ABSTRACT

BRADY, CHRISTOPHER LEE. Criticality Safety Analysis of a Spiral Plate Heat Exchanger for Molten Salt Reactors. (Under the direction of Xu Wu).

Spiral plate heat exchangers (SHE) have been proven in industrial applications involving viscous and fouling fluids, possess reduced maintenance requirements, and feature high heat transfer capacity making them a great candidate for Molten Salt Reactor (MSR) applications. While traditional tube-and-shell heat exchangers also have proven industrial success, their complexity and significant maintenance requirements are disadvantageous. Because the combined fuel and coolant of liquid fueled MSRs often passes through an external heat exchanger in a compact geometry with a potentially moderating secondary fluid, criticality safety analysis is necessary. The Monte Carlo N-Particle® (MCNP) Transport Code System allows simulation of the criticality of the system and the neutron flux across the system. We evaluate the system multiplication factor for several geometries and materials through parametric studies varying SHE size, hot/cold channel gaps, and plate thickness for selected structural materials, fuel salts, and secondary loop heat transfer fluids. We determine that multiple SHE configurations exist that ensure the system remains deeply sub-critical and identify some of the important SHE design considerations from a criticality perspective.
BIOGRAPHY

Christopher Brady was born in Evanston, WY and raised across multiple states in the US. He graduated from the United States Military Academy in 2007 with a Bachelor's of Science in Nuclear Engineering. After ten years of military service, he returned to North Carolina for continued education and pursuit of a career in the nuclear industry. Following completion of his Master of Science degree, Chris will continue his education at North Carolina State University in pursuit of a PhD.
ACKNOWLEDGEMENTS

Special thanks to Dr. Xu Wu and Dr. John Zino for their advice and mentorship as well as the team from GE for their collaboration on this project.
# TABLE OF CONTENTS

List of Tables ................................................................................. v

List of Figures ................................................................................ vi

Chapter 1 INTRODUCTION ................................................................. 1
  1.1 Motivation .............................................................................. 1
  1.2 Industrial Heat Exchangers ..................................................... 4
  1.3 Molten Salt Reactor Designs of Interest ................................. 6
  1.4 Problem Statement and Organization .................................... 8

Chapter 2 METHODS ......................................................................... 9
  2.1 SHE Materials Selection .......................................................... 9
     2.1.1 Structural materials ....................................................... 9
     2.1.2 Fuel salts ........................................................................ 11
     2.1.3 Secondary fluids ............................................................ 14
  2.2 Monte Carlo N-Particle Simulation .......................................... 15
     2.2.1 Simulation process ......................................................... 15
     2.2.2 Model geometry ............................................................ 19
     2.2.3 Simulation parameters .................................................. 21

Chapter 3 RESULTS ......................................................................... 23
  3.1 System Characterization .......................................................... 23
     3.1.1 Material cross sections .................................................. 23
     3.1.2 Neutron flux .................................................................... 26
  3.2 Parametric Studies ................................................................. 29
     3.2.1 Density studies ............................................................... 29
     3.2.2 Geometry studies ............................................................ 31
     3.2.3 Material comparisons ..................................................... 33
  3.3 Simulation Evaluation ............................................................. 37

Chapter 4 CONCLUSIONS ................................................................. 41
  4.1 Summary of Results ............................................................... 41
  4.2 Overarching Conclusions ....................................................... 42
  4.3 Future Work ............................................................................. 43

References ..................................................................................... 45

Appendices ...................................................................................... 47
  Appendix A Acronyms ................................................................. 48
  Appendix B Variables ................................................................. 50
  Appendix C Material Cross Sections ........................................... 52
  Appendix D Flux Plots ................................................................. 58
LIST OF TABLES

Table 2.1 SHE structural material composition. ........................................ 11
Table 2.2 Fuel salt compositions. .............................................................. 14
Table 2.3 Secondary loop heat transfer fluid operating conditions. .......... 15
Table 2.4 SHE nominal and parametric study dimensions. .................... 21
Table A.1 A summary of acronyms used in alphabetical order. .............. 48
Table B.1 A summary of variables and their abbreviations in alphabetical order. . . 50
Table C.1 Material Cross Section Legend Key. ....................................... 52
## LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>Tube-and-shell heat exchanger (Enerfab 2023)</td>
<td>4</td>
</tr>
<tr>
<td>1.2</td>
<td>Industrial Spiral Plate Heat Exchanger (Elanco 2022)</td>
<td>5</td>
</tr>
<tr>
<td>2.1</td>
<td>Radial and axial cross-sectional views of the SHE MCNP model</td>
<td>20</td>
</tr>
<tr>
<td>2.2</td>
<td>Geometry confirmation and cell configuration plots</td>
<td>21</td>
</tr>
<tr>
<td>3.1</td>
<td>Material Cross Sectional Data</td>
<td>25</td>
</tr>
<tr>
<td>3.2</td>
<td>Radial neutron flux for secondary fluids at nominal parameters. From left to right: thermal (&lt; 0.625 eV), intermediate (0.625 eV - 100 keV), fast (&gt; 100 keV)</td>
<td>27</td>
</tr>
<tr>
<td>3.3</td>
<td>Axial neutron flux for secondary fluids at nominal parameters. From left to right: thermal (&lt; 0.625 eV), intermediate (0.625 eV - 100 keV), fast (&gt; 100 keV)</td>
<td>28</td>
</tr>
<tr>
<td>3.4</td>
<td>Heat transfer fluid density influence on multiplication factor</td>
<td>30</td>
</tr>
<tr>
<td>3.5</td>
<td>SHE size influence on multiplication factor</td>
<td>31</td>
</tr>
<tr>
<td>3.6</td>
<td>Channel gap influence on multiplication factor</td>
<td>32</td>
</tr>
<tr>
<td>3.7</td>
<td>SS316 hot channel gap parametric studies</td>
<td>34</td>
</tr>
<tr>
<td>3.8</td>
<td>Hastelloy-N hot channel gap parametric studies</td>
<td>34</td>
</tr>
<tr>
<td>3.9</td>
<td>SS316 cold channel gap parametric studies</td>
<td>35</td>
</tr>
<tr>
<td>3.10</td>
<td>Hastelloy-N cold channel gap parametric studies</td>
<td>35</td>
</tr>
<tr>
<td>3.11</td>
<td>SS316 plate thickness parametric studies</td>
<td>36</td>
</tr>
<tr>
<td>3.12</td>
<td>Hastelloy-N plate thickness parametric studies</td>
<td>36</td>
</tr>
<tr>
<td>3.13</td>
<td>$k_{eff}$ plus one standard deviation for secondary fluids at nominal parameters</td>
<td>38</td>
</tr>
<tr>
<td>3.14</td>
<td>Source entropy for secondary fluids at nominal parameters</td>
<td>38</td>
</tr>
<tr>
<td>3.15</td>
<td>Relative error for secondary fluids at nominal parameters</td>
<td>39</td>
</tr>
<tr>
<td>3.16</td>
<td>Figure of merit for secondary fluids at nominal parameters</td>
<td>40</td>
</tr>
</tbody>
</table>
CHAPTER

1

INTRODUCTION

1.1 Motivation

The Generation IV International Forum (GIF) has selected Molten Salt Reactors (MSR) as one of six reactor systems on which to focus international research and development collaboration. Although there are currently some technological challenges that need to be addressed, MSRs have several promising features. They have a diverse array of configurations that boast inherent safety, high operating temperatures, and fuel cycle flexibility. The MSR name is derived from its use of liquid molten salts circulated through the reactor core as a combined reactor fuel carrier and coolant. In a liquid fuel MSR, the fuel is dissolved directly into the molten salt, which we will refer to as a fuel salt; however, in a solid fuel MSR the fuel is either in a static array or circulated through the core in a solid form, such as Tri-structural Isotropic (TRISO) particles
suspended in graphite pebbles. In this paper, we focus on liquid fuel MSRs because solid fuel MSRs generally prevent fuel or fission products from leaving the reactor vessel to minimize radiation exposure beyond the reactor core, which eliminates the need to perform criticality safety analysis of the heat exchanger. MSRs can operate in a thermal or fast neutron spectrum using a variety of fissile/fissionable isotopes as fuel, or even include transuranic elements to breed additional fuel material. A variety of fuel salts have been explored to carry fuel through reactor core but are typically a Fluoride or Chloride based salt.

The physical properties of the MSR create a system that has several inherent safety features. The first is a large negative temperature and void coefficient that results from a decrease in the density of the fuel salt as temperature increases. If the reactor begins to overheat the fuel salt expands and the amount of fuel in the core decreases, introducing negative reactivity and reducing the power of the core back to safe levels. Additionally, a freeze plug is typically employed that will melt before any damage is done to reactor component structural materials, allowing the fuel salt to be gravity fed into separate subcritical holding vessels capable of managing decay heat. The thermophysical properties of molten salts make them very efficient heat transfer fluids and contribute to effective decay heat rejection. The low vapor pressure of typical fuel salts does not require a significantly pressurized reactor vessel to prevent phase change. This not only reduces the dispersion of radionuclides in the event of an accident, but also reduces the cost of the reactor vessel and increases its operational lifetime because it is not under constant heavy stress loads.

In addition to safety features, MSRs have multiple operational advantages. High vaporization temperatures allow MSRs to operate at higher temperatures than light water reactors (LWR) which enables increased efficiency in electricity generation or application to other industrial processes such as cogeneration of hydrogen. Additionally, because MSRs typically have online refueling capability, there is a reduced need to manage excess reactivity in order to extend time between refueling as LWRs require. Online refueling also means reactor outages are limited to those required for maintenance. Some configurations can take advantage of higher fuel
utilization or fuel breeding to reduce fuel cycle costs.

Several challenges exist that MSRs must overcome before wide implementation. MSRs differ significantly from the current fleet of LWRs and will need to meet different safety and regulatory requirements that are not fully established. The thermophysical properties of molten salts still need to be established and appropriate tools developed to model their thermo-hydraulic behavior. In liquid fuel MSRs, the already corrosive molten salts are made more corrosive as fission products are produced and dissolved into the molten salt. As a result, specialized materials must be developed, evaluated, and codified for use in reactor components. Fission product production also creates the need for online fuel salt chemical processing to maintain the desired salt composition to allow predictable neutron behavior in the reactor core (Caponiti et al. 2022).

The heat generated in the reactor core must be transferred to a secondary fluid before it can be used for an industrial process or electricity generation because the dissolved fission products make the fuel salt highly radioactive. This is traditionally accomplished with a tube-and-shell heat exchanger. However, the highly corrosive nature of the fuel salt and its high viscosity can block or damage the tubes requiring maintenance and causing operational down time. Furthermore, this maintenance must be performed remotely because the heat exchanger is irradiated as the liquid fuel salt and fission products pass through it, adding additional cost and complexity.

Liquid fuel MSRs have the unique characteristic that the reactor fuel, combined with the reactor coolant, passes through the heat exchanger. This characteristic requires a criticality safety analysis because the fuel salt will collect in a compact geometry with a potentially moderating secondary fluid which might result in an critical excursion. Some MSRs, such as the integral molten salt reactor, (IMSR) integrate the heat exchanger into the reactor vessel in order to reduce the footprint of components containing radioactive material. While SHEs might also be applicable in these scenarios, this study will only consider a heat exchanger that is decoupled from the reactor vessel.
1.2 Industrial Heat Exchangers

One of the most common heat exchangers seen in the nuclear industry is the tube-and-shell heat exchanger, shown in Fig. 1.1. These heat exchangers are capable of operating at high temperatures and pressures and come in many configurations. The tubes can pass once through the shell, be bent in a u-turn within the shell, or create a helical coil within the shell. The flow can be characterized as parallel, cross, or counter flow depending on the configuration. The nature of the small tubes enables them to contain high pressure fluids during the heat transfer process. These heat exchangers have a long proven history in the many industries, including nuclear, and their performance is well understood.

![Figure 1.1: Tube-and-shell heat exchanger (Enerfab 2023).](image)

However, the large array of often hundreds of small tubes has several operational and maintenance drawbacks. Over time, the tubes may become fouled from precipitate deposits or corrosion reducing the heat transfer capacity. Some tubes may even become completely blocked by impurities or debris in the fluid causing reduced heat transfer capacity and unwanted pressure drop across the heat exchanger. Furthermore, ruptures in the tubes can be caused over time from stress-corrosion cracking and fatigue resulting in unwanted fluid transfer between loops. These factors require regular maintenance to ensure the heat exchanger is
functioning as designed. The extensive network of very small tubes in a compact array makes cleaning, diagnosing problems, and repair a complex and laborious task adding to the regularity and extent of maintenance downtime. When used with liquid fuel MSRs, fouling and blockages are a greater concern and the task of maintenance is further complicated by the requirement for remote maintenance because the heat exchanger structure is irradiated (Trafczynski et al. 2021).

Figure 1.2: Industrial Spiral Plate Heat Exchanger (Elanco 2022).

Spiral Plate Heat Exchangers (SHE) have proven performance in the petrochemical and other industrial processes involving highly viscous and fouling fluids. They offer a true counter-flow configuration that typically exceeds the heat transfer capacity of similarly sized heat exchangers. The nature of the continually changing flow direction creates a self cleaning characteristic that can substantially reduce required maintenance intervals. Furthermore, easy access to the flow channels allows for significantly simplified maintenance and cleaning (Memon et al. 2019). However, one drawback of the SHE is that it cannot sustain large pressure differentials between the operating fluids. The diagram of the flow in a typical SHE alongside an actual SHE with the flow channels exposed as it would be for maintenance is depicted in Fig. 1.2.
1.3 Molten Salt Reactor Designs of Interest

There is a diverse assortment of MSR designs resulting from the flexibility of their operation. MSRs can operate in fast or thermal neutron spectrum either burning or breeding fuel from a variety of fuel types. This operational flexibility gives rise to numerous distinct MSR designs intended to take advantage of specific characteristics in light of the energy demand, fuel cycle costs, safety considerations, regulatory constraints, and counterproliferation concerns. Because of the diversity of MSR designs, we make some distinctions between designs and terminology, then examine several specific MSR designs to understand the materials and operating conditions for which a MSR heat exchanger might need to be designed.

We have already distinguished between liquid and solid fueled MSRs, but will briefly discuss their merits here before making further delineations. Liquid fuel designs allow significant flexibility and control of fuel concentration in the fuel salt and simplifies high fuel utilization, fuel recycling, or fuel breeding. Liquid fuel designs have the added benefit that noble gas fission products, such as the neutron absorber Xenon, are easily out-gassed and separated from the fuel salt. This comes at the cost of other fission products being dissolved directly into the fuel salt making it radioactive and more corrosive. Solid fuel designs seek to reduce the need for online fuel salt chemical processing by containing the fission products to prevent mixing with the fuel salt. Some MSR designs incorporate two fuel loops in the reactor core, one with a fissile fuel salt and an adjacent loop with fertile fuel salts meant to breed fuel. Other MSR designs operate in the fast neutron spectrum which eliminates the need for a neutron moderator in the core which can be inconvenient to maintain and costly to replace. Fast spectrum MSRs also frequently seek to take advantage of neutron absorption in fertile materials to recycle or breed fuel. It is important to note that fuel breeding and recycling are potentially possible with MSRs, but these capabilities face significant challenges primarily due to proliferation concerns.

No study involving MSRs would be complete without mentioning the Molten Salt Reactor Program (MSRP) at Oak Ridge National Labs (ORNL) which consisted of the operation of the Aircraft Reactor Experiment (ARE) and the Molten Salt Reactor Experiment (MSRE) as well
as the conceptual design of the Molten Salt Breeder Reactor (MSRB). The ARE was part of an effort to design a nuclear propelled aircraft. It used NaF-ZrF$_4$-UF$_4$ fuel salt with 93.4% enriched $^{235}$U at 34.47 kPa and 860 °C outlet temperature with a 180 °C drop across the reactor core. The fuel salt was pumped through Inconel tubes in a beryllium oxide moderator contained in an Inconel reactor vessel. It achieved a maximum sustained power output of 2.5 MW$_{th}$ operating for a total of 221 hours at various power levels in 1954 (Bettis et al. 1957). The MSRE used LiF-BeF$_2$-ZrF$_4$-UF$_4$ fuel salt with 33% enriched $^{235}$U (and later $^{233}$U) at 34.47 kPa and 650 degree C. The fuel salt passed directly through graphite blocks contained by a Hastelloy-N container within the reactor vessel. The MSRE was 8 MW$_{th}$ and operated for 11,555 equivalent full power hours between 1965-1968. (Haubenreich and Engel 1970). These experiments very successfully demonstrated the feasibility of MSRs, and provided data on fuel salt behavior and structural material performance that is frequently cited.

The Chinese Academy of Sciences (CAS), in coordination with the Shanghai Institute of Applied Physics (SINAP), is undertaking the Thorium-based Molten Salt Reactor-Liquid Fuel (TMSR-LF1) experiment which has operating parameters remarkably similar to the MSRP and plans to incorporate Thorium into the fuel salt. The TMSR-LF1 will use LiF-BeF$_2$-ZrF$_4$-UF$_4$-ThF$_4$ fuel salt with 19.75% enriched $^{235}$U at low pressure and 650 °C outlet temperature and a 20 °C drop across the reactor core. The fuel salt will pass directly through tubes in a graphite core contained in a Hastelloy-N sleeve to channel the fuel salt. The TMSR-LF1 is designed to produce 2 MW$_{th}$. (Liu et al. 2020).

There has been recent discussion of Molten Chloride Fast Reactors (MCFR) with the US Department of Energy funding the Molten Chloride Reactor Experiment (MCRE) to be operated by Southern Company in partnership with TerraPower. Additionally, TerraPower currently has pre-application actions with the US Nuclear Regulatory Commission for a MCFR using a NaCL-UCl$_3$ fuel salt. One proposed design for a MCFR uses NaCL-UCl$_3$ fuel salt with 15.5% enriched $^{235}$U at low pressure and 677 °C outlet temperature with a 100 °C drop across the reactor core. The fuel salt in the core is contained in a type-316 stainless steel (SS316) reflector and shield.
This reactor design is intended to produce $3,000\text{ MW}_{\text{th}}$ (Mausolff et al. 2021).

This collection of MSR designs is far from exhaustive but was selected to demonstrate some of the common operating parameters and materials that should be considered in analyzing the aspects of the heat exchanger. Because we are only analyzing the criticality of the heat exchanger and do not analyze its heat transfer capacity we do not specifically discuss the fuel salt flow rates or viscosity, but some thermophysical properties are briefly discussed when we consider the composition of the fuel salts.

### 1.4 Problem Statement and Organization

In this study, we seek to analyze a horizontal spiral plate heat exchanger for a liquid fuel molten salt reactor to determine the effects of geometry, structural material, fuel salt, and secondary fluid composition on the system beginning of cycle (BOC) criticality. In this process we identify materials and operating conditions commonly used in molten salt reactors. Then apply this information to build a model in Monte Carlo N-Particle® Transport Code System (MCNP) and conduct parametric studies to determine the multiplication factor of a SHE in various design configurations.

The rest of this paper is organized as follows: Chapter 2 presents details of the SHE design and the MCNP modeling process. Chapter 3 presents the neutronics analysis results and simulation evaluation. Finally, Chapter 4 summarizes the findings and concludes this paper.
2.1 SHE Materials Selection

2.1.1 Structural materials

While evaluating viable structural materials for MSR applications is beyond the scope of this study, it is important to use materials that are currently being considered for this purpose in order to understand their influence on the system. We will briefly discuss the characteristics important in selecting structural materials for MSR applications then present the materials selected for this study. Structural materials used in MSR heat exchangers must endure very high temperatures, corrosive environments, and radiation damage while maintaining their mechanical integrity. These conditions make it difficult to design materials with long opera-
tional lifetimes. Several structural materials capable of withstanding the corrosive nature of MSR liquid fuel salts have been considered in practice (Bettis et al. 1957; Haubenreich and Engel 1970) as well as in the literature (Busby et al. 2019; Wright and Sham 2018).

The high temperatures generally increase the creep rate and reduces the yield stress of potential structural materials. As a result high pressure systems will have reduced operational lifetimes and require increased material to withstand the higher stresses, making them more costly to produce and maintain. Nickle based alloys consistently outperform iron based alloys in both creep rate and maximum yield stress at high temperatures.

In general, the corrosive nature of the fuel salt will preferentially dissolve the least noble elements of the alloy where the fuel salt contacts the surface. Since Ni is more noble than Fe, Ni based alloys are commonly used in corrosive environments. The least noble component in common structural materials is often Chromium which is added to reduce oxidation, thus low chromium alloys are routinely selected for use with molten salts (Busby et al. 2019).

When considering the effects of irradiation on structural materials it is important to understand the the neutron spectrum and the temperature of the structural material. Neutrons are primarily responsible for radiation damage in structural materials and their energy heavily influences their interaction types. High energy neutrons are responsible for creating point defects in the material when they collide with an atom with sufficient energy to knock it out of the crystalline lattice. While this can cause hardening and embrittlement, these effects are minimized at high temperatures due to the heightened diffusion kinetics enabling the material to return to the original lattice structure for most defects. However, lower energy neutron absorption can cause transmutation and He production in the structural material. Transmutation to undesirable elements can have adverse effects on the mechanical properties as well as corrosivity resistance. Perhaps the most damaging interaction is He production through \((n,\alpha)\) reactions. In this case, the heightened diffusion kinetics at high temperatures allows He to collect into bubbles at grain boundaries causing embrittlement and swelling. This is particularly problematic in Ni based alloys because Ni is prone to \((n,\alpha)\) reactions (Wright...
One must also consider availability and code qualification when selecting industrial structural materials. Many materials discussed in literature are not fully code qualified across the desired operating temperatures or for slight alloy composition variations. This study examines type 316 stainless steel (SS316) as an iron-based alloy and Hastelloy-N as a nickel-based alloy due to their extensive operating experience, established standards, and commercial availability. The exact composition of these alloys varies depending on purpose, grade, and manufacturer but generally aligns with those selected. The specific elemental composition of the selected structural materials is outlined in Table 2.1 assuming natural isotopic abundances for each element.

Table 2.1: SHE structural material composition.

<table>
<thead>
<tr>
<th>Elements</th>
<th>Weight fractions</th>
<th>Elements</th>
<th>Weight fractions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ni</td>
<td>12.00%</td>
<td>Ni</td>
<td>70.65%</td>
</tr>
<tr>
<td>Fe</td>
<td>65.35%</td>
<td>Fe</td>
<td>3.97%</td>
</tr>
<tr>
<td>Mn</td>
<td>2.00%</td>
<td>Mn</td>
<td>0.52%</td>
</tr>
<tr>
<td>Mo</td>
<td>2.50%</td>
<td>Mo</td>
<td>16.28%</td>
</tr>
<tr>
<td>Si</td>
<td>1.00%</td>
<td>Si</td>
<td>0.50%</td>
</tr>
<tr>
<td>Cr</td>
<td>17.00%</td>
<td>Cr</td>
<td>7.50%</td>
</tr>
<tr>
<td>C</td>
<td>0.08%</td>
<td>Ti</td>
<td>0.26%</td>
</tr>
<tr>
<td>P</td>
<td>0.05%</td>
<td>Al</td>
<td>0.26%</td>
</tr>
<tr>
<td>S</td>
<td>0.03%</td>
<td>W</td>
<td>0.06%</td>
</tr>
</tbody>
</table>

### 2.1.2 Fuel salts

The ability to dissolve actinides into the fuel salt is the essential characteristic that makes liquid fueled MSRs possible, though this same property is what makes them corrosive. However, molten salts also have many other desirable thermophysical properties. Favorable characteristics of a fuel salt include low melting temperature, high evaporation temperature, low
vapor pressure, high thermal conductivity, high heat capacity, favorable neutronics, limited corrosivity, and low toxicity. We will briefly discuss these properties and common fuel salts used in MSRs to inform our fuel salt selections for this study. The viscosity of the fuel salt is also an important parameter in determining the heat transfer capacity of the heat exchanger but is not discussed in detail here.

Solution of fuel into the molten salt raises the issue of fuel precipitating out of the fuel salt solution and creating hot spots in the reactor or even localized criticality excursions outside the reactor. This can be caused by moisture or oxygen impurities in the fuel salt leading to UO$_2$ formation and precipitation. During the MSRE, ZrF$_4$ was added to the fuel salt mixture to preferentially form ZrO$_2$ as a buffer before formation of UO$_2$. However, it is claimed that proper precautions to preserve fuel salt purity makes this addition unnecessary (Haubenreich and Engel 1970).

Low melting temperature and high evaporation temperature increase the operational range of the fuel salt. Low melting temperatures reduce the energy required to maintain the salt in a liquid form throughout all components when the reactor is shut down or in low power. Many MSR designs employ a eutectic salt mixture to reduce the melting temperature of the fuel salt. Common eutectic mixtures include LiF-BeF$_2$ (FLiBe) and LiF-NaF-KF (FLiNaK). High operating temperatures contribute to more efficient electricity generation or application to high temperature industrial processes. As previously discussed, low vapor pressure contributes to safety and reduced stress on structural components. High thermal conductivity and heat capacity contribute to safety with passive decay heat removal as well as increased power density. In fact, the idea to use molten salts with a nuclear reactor can be linked to the ARE which required an extremely high power density to sufficiently power an aircraft (Bettis et al. 1957).

The desired neutronics is dependent on the fuel cycle and neutron spectrum of the MSR, though neutron capture is generally undesirable in the fuel salt in both fast and thermal reactors. Thermal reactor designs prefer fuel salts composed of elements with small atomic masses due
to their ability to moderate neutrons. FLiBe and FLiNaK are often selected for these purposes. However, natural Li is generally enriched above 99.95% $^7\text{Li}$ to reduce neutron absorption and prevent the tritium formation from $(n,\alpha)$ reactions with $^6\text{Li}$ (Liu et al. 2020). Tritium formation is prevented because it is a radioactive element that is difficult to contain. In contrast, fast reactor designs seek fuel salts composed of elements with larger atomic masses as they are less effective neutron moderators. A typical fuel salt in a fast reactor is composed of NaCl. In this case, natural Cl is often enriched to various amounts of $^{37}\text{Cl}$ to avoid the large fast neutron absorption cross section of $^{35}\text{Cl}$ (Mausolff et al. 2021).

Limited corrosivity and toxicity reduce the special materials and procedures required to control the fuel salt. The toxicity and special handling requirement of Be have motivated some MSR designs to avoid FLiBe based fuel salts usually in favor or FLiNaK (Serrano-López et al. 2013). Corrosivity of the salt is often managed through online chemical processing of the fuel salt to reduce the amount of free anions resulting from the fission of fuel atoms. As the amount of anions freed from fissioned atoms increases a free cation can be added to limit corrosivity (Haubenreich and Engel 1970).

This study examines the 5 fuel salts outlined in Table 2.2 with the $^{235}\text{U}$ column indicating isotopic enrichment. The fuel salts are considered to have an average temperature of 650 °C and 34.47 kPa. The isotopic composition of FLiBe-based fuel salts is enriched to 99.95% $^7\text{Li}$ to avoid tritium production and the isotopic composition of NaCl-based fuel salt is enriched to 90% $^{37}\text{Cl}$ to avoid the large neutron absorption cross section of $^{35}\text{Cl}$. This study only examines the SHE criticality at BOC and does not examine the effects of fission product accumulation over the course of the cycle. This assumption will likely yield a conservative estimate of the multiplication factor due to larger neutron absorption cross section in several fission products that are capable of remaining in the fuel salt such as $^{149}\text{Sm}$, but this is heavily dependent on the fuel composition maintained by the online chemical processing.
Table 2.2: Fuel salt compositions.

<table>
<thead>
<tr>
<th>Salt</th>
<th>LiF mol%</th>
<th>BeF₂ mol%</th>
<th>ZrF₄ mol%</th>
<th>UF₄ mol%</th>
<th>ThF₄ mol%</th>
<th>NaCl mol%</th>
<th>UCl₃ mol%</th>
<th>²³⁵U wt%</th>
<th>ρ g/cm³</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>65.39</td>
<td>28.34</td>
<td>4.72</td>
<td>1.55</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>5.0</td>
<td>2.307</td>
</tr>
<tr>
<td>2</td>
<td>65.39</td>
<td>28.34</td>
<td>4.72</td>
<td>1.55</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>19.9</td>
<td>2.307</td>
</tr>
<tr>
<td>3</td>
<td>65.39</td>
<td>28.34</td>
<td>4.72</td>
<td>1.55</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>93.0</td>
<td>2.307</td>
</tr>
<tr>
<td>4</td>
<td>65.39</td>
<td>27.34</td>
<td>4.72</td>
<td>1.55</td>
<td>1.0</td>
<td>-</td>
<td>-</td>
<td>19.9</td>
<td>2.412</td>
</tr>
<tr>
<td>5</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>66</td>
<td>34</td>
<td>15.5</td>
<td>3.112</td>
</tr>
</tbody>
</table>

2.1.3 Secondary fluids

Many of the characteristics that are desirable in a fuel salt are also desirable in the secondary loop heat transfer fluid. Important traits for the secondary fluid include low operating pressure, high thermal conductivity, high heat capacity, low reactivity with the fuel salt, low activation potential, limited corrosivity, and low toxicity. As previously discussed, a low operating pressure reduces stress on the structure reducing cost and increasing component lifetime. Desirable thermophysical properties will significantly influence the heat transfer capacity and overall size of the the heat exchanger. It is important that the secondary fluid does not violently react with the fuel salt in the event of a leak in the heat exchanger and that the secondary fluid experiences limited activation from close proximity with the fuel salt. As with the fuel salt low corrosivity and and toxicity simplify operations and reduce cost.

Several common secondary fluids are frequently used given their thermophysical properties, availability, and inert nature. We select the five secondary fluids outlined in Table 2.3 at the provided operating conditions assuming natural isotopic abundances. The operating conditions are estimated by the fuel salt temperatures leaving the core and the typical industrial SHE design capabilities. We use the advertised SHE maximum operating pressure of 4.5 MPa as a design limitation (GoochThermal 2021). Although the case of liquid water is beyond the nominal pressure capabilities of a SHE and unrealistic, we simulate this case as an extreme scenario to understand the system with a strong moderator as the secondary fluid.
Table 2.3: Secondary loop heat transfer fluid operating conditions.

<table>
<thead>
<tr>
<th>Secondary Fluid</th>
<th>$T_{avg}$ (°C)</th>
<th>P (MPa)</th>
<th>$\rho$ (g/cm$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air (Detwiler et al. 2021)</td>
<td>540</td>
<td>4.48</td>
<td>0.01919</td>
</tr>
<tr>
<td>Helium (Detwiler et al. 2021)</td>
<td>540</td>
<td>4.48</td>
<td>0.00264</td>
</tr>
<tr>
<td>Solar Salt (Serrano-López et al. 2013)</td>
<td>540</td>
<td>0.03447</td>
<td>1.74656</td>
</tr>
<tr>
<td>Steam (Detwiler et al. 2021)</td>
<td>540</td>
<td>4.48</td>
<td>0.01257</td>
</tr>
<tr>
<td>Water (Detwiler et al. 2021)</td>
<td>325</td>
<td>14.0</td>
<td>0.66740</td>
</tr>
</tbody>
</table>

2.2 Monte Carlo N-Particle Simulation

2.2.1 Simulation process

MCNP is a stochastic general purpose particle transport code capable of computing the eigenvalues for critical systems. A general input file consists of cell, surface, and material cards to define the problem geometry and material compositions. Next the desired particle source and tally cards are defined to obtain the desired parameter estimators. The code records the history of particles taken on a random walk through the problem geometry, using physics and random numbers to sample the probability of events along the path. Events are sequentially simulated and follow the entire life a particle and its progeny from birth to death. Relevant events are tallied to produce an estimator of the desired parameter.

In MCNP the criticality eigenvalue $k_{\text{eff}}$, often referred to as the multiplication factor, is defined as

$$k_{\text{eff}} = \frac{\text{fission neutrons in generation } C + 1}{\text{fission neutrons in generation } C}$$

(2.1)

The value of $k_{\text{eff}}$ indicates the criticality of a system with $k_{\text{eff}} < 1$ being sub-critical, $k_{\text{eff}} = 1$ being critical, and $k_{\text{eff}} > 1$ being super-critical. A critical or super-critical system will self sustain the fission chain reaction, but a sub critical system will not sustain fission reactions (Sweezy et al. 2003). Criticality safety analysis involves ensuring the system in question will remain in a sub-critical configuration.

MCNP solves the k-eigenvalue transport equation using the standard power method as
outlined by Brown (2009). The standard form of the k-eigenvalue transport equation follows

\[
\Omega \cdot \nabla \Psi = \int \int \int \Omega (\vec{r}', E', \Omega') \Sigma_S(\vec{r}, \Omega \rightarrow \Omega', E \rightarrow E') d\Omega' dE' + \int \int \frac{1}{k_{\text{eff}}} \chi (E) \int \nu \Sigma_F(\vec{r}, E') \Psi(\vec{r}, E', \Omega') d\Omega' dE'
\]

where the first term on the left represents neutrons entering the volume of interest and the second term on the left represents all neutron interactions in the phase space which is composed of position, energy, and solid angle direction. The first term on the right represents neutrons scattering into the phase space and the second term on the right represents neutron production from fission in the phase space. The k-eigenvalue transport equation is rewritten

\[
(L + T)\Psi = S\Psi + \frac{1}{k_{\text{eff}}} P\Psi
\]

then rearranged as

\[
\Psi = \frac{1}{k_{\text{eff}}} (L + T - S)^{-1} P\Psi = \frac{1}{k_{\text{eff}}} F\Psi
\]

This form is solved numerically using the standard power iteration method.

\[
\Psi^{(c+1)} = \frac{1}{k_{\text{eff}}}^{(c)} F\Psi^{(c)} \quad \text{for } c = 0, 1, ..., C \quad \text{given } k_{\text{eff}}^{(0)} \text{ and } \Psi^{(0)}
\]

where \(k_{\text{eff}}^{(0)}\) and \(\Psi^{(0)}\) are the user provided multiplication factor estimate and neutron source distribution. Here a single simulated fission generation corresponds to an iteration cycle. The user specifies the number of neutrons, \(N\), per generation or cycle, which will undergo a simulated random walk to estimate the new \(k_{\text{eff}}\) and source distribution. The user must ensure that the \(k_{\text{eff}}\) and source distribution have converged before the simulation starts recording tallies and that sufficient tallies are recorded to achieve the desired confidence in the simulated \(k_{\text{eff}}\). To do this, the user supplies the the number of inactive cycles, which must be sufficient to ensure convergence, and the total number of cycle iterations to perform, \(C\). Active cycles are
those cycles in which tallies are recorded and are equal to the total number of cycles minus the
inactive cycles. The power iteration method is known to produce a bias in $k_{\text{eff}}$ estimates that is
proportional to $1/N$, thus it is also important for the user to specify a sufficiently large $N$ to
reduce the bias to negligible levels. While the exact number of neutrons required depends on
the problem it is generally advised to have $N > 5,000$ Brown (2009).

In the first cycle of the simulation, $N$ source particles are initiated according to the user
supplied source distribution estimate. This estimate defines the distribution of source point
locations, source particle energy, and source particle direction that will be sampled for each
initiated particle. This source distribution is updated each cycle according fission locations
and resultant neutron energies determined during the cycle. During each active cycle, source
particles are transported through the geometry on a random walk with collision points de-
termined by particle energy and material cross section of the cell through which the particle
is passing. The simulation performs four steps at each collision point. First, it tallies the the
prompt neutron lifetime. Second, if fission is possible, $k_{\text{eff}}$ estimates are tallied. Third, if fission
is possible, $m$ fission sites are recorded for future cycle source points with next cycle neutron
energy sampled according to incident neutron energy. Here $m$ is a function of particle weight,
$f$, fission probability, $k_{\text{eff}}$, and a random number. Fourth, the collision type is sampled to
determine reaction type, but fission is treated as capture. Unlike other MCNP simulations,
criticality simulations do not allow fission reaction events to produce neutrons, transport them
with a random walk, and record the history of those neutrons during that cycle. Instead, those
neutrons are accounted for in the $k_{\text{eff}}$ estimates from step two and the source points from step
three. At cycle termination, a new set of $M = \sum m$ source particles determined from step three
is recorded for use in the next cycle and is weighted such that normalization occurs for $N$
particles instead of $M$ particles (Sweezy et al. 2003).

MCNP criticality calculations compute three separate multiplication factor estimators.
These are the collision estimator, the absorption estimator, and the track length estimator.
These estimators are reported as individual and combined estimates in the simulation output.
While each of the three estimates has some advantages in specific scenarios, the MCNP documentation recommends the three combined estimates as the best final estimate of a criticality simulation. In order to combine the estimates, MCNP produces a maximum likelihood estimate for the combined average of $k_{\text{eff}}$ using the almost-minimum variance estimate (Sweezy et al. 2003).

The collision estimator is shown in Eqn. (2.6)

$$k_{\text{eff}}^C = \frac{1}{N} \sum_i W_i \left[ \frac{\sum_j \nu_j f_j \sigma_{f_j}}{\sum_j f_j \sigma_{c_j}} \right]$$  \hspace{0.5cm} (2.6)

where $i$ is summed over all collisions where fission is possible in a cycle, $j$ is summed over all nuclides of the colliding material, $W$ indicates the particle weight, and $f$ is the atom fraction. We can see this provides the average number of neutrons produced from all possible fission processes of each collision for all collision events divided by the number of source neutrons. That is to say, the ratio of the number of neutrons in the next generation to the number of neutrons in this generation, which is $k_{\text{eff}}$ (Sweezy et al. 2003).

The absorption estimator is shown in Eqn. (2.7)

$$k_{\text{eff}}^A = \frac{1}{N} \sum_i W_i \nu_j \frac{\sigma_{f_j}}{\sigma_{c_j} + \sigma_{f_j}}$$  \hspace{0.5cm} (2.7)

where $i$ is summed over each absorption event in the $j$ nuclide. This estimator is very similar to the collision estimator except that it only considers neutrons produced from absorption events with the specific absorbing nuclide, as opposed to the average number of neutrons produced from all possible fission processes in every nuclide of the material (Sweezy et al. 2003).

The track length estimator is shown in Eqn. (2.8)

$$k_{\text{eff}}^{TL} = \frac{1}{N} \sum_i W_i \rho d \sum_j f_j \nu_j \sigma_{f_j}$$  \hspace{0.5cm} (2.8)

where $i$ is summed over all neutron trajectories in fissionable material, $\rho$ is the cell atom
density, and $d$ is the track length from the last event. We can see that this provides the number of neutrons produced over a track length $d$ for every neutron track length through fissionable material divided by the number of source particles. Again this is the number of neutrons produced per cycle or the ratio of the number of neutrons in the next generation to the number of neutrons in this generation (Sweezy et al. 2003).

### 2.2.2 Model geometry

A model geometry in MCNP is generally specified using surfaces or meshes to define cell volume boundaries with assigned material compositions. We are able to model the complex spiral channels in the SHE using only basic surfaces. To do this we divide the SHE into top and bottom halves and create a series of concentric cylinders with increasing radii and slightly offset axes for the top and bottom series of cylinders. Care is needed to perfectly align the top and bottom cylinders in order to form smooth spiral channels throughout the volume of the SHE. As shown in Fig. 2.1, the model consists of the SHE shell surrounded by dry air at standard temperature and pressure sitting on a concrete pad. The SHE shell has axial and radial inlets/outlets (radial in/outlets not shown). Along the center of the spiral heat exchanger are the central fuel salt inlet and secondary fluid outlet core surrounded by hot/cold channels divided by the plate. Various manufacturers have different designs for the geometry of the SHE core, so we select a typical geometry used in industrial applications for this model. Not included in this model are structural supports that resemble studs or pillars in the hot/cold channels that maintain proper channel width. While these will significantly affect the fluid flow, they should have limited influence on the neutronics modeling. Because the structural supports will behave as neutron absorbers more than neutron moderators, this assumption will likely cause a slightly increased simulated multiplication factor which serves as a conservative estimation of the criticality safety analysis.

MCNP6.2 comes with a built in capability to run perturbation studies, but we are unable to take advantage of this capability due to the changing number of surfaces and cells in the spiral...
Figure 2.1: Radial and axial cross-sectional views of the SHE MCNP model.

channels as we vary the channel gaps. Nevertheless, it is possible to automate the production of MCNP input files with slightly perturbed geometries for use in parametric studies because the radius of each cylindrical surface is a function of the hot/cold channel gap and plate thickness. However, this process becomes very complicated when defining the outermost channel and plate cells as they meet the SHE shell. But the cylinders do follow a semi-complicated relationship with the SHE shell inner radius that allows cell boundaries to be identified with automation in all scenarios. In Fig. 2.2, we use geometry plots to confirm cells composing complicated sections of the geometry have been properly defined. This is an important step in model validation because overlapping cells will create lost particles in the simulation and interfere with tallies.

The automation process enables us to conduct parametric studies varying the inner SHE radius, length, hot channel gap, cold channel gap, and plate thickness. Additionally, we can easily select the composition of structural materials, fuel salt types/enrichments, and secondary loop fluids from our material library. The script was designed to be flexible for future studies and can be easily modified to adjust any parameter of the SHE. The dimensions examined for
these parametric studies are detailed in Table 2.4. These dimensions slightly exceed common advertised manufacturing limitations in order to provide a better understanding of design extremes and encompass the dimensions that would likely be required for use with most MSR designs.

Table 2.4: SHE nominal and parametric study dimensions.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Nominal (cm)</th>
<th>Minimum (cm)</th>
<th>Maximum (cm)</th>
<th>Step Size (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SHE radius</td>
<td>( R_i )</td>
<td>107</td>
<td>60</td>
<td>150</td>
<td>10</td>
</tr>
<tr>
<td>SHE length</td>
<td>( L_i )</td>
<td>183</td>
<td>120</td>
<td>300</td>
<td>20</td>
</tr>
<tr>
<td>Plate thickness</td>
<td>( t_p )</td>
<td>0.4</td>
<td>0.1</td>
<td>2.8</td>
<td>0.3</td>
</tr>
<tr>
<td>Hot gap</td>
<td>( h_g )</td>
<td>5.0</td>
<td>0.5</td>
<td>14</td>
<td>1.5</td>
</tr>
<tr>
<td>Cold gap</td>
<td>( c_g )</td>
<td>5.0</td>
<td>0.5</td>
<td>14</td>
<td>1.5</td>
</tr>
</tbody>
</table>

### 2.2.3 Simulation parameters

This simulation uses the evaluated nuclear data file ENDF71x library evaluated at 627 °C with the ENDF71SaB thermal scattering data on available materials. Because operating temperatures of 650 °C are very near temperatures available in the data libraries we do not employ the \( makxsf \)
utility program to create nuclear data sets at new temperatures.

We also create two mesh tallies to determine the neutron flux across the SHE. We use the tmesh flux tally to create 1x1x1 cm meshes across the axial and radial center lines of the SHE which tally the total, thermal (< 0.625 eV), intermediate (0.625 eV - 100 keV), and fast (> 100 keV) neutron flux. These tallies are used to plot the neutron flux across the SHE.

The initial neutron source estimate samples $10^4$ particles per cycle uniformly distributed through the interior of the SHE, with isotropic angular distribution, and energy sampled from the recommended watt fission spectrum for thermal fission of $^{235}$U, as outlined in the MCNP manual. While this causes some initial source particles in non-fissionable material we observe that our source entropy converges quite rapidly for this system. The simulation discards the first 100 cycles then tallies 2000 active cycles with both the $k_{\text{eff}}$ and source distribution typically converging in < 20 cycles. Further discussion on the performance of the simulations is conducted in Chapter 3.3.
3.1 System Characterization

3.1.1 Material cross sections

We begin the analysis by characterizing the system to provide insight into system neutronics behavior. We have established the materials we are interested in studying and now plot their neutron cross sections to compare materials in Fig. 3.1. Because we want to easily compare materials, the scale of the plots is not ideal, so we also include full scale plots in Appendix C. MCNP makes it relatively easy to examine the cross sections of specific nuclides or the combined cross sections of all nuclides in a material card. While we compare our combined material cross sections, we do not examine specific nuclides contributions to these cross sections. It is
important to note that we label the special reaction number -2 as the capture capture cross section but the MCNP manual labels it as both capture and absorption in different locations and we have not been able to verify the correct label, however we will continue to refer to these as capture cross sections for consistency.

We first compare the structural materials in Figs. 3.1a-3.1c. Overall the cross sections are very similar with slightly increased cross sections across the board in Hastelloy-N compared to SS316. We note that the increased capture cross section will likely lead to slightly reduced multiplication factor in Hastelloy-N but this could also contribute to potential structural material problems that will need to be examined in depth. Their similar atomic masses indicates that neutron moderation will be comparable but slightly increased in Hastelloy-N due to the increased scattering cross section.

The secondary fluid cross sections in Figs. 3.1d-3.1f have much more variation due to significantly different nuclide compositions. We first note that water and steam have the same cross sections because they share the same nuclide composition. More importantly they have the highest scattering cross sections combined with the second lowest capture cross sections and very low atomic masses indicating that it will be an excellent moderator, part of why we chose to model it in the first place. Helium has significantly lower cross sections across the board, indicating it will have the least influence on the neutron flux, especially when we include density into the consideration. Air has highest capture cross section and a comparably significant scattering cross section, however its low density will likely cause limited impact on the neutron flux. Solar salt has relatively mid range capture and scattering cross sections combined with the highest density of the secondary fluids. As a result it will likely follow closely behind water in reducing overall neutron flux and energy. Additionally, there may be some concern with activation in the solar salt that suggests the need for study of component nuclide cross sections.

The fuel salt cross sections in Figs. 3.1f-3.1d show vastly increased resonance regions due to the large atomic mass nuclides present in these materials. We note that the FLiBe-Th+U(19.9%)
Figure 3.1: Material Cross Sectional Data
has a slightly higher capture cross section and fast fission cross section than FLiBe-U(19.9%) but virtually unchanged cross sections for fission and scattering. This is not entirely surprising given that Th is often used to breed $^{233}$U. Next we compare FLiBe-U 5%, 19.9%, and 93%. As enrichment increases we see virtually unchanged scattering cross sections with nearly uniformly increasing capture and fission cross sections with slight variations in the fast energy spectrum. Lastly we examine NaCl-U(15.5%) where we note significantly increased fission and capture cross sections, exceeding even FLiBe-U(93%), despite the lower enrichment. This is easily explained by the much higher molar concentration of UCl$_3$ in the NaCl salt which causes a significantly higher atom density of $^{235}$U in the fuel salt.

### 3.1.2 Neutron flux

Next we characterize the neutron flux for all secondary fluids with SS316 structural material and FLiBe-U(19.9%) fuel salt at nominal dimensions. We use the mesh flux tallies to plot the flux along the center of axial and radial cross sections of the SHE in Figs. 3.3-3.2. Again, we present these plots at reduced scale to allow easy comparison but include full scale plots in Appendix D. It is also important to note that the color scale is not uniform across plots but are sufficiently close to conduct visual comparisons.

We first compare the air and helium flux plots observing the overall similarity despite the significantly larger capture and scatter cross sections. We also notice very low thermal neutron flux in these systems with the largest neutron flux in the intermediate energy range. In the thermal plot we can also tell there is significant neutron leakage from the SHE by observing the relatively high flux in the concrete pad. We attribute these observations primarily to the low density of air and helium. Though steam has comparable density to air and helium we see a significantly higher thermal neutron flux which is easily accounted for by recalling its very high scattering cross section and low capture cross section. In the solar salt and water flux plots we can begin to see spiral striations in the neutron flux resulting from the material properties in the spiral flow channels. In the solar salt and water fast flux plots we see high neutron flux in
Figure 3.2: Radial neutron flux for secondary fluids at nominal parameters. From left to right: thermal ($< 0.625$ eV), intermediate (0.625 eV - 100 keV), fast ($> 100$ keV)
Figure 3.3: Axial neutron flux for secondary fluids at nominal parameters. From left to right: thermal (< 0.625 eV), intermediate (0.625 eV - 100 keV), fast (> 100 keV)
the fuel salt channel and in the thermal flux plots we see high flux in the secondary fluid channels. We also see significantly less neutron leakage in these systems. Overall, we can characterize the cases of air, helium, and steam as lightly moderated. Solar salt likely to be lightly moderated as well but it is difficult to make this claim based solely on the flux plots. The case of water appears to be quite well moderated but we will want to examine the parametric studies to fully evaluate this statement.

3.2 Parametric Studies

The number of parameters studied requires the parametric studies to be well organized for easy comparison. We first conduct density parametric studies of the fuel salt and secondary fluid with SS316 and nominal dimensions. Next we conduct parametric studies of the SHE overall size and channel gap widths with SS316 and nominal dimensions to understand the effects of geometry. Finally, we perform parametric studies of the plate thickness and channel gaps for all materials of interest in order to make material comparisons. These studies will be grouped first by the parameter studied, then by structural material, and then by fuel salt for each secondary fluid. The reader is reminded that the nominal SHE design uses the dimensions listed in Table 2.4 and when necessary nominal materials are considered to be SS316, FLiBe-U(19.9%), and solar salt. It is important to note that with the exception of the SHE radius/length parametric study, these results are for a fixed volume system. As such, it is useful to consider how the ratio of fuel salt to secondary fluid changes over the parametric studies.

3.2.1 Density studies

One of the safety features touted in most MSR designs is the large negative reactivity feedback with temperature rise which is caused by the decrease in fuel salt density as the temperature rises. This becomes a risk factor in the heat exchanger because the fuel salt temperature is deceasing and the density is increasing which will cause a positive reactivity insertion into
the system. Thus we need to evaluate how rapidly the multiplication factor will change with increasing density. To do this, we perturb the fuel salt and secondary fluid densities by 10% of their nominal densities and plot the results in Fig. 3.4. We do not examine more significant transients or full accident scenarios, such as fuel salt solidification.

![Figure 3.4: Heat transfer fluid density influence on multiplication factor.](image)

We first turn to the fuel salt density parametric study and note that a 10% change in the density roughly corresponds to a 100 °C change in temperature in either direction. While the density variation is enough to cause the case of FLiBe-U(93%) to transition between sub-critical and super critical, we note that the rate of change across all fuel types is quite low which is desirable. We also observe that the rate of change is increased with increasing enrichment or fuel concentration in the fuel salt. The secondary fluid density studies show extremely flat multiplication factor across the prescribed densities indicating little influence on $k_{\text{eff}}$. It would be interesting to explore more extreme cases in both of these studies.
3.2.2 Geometry studies

We now examine the influence of the SHE size on the criticality of the system. Here we vary both the inner length and the inner radius of the SHE and plot the resultant multiplication factor as a surface in Fig. 3.5. Despite the expansive range of sizes examined, the multiplication factor remains quite flat for each secondary fluid. We do note that the multiplication factor increases with size more rapidly for those systems identified to have lower moderation in the flux plot analysis. While these plots generally indicate that a wide range of SHE sizes can be selected without significantly increasing criticality risks, we would want to conduct additional studies using other channel gap widths and extreme channel gap ratios to fully validate this claim.

Figure 3.5: SHE size influence on multiplication factor.
Next we assess the influence of the channel gap on the criticality of the system. We vary both the hot and cold channel gaps and plot the resultant multiplication factor as a surface in Fig. 3.6. We generally observe that multiplication factor increases with increased hot channel gap and decreased cold channel gap. This is intuitive when we recall that the SHE interior is a fixed volume system and increasing the cold channel gap implies an overall increase in the fuel salt volume contained in the hot channel. In the case of water, we note an initial increase in the multiplication factor as the cold channel gap increases before it begins to decrease. We claim that this is because the system is initially under moderated before reaching optimal moderation for peak multiplication factor and eventually becoming over moderated and reducing the multiplication factor. We can also claim that the system with other secondary fluids appears to be deeply under moderated. Another observation is that increasing the
channel gap while maintaining the same channel gap ratio results in higher multiplication factor. Again, because the system is a constant volume, the small channel gaps cause a larger proportion of the SHE interior volume to be occupied by the dividing plate relative to the amount of fuel and secondary fluid.

### 3.2.3 Material comparisons

We now compare the influence of selected materials on the multiplication factor for hot gap, cold gap, and plate thickness parametric studies. These studies will be grouped first by the parameter studied, then by structural material, and then by fuel salt for each secondary fluid.

In Figs. 3.7-3.12 we make the following general observations about the materials’ influence on the multiplication factor. The multiplication factor of Hastelloy-N is slightly lower than that of SS316 which conforms with our analysis of the structural material cross sections. The fuel enrichment and the molar concentration of the fuel carrier in the fuel salt have the strongest influence on the multiplication factor and must be carefully analyzed in the design process. This is primarily observable in the FLiBe-U(93%) and the NaCl-U(15.5%) fuel salts and also conforms with the fuel salt cross section analysis of these materials. As we noticed in the fuel salt cross section analysis, the addition of Thorium to the fuel salt had very little influence on the multiplication factor at BOC. With the exception of water, the secondary fluids behave very similarly, especially helium and air.

In Figs. 3.7-3.8, we observe increasing multiplication factor as the ratio of fuel to moderator increases. With the exception of the case of water, all of these systems remain deeply under-moderated with approximately 3/4 of all simulated fissions caused by neutrons in the intermediate energy range (0.625 eV-100 keV). The fuel salt FLiBe-U(93%) reaches unsafe criticality levels for all secondary fluids at large hot channel gap widths, and the fuel salt NaCl-U(15.5%) reaches unsafe criticality levels only for the case of water, which we noted earlier is an extreme case that does not represent realistic operating conditions. All other configurations remain deeply sub-critical.
Figure 3.7: SS316 hot channel gap parametric studies.

Figure 3.8: Hastelloy-N hot channel gap parametric studies.
Figure 3.9: SS316 cold channel gap parametric studies.

Figure 3.10: Hastelloy-N cold channel gap parametric studies.
Figure 3.11: SS316 plate thickness parametric studies.

Figure 3.12: Hastelloy-N plate thickness parametric studies.
In Figs. 3.9-3.10, as we previously commented, the case of water is initially under-moderated but quickly becomes over moderated, while all other cases remain deeply under-moderated. It is desirable to maintain an under-moderated configuration to prevent increased reactivity due to loss of the secondary fluid. As with the hot gap parametric studies, we observe increasing multiplication factor as the ratio of fuel to moderator increases. Again all secondary fluid cases are super-critical in small cold channel gap widths for FLiBe-U(93%) and in the case of water for NaCl-U(15.5%), with the remaining cases remaining deeply sub-critical.

In Figs. 3.11-3.12, we observe the increase in plate thickness drastically decreases the multiplication factor because the volume of both fuel salt and secondary fluid are replaced by the structural material. This indicates that increasing the number or size of channel structural supports can be used to decrease the multiplication factor of the system without significant cost the total heat transfer capacity of the SHE.

### 3.3 Simulation Evaluation

We now evaluate some important simulation metrics to provide some confidence in our results. While it is not feasible to present these metrics for every simulation, we provide the metrics for nominal dimensions using SS316 structural material and FLiBe-U(19.9%) fuel salt for all secondary fluids. The metrics we examine are the convergence of source entropy, convergence of $k_{\text{eff}}$, relative error, and figure of merit. In the course of this study, over 2500 simulations were conducted, each requiring approximately 90-600 minutes of computer time, and achieving standard deviations in simulated $k_{\text{eff}}$ ranging from 0.00003-0.00012.

As discussed in Chapter 2.2, it is important to ensure both the source entropy and $k_{\text{eff}}$ have converged before beginning tallies. The MCNP output will provide assessments to confirm the simulation achieves convergence, but plotting these tallies over all simulation cycles provides quick visual confirmation. In Fig. 3.13 we see that $k_{\text{eff}}$ has arguably converged by the 100 cycle cutoff. We also tested cutoffs up to 500 cycles with similar results on those shown here.
Figure 3.13: \( k_{\text{eff}} \) plus one standard deviation for secondary fluids at nominal parameters.

(a) SS316 - FLiBe19 - Air  
(b) SS316 - FLiBe19 - Helium  
(c) SS316 - FLiBe19 - Solar Salt  
(d) SS316 - FLiBe19 - Steam  
(e) SS316 - FLiBe19 - Water

Figure 3.14: Source entropy for secondary fluids at nominal parameters.

(a) SS316 - FLiBe19 - Air  
(b) SS316 - FLiBe19 - Helium  
(c) SS316 - FLiBe19 - Solar Salt  
(d) SS316 - FLiBe19 - Steam  
(e) SS316 - FLiBe19 - Water
In Fig. 3.14 we see that the source entropy converges very quickly, indicating that some initial source points in non-fuel material does not interfere with source distribution convergence. We note that the source entropy can be significantly influenced by the initial source distribution estimate and the number of particles per cycle.

The relative error is defined as the ratio of the standard deviation to the mean of the tally and should be proportional to \(1/\sqrt{C_a}\). This metric gives an indication to the precision of the simulation, not a comparison to the actual physical process. In Fig. 3.15, we see the final relative error is on the order of \(10^{-3}\) and generally decreases as the number of cycles increases indicating a well behaved tally (Sweezy et al. 2003).

![Graphs showing relative error for different secondary fluids](image)

**Figure 3.15:** Relative error for secondary fluids at nominal parameters

The figure of merit (FOM), defined in Eqn. (3.1), indicates reliability in a tally.

\[
FOM \equiv \frac{1}{R^2T} \tag{3.1}
\]
where $R$ is the relative error and $T$ is the computer time in minutes. Because $R^2$ should be proportional to $1/C_a$ and $T$ should be proportional to $C_a$, the FOM should be constant if the tally is well behaved. A FOM that is not constant might indicate that influential particle paths are not being properly sampled (Sweezy et al. 2003). While these tallies do approach a constant, they are not within the desired fluctuations of the FOM. As a test, we ran the same simulation with increased particles per cycle which achieved well behaved FOM, and our confidence intervals for the $k_{\text{eff}}$ estimate significantly overlapped. We assess that this might have a small impact on the simulated confidence interval of $k_{\text{eff}}$ but the expected value of $k_{\text{eff}}$ is still quite reliable.

Figure 3.16: Figure of merit for secondary fluids at nominal parameters

(a) SS316 - FLiBe19 - Air  (b) SS316 - FLiBe19 - Helium  (c) SS316 - FLiBe19 - Solar Salt
(d) SS316 - FLiBe19 - Steam  (e) SS316 - FLiBe19 - Water
4.1 Summary of Results

We conclude that fuel salt and secondary fluid density are not significant contributors to the criticality of the system at nominal operating parameters but further studies need to confirm transients and accident scenarios potentially involving fuel salt solidification. However, the fuel salt enrichment and fuel carrier concentration are very important and must be selected in coordination with design of the reactor. Addition of Th at concentrations in this study had insignificant effects on the criticality of the SHE at BOC.

Low pressure working fluids are generally preferable for use with SHEs which will likely require secondary fluids to be molten salts or metals. Secondary fluids with reduced moderating capacity are preferable for use with the fuel salts considered here. This means secondary
fluids with constituent nuclides of higher atomic mass and lower scattering cross sections are preferable. This assessment will need to be reevaluated for other fuel compositions. Additionally, secondary fluids with low absorption cross sections and preferable decay chains should be selected to reduce activation of the secondary fluid. However, thermophysical properties of the secondary fluid should not be forgotten when selecting for preferable neutron interaction properties.

The overall size of the SHE only has moderate influence on the criticality of the SHE, but extreme configurations will require specific analysis. Hastelloy-N demonstrated slightly lower multiplication factors than SS316 but may have reduced service life due to radiation induced He embrittlement, depending on the scale of the neutron flux. The structural configuration of inter-channel supports can be used as multiplication factor reduction tool to the extent that it does not interfere with mechanical and heat transfer properties.

Analysis of the relative volume of fuel salt, secondary fluid, and structural material appears to be one of the best indications of the resultant multiplication factor. While a direct relationship is not identified in this work, one likely exists.

There are minor issues in this study regarding the FOM. Secondary simulations using more particles per cycle demonstrate $k_{\text{eff}}$ estimated intervals are statistically similar to this study, serving as anecdotal evidence that the tallies are still quite precise. Future studies using this model should employ 15,000-20,000 particles per cycle.

4.2 Overarching Conclusions

SHEs have been proven in industrial applications involving fouling fluids, boast reduced maintenance requirements, and high heat transfer capacity making them a great candidate for MSR applications. In this work we use MCNP to perform criticality safety simulations of SHEs for liquid fuel MSRs at BOC in order to determine the effects of geometry and materials on the multiplication factor of the system. We found that deeply subcritical configurations
can be achieved using established industrial materials, but special attention should be paid to fuel salt enrichment and concentration. Furthermore, limiting the moderating potential of the secondary fluid significantly contributes to maintaining a subcritical system for the fuel. Overall system criticality can easily be influenced by the volume of structural material replacing fuel in the system, to the extent acceptable, given mechanical and heat transfer considerations. Corrosion and radiation damage need to be considered when selecting structural materials.

4.3 Future Work

Future research on SHE use in MSR applications includes sensitivity analysis of the fuel salt enrichment. This is important as the inventory of fissile material might change over the life of the reactor or might not be perfectly distributed through the fuel salt.

A study of coupled computational fluid dynamics analysis or multi-physics simulations will allow identification of localized criticality risks and inform configurations that are unsuitable due the heat transfer capacity constraints.

Significant work is still required in evaluating and code qualifying structural materials for use with MSRs. The compositions of feasible materials have significant implications on SHE criticality analysis. Thorough analysis of the material cross-sections for each involved nuclide will provide further insight into the behavior of this system. Specific materials investigated could be expanded, to include additional alloys, other fuel salts such as FLiNaK, or other secondary fluids such as other molten salts or even liquid metals.

Some of the extremes of this system could be better explored, for example the effect of the SHE size on higher multiplication factor configurations or various channel gap ratios would be informative. Transients such as flood, fire sprinkler, and fuel salt solidification should be simulated.

Little is currently known how the fission products affect the composition or thermophysical properties of the fuel salt over the life of the fuel. These factors will heavily influence both the
criticality and heat transfer capacity of the SHE. Approximated EOC fuel compositions could be modeled, however, these compositions will be heavily influenced by the chemical processing performed on the fuel salt.
REFERENCES


45

Table A.1: A summary of acronyms used in alphabetical order.

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Abbreviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aircraft Reactor Experiment</td>
<td>ARE</td>
</tr>
<tr>
<td>Beginning of Cycle</td>
<td>BOC</td>
</tr>
<tr>
<td>Chinese Academy of Science</td>
<td>CAS</td>
</tr>
<tr>
<td>End of Cycle</td>
<td>EOC</td>
</tr>
<tr>
<td>Evaluated Nuclear Data File</td>
<td>ENDF</td>
</tr>
<tr>
<td>Generation IV International Forum</td>
<td>GIF</td>
</tr>
<tr>
<td>Integral Molten Salt Reactor</td>
<td>IMSR</td>
</tr>
<tr>
<td>Light Water Reactor</td>
<td>LWR</td>
</tr>
<tr>
<td>Term</td>
<td>Abbreviation</td>
</tr>
<tr>
<td>-----------------------------------------------------------</td>
<td>--------------</td>
</tr>
<tr>
<td>Molten Chloride Fast Reactor</td>
<td>MCFR</td>
</tr>
<tr>
<td>Molten Chloride Reactor Experiment</td>
<td>MCRE</td>
</tr>
<tr>
<td>Molten Salt Breeder Reactor</td>
<td>MSBR</td>
</tr>
<tr>
<td>Molten Salt Reactor</td>
<td>MSR</td>
</tr>
<tr>
<td>Molten Salt Reactor Experiment</td>
<td>MSRE</td>
</tr>
<tr>
<td>Molten Salt Reactor Program</td>
<td>MSRP</td>
</tr>
<tr>
<td>Monte Carlo N-Particle Transport Code</td>
<td>MCNP</td>
</tr>
<tr>
<td>Oak Ridge National Lab</td>
<td>ORNL</td>
</tr>
<tr>
<td>Shanghai Institute of Applied Physics</td>
<td>SINAP</td>
</tr>
<tr>
<td>Spiral Plate Heat Exchanger</td>
<td>SHE</td>
</tr>
<tr>
<td>Stainless Steel Type-316</td>
<td>SS316</td>
</tr>
<tr>
<td>Thorium-based Molten Salt Reactor - Liquid Fuel 1</td>
<td>TMSR-LF1</td>
</tr>
<tr>
<td>Tri-structural Isotropic Particle</td>
<td>TRISO</td>
</tr>
</tbody>
</table>
Table B.1: A summary of variables and their abbreviations in alphabetical order.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Abbreviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Absorption estimator</td>
<td>$k^A_{\text{eff}}$</td>
</tr>
<tr>
<td>Angular neutron flux</td>
<td>$\Psi$</td>
</tr>
<tr>
<td>Atomic density</td>
<td>$\rho$</td>
</tr>
<tr>
<td>Atomic fraction for nuclide $j$</td>
<td>$f_j$</td>
</tr>
<tr>
<td>Cold channel gap</td>
<td>$c_g$</td>
</tr>
<tr>
<td>Collision estimator</td>
<td>$k^C_{\text{eff}}$</td>
</tr>
<tr>
<td>Energy</td>
<td>$E$</td>
</tr>
<tr>
<td>Fission neutron energy density</td>
<td>$\chi$</td>
</tr>
<tr>
<td>Term</td>
<td>Symbol</td>
</tr>
<tr>
<td>----------------------------------------------------------------------</td>
<td>--------</td>
</tr>
<tr>
<td>Fission neutron yield for nuclide $j$ (prompt or total)</td>
<td>$\bar{\nu}_j$</td>
</tr>
<tr>
<td>Fission neutron yield</td>
<td>$\nu$</td>
</tr>
<tr>
<td>Hot channel gap</td>
<td>$h_g$</td>
</tr>
<tr>
<td>Microscopic capture cross section for nuclide $j$</td>
<td>$\sigma_{c_j}$</td>
</tr>
<tr>
<td>Microscopic fission cross section for nuclide $j$</td>
<td>$\sigma_{f_j}$</td>
</tr>
<tr>
<td>Microscopic total cross section for nuclide $j$</td>
<td>$\sigma_{T_j}$</td>
</tr>
<tr>
<td>Macroscopic fission cross section</td>
<td>$\Sigma_F$</td>
</tr>
<tr>
<td>Macroscopic scattering cross section</td>
<td>$\Sigma_S$</td>
</tr>
<tr>
<td>Macroscopic total cross section</td>
<td>$\Sigma_T$</td>
</tr>
<tr>
<td>Multiplication factor</td>
<td>$k_{\text{eff}}$</td>
</tr>
<tr>
<td>Number of cycles</td>
<td>$C$</td>
</tr>
<tr>
<td>Number of active cycles</td>
<td>$C_a$</td>
</tr>
<tr>
<td>Particle weight</td>
<td>$W$</td>
</tr>
<tr>
<td>Particles per cycle</td>
<td>$N$</td>
</tr>
<tr>
<td>Position vector</td>
<td>$\vec{r}$</td>
</tr>
<tr>
<td>SHE Length (inner)</td>
<td>$L_i$</td>
</tr>
<tr>
<td>SHE Radius (inner)</td>
<td>$R_i$</td>
</tr>
<tr>
<td>Solid angle direction</td>
<td>$\Omega$</td>
</tr>
<tr>
<td>Thickness of plate</td>
<td>$t_p$</td>
</tr>
<tr>
<td>Track length estimator</td>
<td>$k_{\text{eff}}^{T_L}$</td>
</tr>
<tr>
<td>Trajectory track length</td>
<td>$d$</td>
</tr>
</tbody>
</table>
## MATERIAL CROSS SECTIONS

Table C.1: Material Cross Section Legend Key.

<table>
<thead>
<tr>
<th>Material</th>
<th>Legend Label</th>
</tr>
</thead>
<tbody>
<tr>
<td>SS316</td>
<td>m11</td>
</tr>
<tr>
<td>Hastelloy-N</td>
<td>m12</td>
</tr>
<tr>
<td>FLiBe-U(5%)</td>
<td>m21</td>
</tr>
<tr>
<td>FLiBe-U(19.9%)</td>
<td>m22</td>
</tr>
<tr>
<td>FLiBe-U(93%)</td>
<td>m23</td>
</tr>
<tr>
<td>FLiBe-Th-U(19.9%)</td>
<td>m24</td>
</tr>
<tr>
<td>NaCl-U(15.5%)</td>
<td>m25</td>
</tr>
<tr>
<td>Air</td>
<td>m31</td>
</tr>
<tr>
<td>Helium</td>
<td>m32</td>
</tr>
<tr>
<td>Solar Salt</td>
<td>m33</td>
</tr>
<tr>
<td>Steam</td>
<td>m34</td>
</tr>
<tr>
<td>Water</td>
<td>m35</td>
</tr>
</tbody>
</table>
Neutron Total Cross Section

Structural Material

mcnp 6
probid: 05/08/23 12:34:04
m11
nuclides
6000.82c
20055.82c
16032.82c
16033.82c
16034.82c
16036.82c
14028.82c
14029.82c
14030.82c
24050.82c
24052.82c
24053.82c
24054.82c
28058.82c
28060.82c
28061.82c
28062.82c
28064.82c
28066.82c
28068.82c
42092.82c
42095.82c
42096.82c
42097.82c
42098.82c
42100.82c
26054.82c
26056.82c
26057.82c
26058.82c

Cross section (barns)

mt xs
-1 m11

Energy (MeV)

Neutron Capture Cross Section

Structural Material

mcnp 6
probid: 05/08/23 12:34:04
m11
nuclides
6000.82c
20055.82c
16032.82c
16033.82c
16034.82c
16036.82c
14028.82c
14029.82c
14030.82c
24050.82c
24052.82c
24053.82c
24054.82c
28058.82c
28060.82c
28061.82c
28062.82c
28064.82c
28066.82c
28068.82c
42092.82c
42095.82c
42096.82c
42097.82c
42098.82c
42100.82c
26054.82c
26056.82c
26057.82c
26058.82c

Cross section (barns)

mt xs
-2 m11

Energy (MeV)
Neutron Elastic Cross Section

Fuel Salt

Neutron Total Cross Section

Secondary Fluid

mcnp
probid:05/08/23 12:34:04
m21
nuclides
3006.82c
3007.82c
4009.82c
9019.82c
40090.82c
40091.82c
40092.82c
40094.82c
40096.82c
92234.82c
92235.82c
92238.82c

mcnp
probid:05/08/23 12:34:04
m31
nuclides
6000.82c
7014.82c
7015.82c
8016.82c
8017.82c
18036.82c
18038.82c
18040.82c
Flux Plots must be normalized for $10^4$ source particles.

Unit: $\frac{\text{neutrons}}{cm^2 \cdot s}$ per source particle
Intermediate Neutron Flux (0.625eV - 100keV) - Radial View
SS316 - FLiBe19 - Air

Fast Neutron Flux (> 100keV) - Radial View
SS316 - FLiBe19 - Air
Total Neutron Flux - Radial View

SS316 - FLiBe19 - Helium

-100 -50 0 50 100
Radial Length (cm)

-100 -50 0 50 100
Height (cm)

-100 -50 0 50 100
Radial Length (cm)

-100 -50 0 50 100
Height (cm)

Thermal Neutron Flux (< 0.625eV) - Radial View

SS316 - FLiBe19 - Helium

-100 -50 0 50 100
Radial Length (cm)

-100 -50 0 50 100
Height (cm)

-100 -50 0 50 100
Radial Length (cm)

-100 -50 0 50 100
Height (cm)
Total Neutron Flux - Radial View
SS316 - FLiBe19 - Steam

Thermal Neutron Flux (< 0.625eV) - Radial View
SS316 - FLiBe19 - Steam
Intermediate Neutron Flux (0.625eV - 100keV) - Radial View

SS316 - FLiBe19 - Steam

Fast Neutron Flux (> 100keV) - Radial View

SS316 - FLiBe19 - Steam
Intermediate Neutron Flux (0.625eV - 100keV) - Axial View

SS316 - FLiBe19 - Water

-100 -50 0 50 100
Axial Length (cm)
-100
-50
0
50
100
Height (cm)

Fast Neutron Flux (> 100keV) - Axial View

SS316 - FLiBe19 - Water

-100 -50 0 50 100
Axial Length (cm)
-100
-50
0
50
100
Height (cm)

76