditions at 1.95% and 32.37%, respectively. This is over a ten fold increase for the heat capacity percent difference between the perturbed property temperature and nominal. Thermal conductivity also saw at least a ten fold increase. The viscosity and density both saw at least a twenty fold increase.

The temperature difference between the reactivity insertion transient without any property perturbations compared to steady state is 195.88 K for the mean

Table 5.1: Comparison of maximum percent differences for the steady state and reactivity insertion conditions

Property	Steady State (%)	Reactivity Insertion (%)
Density	0.034	1.01
Thermal Conductivity	0.176	2.14
Heat Capacity	1.95	32.37
Viscosity	0.085	2.00

temperature. This temperature change is much larger than those seen for any of the property perturbations dwarfing the changes that are seen for the property perturbations. The changes in properties will have an impact on how the event is handled in terms of material performance.

The heat capacity sees the highest change for temperatures in both steady state and reactivity insertion scenarios. The temperatures never reach an unsafe temperature. If any thermophysical properties should be investigated further, it should be heat capacity since it sees the highest percent difference and change in temperature with the perturbations. But even this is not of concern since the reactor does not reach unsafe conditions.

5.1.3 Buildup Transient

The buildup transient was modeled to look at how fission product, corrosion product, and other product buildup on the piping effects the reactor behavior and temperature. This was initially planned for four diameters being explored, 12 inch, 9 inch, 6 inch, and 3 inch.

The 3 inch gave interesting results though, which will be discussed here. The 3 inch results are not valid in this case due to the use of a simple mass flow pump, which simply forces the same mass flow through the pump no matter other conditions. This results in the same mass flow rate through the 12 inch pipe and the much smaller 3 inch pipe. This causes a huge pressure drop, which can be seen in Table 5.2. A more sophisticated pump should be used that implements pump curves to account for this much smaller diameter. Further, the piping diameter would never be reduced by this much since all the material that might plate out would result in a much smaller impact.

It was decided that the 3 inch investigation would be dropped from the rest of the analysis and only the results from the 6 inch, 9 inch, and 12 inch would be explored.

Table 5.2: Pressure drop

Diameter (in)	Δp Cold Leg (bar)	Δp Hot Leg (bar)
12	0.50	0.17
9	2.10	0.72
6	16.19	5.6422
5	40.94	14.35
4.5	70.12	24.64
4	128.15	45.12
3.5	254.06	89.51
3	777.96	196.43

In this case, the highest temperature is seen for a diameter of six inches, which is 50% less than the starting diameter of 12 inches. This means that as fission products, corrosion products, and other products build up on the piping and reduce the effective pipe diameter, the temperature will get higher and higher. The difference between the 9 inch temperature and the 12 inch temperature was in the range of 4.56-4.71 K. The difference between the 6 inch temperature and the 12 inch temperature was 8.25-8.39 K. These, of course, happened for heat capacity, but viscosity was not far behind.

This is an extreme example since there is no reason to expect the pipe diameter to drop from 12 inches to 6 inches. Even if there was enough buildup to reduce the pipe diameter by 50%, it would not happen quickly and thus operators would quickly see this happening, especially from the change in flow rates for the system. The amount of heat that is exchanged between the salt and the pipes will change with buildup since it will be exchanging with the deposits as well. This model is not exactly mimicking what would happen with heat transfer from the wall versus heat transfer from the build up deposits.

5.1.4 Two Parameters

The investigation for varying two parameters at the same time was performed to look for adverse effects to temperature that were not seen for the one parameter at a time analysis. The deviations were chosen in Chapter 2 and all the simulations of two parameters at a time are a combination of the maximum deviations considered for each individual parameter. It was found that heat capacity dominated the effect on the temperature when compared to density and thermal conductivity. It was found that thermal conductivity is inversely related to both density and heat capacity with the maximum temperature occurring for the largest thermal conductivity value and the smallest heat capacity and density value. It was also found that density and heat capacity are directly related with the maximum temperature happening

for a combination of the smallest density and the smallest heat capacity. Some of the curvature of the plots depends on how each property behaves independently. Correlation between the thermophysical properties was found, but the effects from this were not adverse. This is another promising finding pointing to the fact that heat capacity is the most important thermophysical property in terms of temperature change. Further, it is promising that there is not much temperature change observed.

5.2 Limitations

This study is limited in its scope due to the lack of experimental data on the MS DR design and the fact it was never built and operated, but is rather a paper design. The main limitation other than lack of experimental data for MS DR is the lack of adequate documentation for TRANSFORM. This lack of documentation made it difficult to parse what equations and assumptions were being used. Further, due to lack of data on the MS DR, neutronics for MS RE were used here. This assumption should not have much bearing on the results, but they do use two different fuel salt combinations, LiF-BeF₂-ZrF₄-UF₄ (65-29.1-5-0.9 mole %) for MS RE and LiF-BeF₂-ThF₄-UF₄ (71.5-16.0-12.0-0.5 mole %) for MS DR. The neutronics should be similar enough, but are not exact. There were also simplifying assumptions made, such as one phase flow, no voids, homogeneous, Newtonian fluid, and the heat transfer correlation. With these assumptions, changes were small, so even a change in assumptions would not affect much.

A heat transfer correlation was chosen, but there could be a better correlation out there. There are limitations on some initial conditions and values and reactivity that were obtained from the MS RE documentation. Although that documentation is extensive, not everything is adequately detailed. These limitations are not great enough to invalidate these results.

Uncertainty is added from these limitations, but I do not believe it is a significant amount and the results here show a small enough change that it does not matter one bit. These results matter since they further the R&D and show a smaller experimental envelop needed for MSRs to be built and eventually commercialized.

5.3 Implications for Future Research

I am reassured by the changes in temperature between the property perturbations being relatively low. From this result, it seems to me that these four thermophysical properties should not be of much concern and experimental efforts should be placed elsewhere. Even though this analysis was focused on the MSDR design, this framework could easily be extended to the MSRE as well as other MSR designs of interest. This type of analysis, especially the basic parts of it, could be easily modified to look at the effect from other phenomena.

The current tools could definitely be improved by having adequate documentation for TRANSFORM and possibly moving TRANSFORM over to the free software OpenModelica instead of the current proprietary software Dymola.

The pressure loss and heat transfer correlations could be better explored and possibly updated and/or made better in the code. Also, investigation on how using other heat transfer models for the same reactor design could be useful to understand how much difference it actually makes and if the difference matters and if it is important.

Using Risk Analysis and Virtual Control Environment (RAVEN) to aid in the sensitivity analysis would definitely be beneficial, but as it currently stands, coupling RAVEN and Dymola is relatively difficult, so it is not very useful at this current moment in time. Using a higher fidelity model could also provide more in-depth insight. I think Object Oriented Modeling is definitely the path forward with MSR investigations of basically any sort.

5.4 Implications for Researchers & Developers

The results of this study can inform people performing thermophysical property measurements and experiments and potentially reduce the scope of their experimental envelope. This study also helps inform people concerned with uncertainty, safety, and licensing. Some aspects that need further investigation and should be looked at include how the composition changing during burnup affects these results and conclusions.

Chapter 6

Conclusion

The aims of this study were to develop an MSDR model that allows for changing thermophysical property values and to use this model to explore reactor behavior, such as temperature, during steady state and transient scenarios. This was done to explore whether thermophysical property uncertainty has a significant effect. The implications of these properties on licensing and regulation is a very important question since we have pure salt measurements for most candidate mixtures, but the moment the reactor starts up they will evolve and not be pure salts anymore. This needed to be done because we cannot measure the thermophysical properties of all the salt compositions that will be seen over the life of the reactor. As a result of this study, changes in temperature were seen for the property perturbations, but they will not affect the safe operation of the reactor. Based on these conclusions, molten salt developers and researchers should not need to worry about the four thermophysical properties investigated here: density, thermal conductivity, heat capacity, and viscosity. It is also concluded based on this study and previous thermophysical property measurements, the measurement techniques used to measure density, thermal conductivity, heat capacity, and viscosity are adequate to measure a new salt composition.

This was one of the first in depth attempts at safety analysis for MSR, in terms of thermophysical properties. This analysis demonstrated that uncertainties in thermophysical properties will not affect the safe operating envelope of the reactor.

6.1 Future Work

I think the most important future work is adequately documenting TRANSFORM. Building a molten salt research reactor and sharing the findings with developers for V&V efforts would be an ideal next step. Also, coupling with a thermochemical analysis tool such as Thermochemica could be of great use. Repeating this analysis for other state variables could also be of great interest to further MSR development.

Nuclear Energy University Program (NEUP) work scopes are interested in several MSR topics for research. These include reducing technical risks for MSRs, transient and safety analysis, thermophysical and thermochemical property determinations, and modeling transport phenomena, materials, fuels, and fluid behavior [72].

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Vita

Sarah Elizabeth Creasman was born to Scotty and Cindy Creasman and raised in East Tennessee. She graduated as salutatorian from Meigs County High School in 2012. Upon graduation, she first attended Middle Tennessee State University until she settled on being a nuclear engineering major provoking a change of college to the University of Tennessee where she graduated with a Bachelor's of Science in 2017. In 2020, Sarah received her Master of Science degree from the University of Tennessee. Ever since, she has continued her collaboration between the University of Tennessee and Oak Ridge National Laboratory for her PhD research. Upon completion of her doctorate, she will join Idaho National Laboratory to continue her work with Modelica and Integrated Energy Systems.