135Xe in LEU Cermet Nuclear Thermal Propulsion Systems

DISSERTATION

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Abstract

Nuclear Thermal Propulsion (NTP) is currently a topic of research for NASA. NASA has the goal of sending humans to Mars and Nuclear Thermal Propulsion (NTP) is an appealing technology to aid in this endeavor. In the simplest terms, an NTP system is a nuclear reactor that utilizes hydrogen that is expanded through a convergent-divergent nozzle and ejected for propulsion. NTP can shorten the travel time to Mars and reduce the mass that must be lifted into low earth orbit. Furthermore, strategies to use low enriched uranium (LEU) in NTP systems have been identified which could make NTP significantly more affordable to develop than for past NTP development efforts. Beyond a human Mars mission, NTP has the potential to assist in other human and robotic missions beyond low earth orbit.

The overarching goal of this work is to better understand NTP technology so that it may one day help with a human Mars mission. This work focuses on a subset of NTP systems that use a combination of LEU and tungsten cermet fuel and addresses the issues related to $^{135}$Xe in these systems. LEU cermet NTP systems have a unique operational regime where $^{135}$Xe has a profound impact on performance and controllability. LEU cermet NTP have extremely high power densities, operate with a thermal neutron spectrum, and the reference human mission to Mars requires restarting the reactor 4 to 8 hour after full power operation.
In this work, two LEU cermet NTP point designs are presented and used as reference systems for the study of $^{135}$Xe in LEU cermet NTP systems. These point designs were produced with a thorough search of the rocket performance design space.

Using infinite lattice burnup calculations, it was found that MCNP 6.1.1 Beta and Serpent 2 produced very similar results and that burnup cells across the fuel element were not needed to capture spatial self shielding effects. The infinite lattice results were used to inform the approach undertaken for the full core burnup calculations. Full core burnup calculations indicate that the reactivity loss during operation of a LEU cermet NTP system has a maximum value of 210 pcm during a 25 minute burn and the maximum reactivity loss after operation peaks at approximately 3500 pcm.

The possible effect of $^{135m}$Xe on xenon worth in LEU cermet NTP systems was found by using the model based TENDL-2014 nuclear data library and Serpent 2. Model based TENDL cross sections were used because no experimentally determined cross sections are available for $^{135m}$Xe.

A relationship to estimate the performance (in terms of Isp loss) as a function of control drum angle is derived and presented. Mitigation strategies are identified that show promise for counteracting the effects of $^{135}$Xe and maximizing the performance of LEU cermet NTP systems.

It is recommended for future work that an integrated reactor systems code be developed to examine $^{135}$Xe in LEU cermet NTP more thoroughly. In addition, this work has identified a need for basic nuclear data experiments to measure the cross section of $^{135m}$Xe instead of relying on models.
This document is dedicated to my parents.
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Chapter 1: Introduction

The NASA Authorization Act of 2010 passed by congress and in the U.S. National Space Policy issued by the Whitehouse also in 2010 directs NASA to develop the technology for a human Mars mission in the 2030s time frame. Nuclear thermal propulsion (NTP) is a promising candidate technology for this 2030s human Mars mission and has been a topic of research at NASA. While testifying to congress in 2016 the current Administrator of NASA said the following about NTP:

“We are on a Journey to Mars and most people believe that—in the end—Nuclear Thermal Propulsion will probably be the most effective form of propulsion to get there”


This work examines a subset of NTP technology, Tungsten Cermet Low Enriched Uranium (LEU) NTP systems. In this subset of Cermet LEU NTP technology, the specific problem of $^{135}$Xe is investigated. $^{135}$Xe has a large impact on the operation of Cermet LEU NTP systems and other NTP technology. The knowledge gained in this effort can help in the development of NTP systems and may one day contribute to human exploration of Mars.
1.1. Overview of NTP technology

In simplest terms a NTP system is a nuclear reactor that is used to heat gas that is expanded through a convergent-divergent nozzle and ejected for propulsion. The NTP core geometry that is studied for this work is loosely based on the core geometry studied at the end of the NERVA NTP program in the 1960s and early 1970s [1]. Historically, the base design for a NTP core uses stacks of hexagonal prism fuel elements and a moderator containing tie tube elements. Figure 1 is a labeled cross section MCNP model of an NTP system showing the stacked configuration of fuel elements and moderator elements. The hexagonal fuel elements have circular coolant channels running down their length. Hydrogen gas is passed through the channels of the fuel and heated to temperatures approaching 3000 K. The tie tube elements contain an annulus of zirconium hydride which is actively cooled by hydrogen that circulates up and down the length of the tie tube. The name “tie tubes” for the moderator containing elements is the common name used in literature and acknowledges the structural support role of the tie tubes. Figure 2 shows the flow of hydrogen though the fuel element and tie tube. For additional clarity a NERVA era drawing of labeled NTP system is presented in Figure 3.

Control drums are located on the periphery of the NTP system’s active core in the reflector. These control drums are a dominant control mechanism for controlling the reactivity in the NTP reactor. The control drums are comprised of a cylinder of neutron reflecting material such as Beryllium with a neutron poison (such as boron carbide) on one side of the cylinder. The control drums rotate the neutron poison closer or further away from the core to control how many neutrons are reflected back into the core.
Figure 1: A MCNP produced cross section of a NTP reactor with a traditional hexagon and fuel and tie tube arrangement.

Figure 2: A diagram showing the flow of hydrogen in NTP fuel elements and tie tubes
NTP systems use turbine powered pumps (a turbopump) to pressurize the propellant through the core and other components. The turbopump is powered by expanding heated H₂ through the turbopump’s turbine. In a NTP system the heated H₂ for the turbopump’s turbine comes from cooling components that need to be actively cooled during operation. Components that need to be actively cooled during NTP operation include: tie tubes, radiation shield, reflector, control drums, vessel, chamber and parts of the nozzle. Figure 4 presents a medium level detail flow diagram of a possible NTP system. There are many ways to configure an NTP system. The specific configuration presented in Figure 4 uses enthalpy gained from the tie tubes to power the turbopump.
Figure 4: A labeled flow schematic of a NTP system with a closed loop cycle. This figure was reprinted from [3].

NTP is an in-space propulsion technology used to propel spacecraft after it has been launched into space. For a human Mars mission several chemically powered heavy lift rockets would be used to launch the components of the spacecraft from earth into Low Earth Orbit (LEO). Once in LEO, the spacecraft would be assembled and nuclear thermal propulsion would be used to take the spacecraft to Mars and back.

1.1.1. Advantages of NTP technology

NTP is in a favorable spot in the propulsion design space for mission beyond low earth orbit when compared to technology of similar technological readiness. In order to understand why NTP is an appealing technology, it is important to introduce the key
figures of merit for a propulsion system: Specific impulse ($I_{sp}$) and thrust to weight ratio (T/W).

T/W is simply the thrust produced by a propulsion system divided by weight of the propulsion system (not including fuel) in earth’s surface gravity. A high T/W indicates that propulsion system has a low mass, a generally favorable thing for space travel.

$I_{sp}$ is a measure of how effective a propulsion system uses propellant. By definition, $I_{sp}$ is the total impulse (N s) given per unit of propellant used (kg) and in this definition has units of m/s. Although, most aerospace literature give Isp units of seconds by dividing by earths gravitational constant $g$ (with units of m/s$^2$). By giving $I_{sp}$ units of seconds, the $I_{sp}$ of a propulsion system can be compared to other propulsion systems regardless if United States customary units or Metric units are reported in the work. For clarity equations 1 and 2 are provided to show how $I_{sp}$ affects rocket system performance. 

Equation 1 is simply amount of thrust produced per unit of propellant used. Equation 2 is the classic Tsiolkovsky rocket equation, which gives how much change in velocity a propulsion system experiences as it uses propellant. In both equations, it can be seen that a higher $I_{sp}$ results in more effective use of propellant. The predicted $I_{sp}$ for a Cermet NTP system is approximately 900 s and the maximum $I_{sp}$ for a chemical rocket is approximately 450 s.
\[ F_{\text{thrust}} = g \dot{m} I_{\text{sp}} \quad (1) \]

\[ \Delta v = I_{\text{sp}} g \ln \left( \frac{m_o}{m_f} \right) \quad (2) \]

where

\( I_{\text{sp}} = \) Specific impulse of propulsion system (s)

\( g = \) Acceleration at the Earth's surface (m/s²)

\( \dot{m} = \) Mass flow rate of propellant (kg/s)

\( F_{\text{thrust}} = \) Thrust (N)

\( m_o = \) Initial mass of spacecraft (kg)

\( m_f = \) Final mass of spacecraft (kg)

\( \Delta v = \) Change in velocity (m/s)

Calculating \( I_{\text{sp}} \) accurately for an NTP system is complicated and best accomplished with aerospace specific software. Figure 5 presents the \( I_{\text{sp}} \) for various gases as a function of temperature as calculated with the methods used in this work. In NTP systems, \( I_{\text{sp}} \) increases with temperature, and increases with lower molecular mass of the propellant. Hydrogen is used in NTP systems, because it gives the highest \( I_{\text{sp}} \) of any gas.
Figure 5: The $I_{sp}$ of an NTP system with various propellants.

NTP offers an appealing combination of high $T/W$ and high $I_{sp}$ that is not currently achievable with any other propulsion technology of similar technological readiness. Propulsion technologies exist with higher $T/W$, but lower $I_{sp}$, such as traditional chemical rocket engines. Other propulsion technologies exist with higher $I_{sp}$, but lower $T/W$, such as electric thrusters. Furthermore technologies like advanced fusion rockets have higher $T/W$ and higher $I_{sp}$ than NTP, but these technologies would require significantly more development effort than NTP technology. The unique
combination of T/W, I<sub>sp</sub>, and technological readiness make NTP appealing for a human Mars mission in the 2030s time frame. Figure 6 compares NTP (here called “Nuclear Fission”) to other propulsion technology with comparable or lower technological readiness levels.

Figure 6: A figure showing where different technology fits in the propulsion design space. Here “Nuclear Fission” refers to NTP. This image is reprinted from [4].

1.2. History of NTP technology

NTP is a not new concept. Between 1955 and 1972 the Rover/NERVA program successfully designed, built and tested over twenty NTP reactors. The Rover/NERVA
program had a budget of $7.7 billion (in 2016 dollars) and was a collaboration between the Atomic Energy Commission, NASA, Westinghouse and Aerojet, and other industrial partners. NASA’s original plans for NERVA NTP systems included a visit to Mars in 1979. The Rover/NERVA program was canceled before a in space demonstration of NTP technology, because there was no clear mission for the NTP technology as a human Mars mission was removed from the nation’s space goals [6]. The Rover/NERVA program focused on coated particles and graphite based fuels.

The Soviets also built and tested a NTP system. The RD-0410 Soviet NTP system underwent more than 30 ground tests and was developed from 1958 to the around the fall of the Soviet Union in 1991 [7]. The RD-0410 used a uranium carbide/tungsten carbide based fuel.

Many other NTP efforts have been imitated in the US that reached a level of development less than Rover/NERVA. One notable project was the Special Nuclear Thermal Propulsion Program (SNTP)/Timberwind which ran from 1987 to 1994 under the Strategic Defense Initiative ("Star Wars") program. The SNTP/Timberwind sought to build a NTP system for a boost phase intercept vehicle that would be capable of disabling Soviet missiles early in the Soviet missile’s flight path. The project was slowed and later canceled with the fall of the Soviet Union and the end of the Cold War. At the time of cancelation, the project had spent $328 million (2016 dollars) and was on the path toward successful development of NTP technology [8]. SNTP/Timberwind used a pebble bed fuel with coated particles in a graphite matrix.
1.3. Current NTP Efforts and LEU NTP Technology

With a human mission to Mars now one of the nation’s space exploration goals, NTP is once again under consideration. The US FY 2016 Omnibus Appropriations Bill appropriated a maximum of $20 million dollars for NASA’s nuclear thermal propulsion research [9]. In recent previous years, the Nuclear Cryogenic Propulsion Stage project involved an approximately 50 person NASA/Department of Energy (DOE) team investigating and developing nuclear thermal propulsion [10]. In addition, as of 2015 the DOE has requested NTP related proposals through its Nuclear Energy University Program and Small Business Innovative Research / Small Business Technology Transfer (SBIR/STTR) program. One of the technologies being considered under recent NTP efforts is LEU cermet NTP systems.

A key element of recent NTP efforts has been establishing an affordable NTP development strategy in a budget constrained environment. Using low enriched uranium (LEU) nuclear fuel has been identified as a potential affordable NTP development strategy. Traditionally, space nuclear systems have used highly enriched uranium (HEU) and were developed in an era where HEU was widespread and acceptable. In brief, the potential reasons why LEU may make NTP systems more affordable to develop include:

- Inclusion of industry partners in the development. There is much more flexibility for a private company to own intellectual property and hardware for a LEU system than an HEU system.
• Less regulatory burden for researching and testing an LEU system. LEU systems require significantly less security than HEU systems and more sites are available to research LEU systems.

• LEU systems are in alignment with the Global Threat Reduction Initiative (GTRI) and are better insulated from political concerns. Political concerns add risk to a development schedule and therefore raise costs.

• Potential inclusion of non-weapon state international partners in the development process.

Initial studies comparing the performance of HEU and LEU NTP systems have found no large difference in performance (in terms of T/W and I_{sp}) between comparable HEU and LEU NTP systems [11] [12] [13]. LEU NTP systems have comparable T/W with HEU NTP systems, because the mass of NTP systems is not primarily driven by minimum critical size. Finding the optimum design of an NTP system is a multifaceted problem and thermal considerations, not neutronic considerations, have a larger impact on the overall size of a NTP core for most thrust classes. Furthermore, the mass of the core is only about one half of the total mass of the NTP system. This means, for example, a 10% increase in mass in the core would only result in a 5% increase in mass of the NTP system.

LEU NTP systems can have comparable I_{sp} with HEU NTP systems because I_{sp} is driven by thermal considerations. To achieve a desired I_{sp} a NTP system needs to heat the propellant to a certain temperature. LEU and HEU fuel in comparable NTP systems
have the same maximum operating temperature and are therefore both equally capable of heating propellant to a desired temperature.

1.3.1. Further Discussion on LEU vs. HEU systems

Like space nuclear systems, HEU fuel was once common in research reactors. From a purely technical standpoint, HEU is a logical choice for research reactors because it allows for more compact and therefore higher flux cores per MW than LEU. Proliferation concerns associated with the use of HEU have led to a steep decline in the number of HEU reactors in the world. The GTRI program states its mission is to convert, remove and protect special nuclear material like HEU. The GTRI program has been effective in shutting down HEU reactors or converting HEU reactors to LEU. Furthermore, in the US every remaining HEU research reactor has a LEU conversion effort underway. Even highly specialized reactors located at secure Department of Energy National Laboratories are subject to HEU to LEU conversion efforts.

An example of the success of the HEU minimization efforts can be seen with the cancelation of the Advanced Neutron Source in 1996. The Advanced Neutron Source (ANS) was to be a next generation research reactor that would produce the world’s largest continuous neutron flux. The project was canceled partially because the ANS used HEU fuel and was deemed to be in conflict with the United States’ non-proliferation policy [14]. Testimony in congress at the time stated that building a HEU reactor would damage the US’s position to credibly urge other nations to not use HEU [15].

Beyond partially insulating NTP from political concerns, using LEU allows NASA to better capitalize on emerging movements in advanced nuclear reactor development.
There is an unprecedented movement in private industry advanced nuclear reactor development. Approximately 40 American companies are working to bring advanced nuclear technology to the market [16]. A number of efforts in both the executive and legislative branches of government have emerged to help these companies succeed [17] [18]. The intellectual and industrial base for the nation’s private industry to develop advanced nuclear technology is quickly rising. By focusing on LEU NTP systems, NASA’s will be better able to leverage these advancements in the emerging nuclear industry.
Chapter 2: The LEU cermet point designs: SCCTE and TRIBLE

It is necessary to have reference point designs for LEU cermet NTP systems, before the role of $^{135}$Xe can be examined in these systems. LEU cermet NTP technology is a recent concept. The preliminary LEU cermet NTP design points used in this work are the SCCTE (Space Capable Cryogenic Thermal Engine) and TRIBLE (Tiny Rocket Investigating Balanced Launch Economics) systems. SCCTE and TRIBLE were produced to enable fundamental research in LEU cermet NTP, such as the $^{135}$Xe related analyses conducted in the work. Much of the work on SCCTE and TRIBLE was completed and directed by students. Both SCCTE and TRIBLE were designed for a human Mars mission in the 2030s time frame. The central difference between SCCTE and TRIBLE is that SCCTE and TRIBLE were designed and optimized for different thrust classes. SCCTE was designed to a 35,000 lbf thrust class and TRIBLE was designed to a 16,000 lbf thrust class.

This chapter introduces the SCCTE and TRIBLE LEU cermet point designs. In addition, to provide context, technical background on LEU cermet systems, history, technology and an overview of the design process is also included.
2.1. LEU Tungsten Cermet Fuel

Cermet refers to a fuel form made of ceramic particles dispersed in a metal matrix. The name cermet is an amalgamation of ceramic and metal. In the case of NTP, the ceramic particles are UO$_2$ with a stabilizer and the metal matrix is tungsten. The stabilizer provides free oxygen to assist in keeping UO$_2$ in the UO$_2$ phase at high temperatures. Proposed stabilizers include ThO$_2$, Gd$_2$O$_3$, and Y$_2$O$_3$. Tungsten is a promising material to use for NTP applications, because $I_{sp}$ increases as a function of outlet temperature and tungsten has one of the highest melting temperatures of any chemical element. In addition, tungsten is unreactive with hydrogen even at high temperatures.

Figure 7 presents pictures of the cermet NTP fuel. The micrograph of cermet fuel in Figure 7 uses ZrO$_2$ as surrogate for UO$_2$. Many cermet fuel concepts, including those used in SCCTE and TRIBLE, have a metal clad on the inside of coolant channels. This clad adds structural integrity to the fuel element and helps prevent hydrogen from interacting with the UO$_2$ in the cermet.

Cermet NTP fuel was first developed in parallel with the Rover/NERVA program’s graphite fuel in the 1960s under the programs at General Electric (GE) and Argonne National Laboratory (ANL). Both the GE and ANL program demonstrated the ability of W-UO$_2$ cermets to survive in a hot hydrogen environment at approximately 3000 K [19]. Recent efforts at NASA Marshal Space Flight Center (MSFC) and Center for Space Nuclear Research (CSNR) have successfully fabricated cermet fuel elements [20].
In order to minimize the mass of a LEU tungsten cermet NTP system and achieve the T/W needed for a human Mars mission, it is necessary to isotopically purify the tungsten to include a large fraction of $^{184}$W. Isotopically purifying $^{184}$W lessens parasitic absorption in the fuel matrix as $^{184}$W has a thermal absorption cross section of 1.5 b, while natural W has a thermal absorption cross section of 18.1 b. Figure 8 compares the cross section of natural tungsten with $^{184}$W. One study found that LEU and HEU cermet NTP reactor systems have comparable mass at a 16,000 lbf thrust class when isotopically purified $^{184}$W is used in the fuel matrix of the LEU cermet NTP system [11].
Figure 8: The absorption cross section of natural tungsten (W-0 in the legend) and W-184.

It should be noted that W-UO₂ cermet fuels is well suited for LEU NTP, because the tungsten fuel matrix can be isotopically purified to lessen parasitic absorption in the fuel matrix. Many high temperature metals such as rhenium, hafnium, tantalum, and niobium do not have naturally occurring isotopes with thermal absorption cross sections as low as ¹⁸⁴W’s thermal absorption cross section.

Using ¹⁸⁴W in NTP systems to enable LEU is a new concept, but using ¹⁸⁴W in NTP systems to improve general neutronic performance is not an entirely new concept. The first documents referencing using ¹⁸⁴W cermet in potential NTP systems date back to the
late 1960’s with NASA’s Tungsten Water Moderated Rocket concept [21]. This was a HEU NTP concept and had a different geometry and it was very different in many other regards to the current LEU cermet NTP concepts being studied. Later in 1996, Brookhaven National Laboratory proposed the Miniature Reactor Engine (MITEE) NTP concept, which called for $^{184}$W cermet fuel elements [22]. The MITEE was an advanced HEU NTP concept that was also different in many regards from the current LEU NTP concepts.

2.2. History and Context of LEU Tungsten Cermet NTP

The first work on LEU NTP systems was published in Spring 2013 and examined graphite based fuels [23]. Over the summer of 2013, NASA funded the first design study of LEU cermet NTP fuels with a design team at CSNR [24]. This pioneering work demonstrated the feasibility of the LEU cermet NTP technology.

In Fall of 2014, NASA Marshal Space Flight Center started the SCCTE (Space Capable Cryogenic Thermal Engine) project with a combination of NASA engineers, outside contractors including CSNR, and the author. This was one of NASA’s first LEU tungsten cermet NTP design efforts. The end result of this project was a design point that received considerable optimization and subject matter input from NASA aerospace engineers. The final SCCTE design was for a 35,000 lbf thrust class engine.

In Spring 2015, Aerojet-Rocketdyne, CSNR, and the author started work on TRIBLE (Tiny Rocket Investigating Balanced Launch Economics) LEU tungsten cermet NTP design point. The project was undertaken in part as fundamental research to compare LEU and HEU systems at a similar thrust class. The central feature of TRIBLE that
separates it from SCCTE is that TRIBLE was designed and optimized for 16,000 lbf thrust class.

Both the SCCTE and TRIBLE point designs, along with much of the supporting work, was a collaboration between multiple people and organizations. The author is the primary author on the reactor related work for both the SCCTE [25] and TRIBLE [11] point designs and where possible the contribution of others is cited.

SCCTE and TRIBLE are preliminary designs that were undertaken in order to demonstrate the feasibility of LEU cement NTP, provide initial performance estimates, and most importantly, offer a reference design for other foundational work and fundamental research on LEU cermet NTP systems. Actual flight hardware will likely vary notably from these initial design points, but maturing LEU cermet NTP to the point of flight hardware requires initial point designs like SCCTE and TRIBLE. The many disparate subfields of nuclear and aerospace engineering need a reference design before their specialized analyses can be effectively undertaken and iteration towards a final design can be made.

SCCTE and TRIBLE have thus far effectively served their purpose as reference design for other foundational work on LEU cermet NTP systems. SCCTE and TRIBLE have been used in a number of mission planning studies, specialized analyses, cost estimations and hardware prototyping. As stated before, the SCCTE and TRIBLE design points were needed for the $^{135}$Xe related work presented later in this document. Some other notable work that use the SCCTE or TRIBLE design points that was presented by others at conferences includes:
• SCCTE reflector design with initial hardware prototyping [26].
• SCCTE “Injectafold” design with initial hardware prototyping [27].
• Two separate efforts to model heat transfer from the fuel elements to the tie tube in SCCTE [28] [29].
• Rocket Engine Cycle Analyses for TRIBLE [30]
• A Neutronic assessment of the impact of using MCNP’s on the fly temperature corrected cross section in SCCTE [31]

2.3. The Design Process and Using SPOC to make SCCTE and TRIBLE

Both SCCTE and TRIBLE were created with similar tools and design processes. This section explains the tools used, the design process that was followed, and some of the many factors considered in the design of SCCTE and TRIBLE.

A key tool used in the creation of the SCCTE and TRIBLE point designs was SPOC (Space Propulsion Optimization Code). SPOC is a collection of user defined MATLAB® functions that serves as a multifunctional NTP analyses tool for modeling nuclear characteristics, rocket performance and thermal hydraulic behavior. Many of the details of SPOC are presented in [32]. The author was a contributor to the creation of SPOC.

Some of the capabilities and details of SPOC are restated here to explain how SPOC was used to create the SCCTE and TRIBLE design points. Other key supporting work for SPOC includes: An independent NASA verification of SPOC’s thermal methods [33], a bench mark of SPOC to a historical design [34], and an example of a design study using SPOC [35].
SPOC creates MCNP 6.1 [36] or Serpent 2 [37] input files for an NTP system using an input file that specifies the defining geometry, thermal-hydraulic characteristics and other defining parameters of the NTP system. A comparison of MCNP and Serpent is presented in Chapter 3. The MCNP input file that is produced by SPOC can be run to create a spatial power deposition distribution. With a spatial power deposition distribution calculated and the parameters set in the input file, thermal-hydraulic calculations can be completed in SPOC to estimate rocket performance criteria, such as T/W and \( I_{sp} \). If desired, the neutronic and thermal-hydraulic calculations can be iterated upon to find a steady state convergent solution.

Some of the defining parameters of a hexagonal NTP fuel element’s geometry are length, flat to flat, number of channels, size of the channels, pitch of the channels, thickness of the clad on the channels, and thickness of the clad on the outside of the fuel elements. Figure 9 shows some examples of this of the geometry that can be created in SPOC.

Figure 9. Three fuel elements that can be created in SPOC with different flat-to-flat distances, coolant channel pitch and with 37, 61 and 331 coolant channels, respectively. Image modified from [34].
The fuel elements are placed in a NTP core, in lattices with different fuel to moderator ratios. Table 1 compares some of the possible lattice configurations. In SPOC, it is possible to combine these lattices when designing a core. Examples of cores with combined lattices are presented in Figure 10. Combining lattices is useful for flattening power profiles and maximizing performance of the NTP system.

Table 1. Some of the different lattice configurations and their moderator-to-fuel element ratios that can be created in SPOC. Table modified from [34].

<table>
<thead>
<tr>
<th>NERVA Pewee</th>
<th>SNRE</th>
<th>Bullseye</th>
<th>Inverted SNRE</th>
<th>Inverted Pewee</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="NERVA Pewee" /></td>
<td><img src="image2" alt="SNRE" /></td>
<td><img src="image3" alt="Bullseye" /></td>
<td><img src="image4" alt="Inverted SNRE" /></td>
<td><img src="image5" alt="Inverted Pewee" /></td>
</tr>
</tbody>
</table>

\[ \frac{F}{M} \text{ Ratio} = 3:1 \quad \frac{F}{M} \text{ Ratio} = 2:1 \quad \frac{F}{M} \text{ Ratio} = 1:1 \quad \frac{F}{M} \text{ Ratio} = 1:2 \quad \frac{F}{M} \text{ Ratio} = 1:3 \]

Figure 10. Examples of cores made with combined lattices of different types. Here the grey elements represent moderator elements and the fuel elements are colored by zone.
The central thermal-hydraulic calculation that SPOC does is calculating the maximum $I_{sp}$ that a specified NTP configuration is capable of producing at a desired thrust, without violating the maximum specified temperature of the fuel. Inlet temperature and inlet pressure are specified in the input file. Mass flow rate is a function of thrust and $I_{sp}$. The calculation relies on routine 1-D compressible-flow finite-volume calculations. A solver written in MATLAB® iterates the 1-D finite-volume calculations so that the maximum $I_{sp}$ is achieved under the stated constraints (i.e. maximum $I_{sp}$ at the desired thrust without violating maximum allowable fuel temperature). The Nusselt Number is calculated using Taylor’s correction to the McCarthy-Wolf correlation as shown in [38]. The friction factors for the Nusselt Number correlation can be found in [39]. Temperature and pressure dependent hydrogen properties are interpolated from work based on [40].

It is necessary to calculate the temperature profile in the fuel element to ensure that the maximum specified temperature of the fuel is met and not exceeded. A unique feature of the hexagonal fuel geometry, used in many NTP concepts, is the inverted triangular stacking of coolant channels in an internally heated medium. This geometry, with a unit cell, is featured in Figure 11. An analytical solution for analyzing conduction in this geometry is given in [41] and was used in the analysis of SCCTE and TRIBLE. Temperature dependent thermal conductivities for cermet fuel were calculated using the most conservative methods described in [42].
Figure 11. The unit cell described in [41] for an inverted triangular stacking of coolant channels in an internally heated medium.

2.3.1. The Design process

A key facet of the design approach behind TRIBLE and SCCTE was the production of approximately one million design points and sorting those design points to find promising designs. These million design points were produced by varying parameters of the NTP system in a combinatorial fashion. This computationally intensive “brute force optimization” approach was made possible by use of the Idaho National Laboratory’s high performance computer (HPC) center and high power desktops. This “brute force optimization” approach was well suited for LEU cermet NTP, as LEU cermet is a recent concept and little was known about optimum systems prior to this modeling effort. Unlike other NTP concepts there are no historical LEU cermet NTP systems to reference.

SPOC was written to be parallelizable, so that file generation and analysis could be conducted using many computer processors. Figure 12 is a top level view of how
SPOC was used to create the TRIBLE and SCCTE design points. This is a simplified linear view that does not capture the degree of iteration that was present at each step. The process described in Figure 12 captures the key elements of the design process and can be used to understand how the “brute force optimization” approach was leveraged.

Figure 12. An overview of how the SCCTE and TRIBLE point designs were made with SPOC.

A brief description of each of the steps in Figure 12 is presented in below:

**Combinatorial Inputs**

Using automated scripts, a very large number of SPOC input files were generated that varied design parameters important to a NTP system in a combinatorial fashion. A notional example of how NTP design parameters were varied is presented below to demonstrate the combinatorial nature of this design process.
• 9 Core Lengths
• 9 Core layouts
• 3 Axial Reflector Thickness
• 3 Radial Reflector Thickness
• 4 Channel Radii
• 4 Fuel Flat to Flat sizes
• 4 Number of channels
• 6 Fuel Zoning configurations
• 5 Axial Enrichments configurations

Producing input files with these factors varied in a combinatorial fashion would result in ~1.1 million input files. Each one of these input files is a NTP point design. The input file was used to create a MCNP input file and later be used in combination with the results of the MCNP analysis to predict the performance of the NTP point design based on the input file.

The NTP design parameters that were varied and the degree to which they were varied was based on subject matter expert input. Early studies on SCCTE had little subject matter expert input and as a result these early studies were very large. Later studies on TRIBLE had more subject matter expert input and therefore included a lower number of varied parameters over a smaller range. Subject matter expert input represents knowledge both gained by the NTP design team and contributed by outside parties. NASA MSFC contributed on subject matter expert input that assisted with many hardware related decisions during the SCCTE effort.
Neutronic Calculations

The primary purpose of the neutronic calculations is to determine the keff and the spatial power distribution in the core. For this initial step, temperature adjusted cross-section for the various materials in the NTP system were assigned based on an informed estimate for the temperature profile. Also for this initial step, a control drum angle was assumed.

The majority of criticality calculations were made with MCNP 6.1.1 beta as it is the newest and fastest version of MCNP and the power deposition tallies for Serpent 2 were not implemented at the time of this work.

Thermal Calculations

Each of the inputs undergoes thermal analysis. The thermal calculations are described above and in [32] and [32]. The thermal analysis is constrained so that each input has the same inlet conditions, maximum fuel temperature, and thrust. To save computation time, thermal analysis is not conducted on cores that were very subcritical.

An assumed power profile can be used to avoid the need to calculate power deposition in the Monte Carlo neutronic calculations and extract it for thermal calculations in SPOC. The assumed power profile can be taken from a representative core. This drastically lessens calculation time but gives a less accurate calculation of $I_{sp}$ and other thermal hydraulic related values. An assumed power profile was used in early calculations, before informed estimates could be made about ranges of parameters to vary.
Not all of the point designs are capable of producing the desired thrust, because there is not sufficient inlet pressure to drive required mass flow through the core. These are excluded from the thermal analysis.

**Make Map of the Design Space then Reduce & Filter**

With the neutronic and thermal analysis completed there are a large number of design points that need to be sorted through, so that promising cases can be identified. Filters that were applied to the design space included:

- Minimum keff
- Maximum mach number in the peak channel
- Maximum Fuel power density.

Figure 13 is an example design space from the SCCTE design effort on a T/W and I<sub>sp</sub> plot. The points in the graph are colored by fuel to moderator ratio in the core. This study did not feature combined lattices. Each point in Figure 13 represents a valid NTP point design in that each point has the:

- Same thrust
- Same maximum fuel temperature
- Meet minimum keff constraints (0.99)
- Meet maximum Mach number constraints (0.30).
Figure 13. An example of the map of the design space visualized on a plot of T/W and $I_{sp}$ colored by fuel to moderator ratio.

Due to the limitations of plotting data on a two dimensional plot, only differences in fuel to moderator ratio is highlighted between point designs on the T/W vs Isp plot in Figure 13. It should be noted that many design parameters change between each point in Figure 13. For clarity, Figures 14 and 15 highlight different design parameters in the design space. These are the same design points that were shown in Figure 13.

In addition, the mass flow rate of each design point is a function of the design point’s $I_{sp}$. The thermal power that each design point operates at is a function of $I_{sp}$ and to a lesser degree pressure drop in the core.
Figure 14. An example of the map of the design space visualized on a plot of T/W and $I_{sp}$ colored by radius of active fuel. R has units of m.
Figure 15. An example of the map of the design space visualized on a plot of T/W and I<sub>sp</sub> colored by thickness of fuel between channels.

**Refinement Iteration**

With promising points in the design space identified, it was necessary to further refine and optimize the design. This process involved examining values between the values chosen for the combinatorial inputs. It may also involve exploring a smaller design space, after a promising range of values have been identified. In addition, not all parameters are best handled by large combinatorial style studies. For example, optimal radial enrichment variation to flatten the power profile can be accomplished by a simple algorithm. This algorithm followed the logic of: lower the enrichment in the highest power fuel elements...
and trade a reduction in radial power peaking for reactivity. Finally, it also is necessary to ensure that the control drums have the necessary criticality worth to shut down the reactor.

2.4. SCCTE and TRIBLE

This section provides an overview of the SCCTE and TRIBLE LEU cermet point designs produced with the design process described above. Sufficient detail is provided so that the role of $^{135}$Xe in the SCCTE and TRIBLE point designs can be understood when discussed in later sections. As stated before the key difference between SCCTE and TRIBLE is thrust level with SCCTE being a 35,000 lbf thrust class system and TRIBLE being a 16,000 lbf thrust class system. Many of the details of the SCCTE system are also reported in [25] [43] and [44]. Many of the details of the TRIBLE system are also reported in in [11] [12] and [45].

SCCTE at 35,000 lbf thrust was designed for a mission similar to the NASA Design Reference Architecture 5 human NTP Mars mission [46]. TRIBLE at 16,000 lbf thrust class was designed to be closer to the historical Small Nuclear Reactor Engine (SNRE) [1] and for the human Mars mission described in [47].

TRIBLE is a smaller more moderated core than SCCTE. This is expected as TRIBLE was optimized for approximately half the thrust of SCCTE. Figures 16 and 17 are scaled cross sections of the MCNP models of SCCTE and TRIBLE. In Figure 17 it can be seen that TRIBLE has a fuel to moderator ratio of 1:2 and SCCTE has a fuel to moderator ratio of 1:1.
SCCTE and TRIBLE use a common geometry for the fuel element and tie tube. The geometry was developed during the SCCTE effort and was largely limited by in-element power peaking effects discussed later. Figure 18 is a MCNP visual editor produced cross section of the fuel element and tie tube.

Table 2 compares many of the key parameters of SCCTE and TRIBLE side by side. It should be noted, TRIBLE has a higher core inlet pressure and a larger area expansion ratio nozzle than SCCTE. These are relatively small differences between the NTP design points that were stated as a boundary condition for the design process. In addition, the core inlet temperature listed in Table 2 for SCCTE were produced by a full power cycle analysis and the inlet temperature for TRIBLE is an assumed value.

Figure 16. A vertical cross section of SCCTE (Left) and TRIBLE (Right) with the respective lengths of the active fuel region dimensioned.
Figure 17. A horizontal cross section of SCCTE (Left) and TRIBLE (Right) with the respective total diameter of the core dimensioned. Not to scale with Figure 16

Figure 18. The Fuel element and tie tube used in SCCTE and TRIBLE.
**Table 2. Key SCCTE and TRIBLE parameters**

<table>
<thead>
<tr>
<th></th>
<th>SCCTE (Space Capable Cryogenic Thermal Engine)</th>
<th>TRIBLE (Tiny Rocket Investing Balance Launch Economics)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Reactor System Mass</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fuel Mass (151 Elements) (kg)</td>
<td>1029.8</td>
<td>Fuel Mass (64 Elements) (kg) 433.4</td>
</tr>
<tr>
<td>Tie Tubes (150 Elements) (kg)</td>
<td>562.5</td>
<td>Tie Tubes (135 Elements) (kg) 501.0</td>
</tr>
<tr>
<td>Radial Reflector + Control Drums (kg)</td>
<td>469.4</td>
<td>Radial Reflector + Control Drums (kg) 412.1</td>
</tr>
<tr>
<td>Axial Reflector (kg)</td>
<td>60.0</td>
<td>Axial Reflector (kg) 49.8</td>
</tr>
<tr>
<td>Barrel+Vessel+Other Core Structure (kg)</td>
<td>255.8</td>
<td>Barrel+Vessel+Other Core Structure (kg) 189.5</td>
</tr>
<tr>
<td><strong>Total Mass (Excluding Shield) (kg)</strong></td>
<td><strong>2377.5</strong></td>
<td><strong>Total Mass (Excluding Shield) (kg)</strong> <strong>1585.8</strong></td>
</tr>
<tr>
<td><strong>Key Performance Parameters</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nominal Isp (150:1 Nozzle)</td>
<td>895</td>
<td>Nominal Isp (300:1 Nozzle) 899</td>
</tr>
<tr>
<td>Nominal Thrust (lbf)</td>
<td>35,000 (155.7 kN)</td>
<td>Nominal Thrust (lbf) 16,000 (71.2 kN)</td>
</tr>
<tr>
<td>Whole Reactor Power(MW)</td>
<td>766.6</td>
<td>Whole Reactor Power(MW) 338.4</td>
</tr>
<tr>
<td>Fuel Temperature Max (K)</td>
<td>2850</td>
<td>Fuel Temperature Max (K) 2850</td>
</tr>
<tr>
<td><strong>Engine System Interface Information</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Interface Point</td>
<td>Flow Rate (kg/s)</td>
<td>Pressure (MPa)</td>
</tr>
<tr>
<td>Core inlet</td>
<td>17.73</td>
<td>6.93</td>
</tr>
<tr>
<td>Core outlet</td>
<td>17.73</td>
<td>4.70</td>
</tr>
<tr>
<td><strong>Fuel Details</strong></td>
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<td></td>
</tr>
<tr>
<td>Fuel Composition</td>
<td>W-UO₂-ThO₂</td>
<td>Fuel Composition</td>
</tr>
<tr>
<td>Volume loading of Oxide (% vol.)</td>
<td>60</td>
<td>Volume loading of Oxide (% vol.)</td>
</tr>
<tr>
<td>ThO₂ in the Oxide (%mol.)</td>
<td>6.0</td>
<td>ThO₂ in the Oxide (%mol.)</td>
</tr>
<tr>
<td>¹⁸⁴W in Tungsten (% atom)</td>
<td>98</td>
<td>¹⁸⁴W in Tungsten (% atom)</td>
</tr>
<tr>
<td>Uranium Enrichment (²³⁵U % atom)</td>
<td>19.75 to 13.13</td>
<td>Uranium Enrichment (²³⁵U % atom)</td>
</tr>
<tr>
<td>Total ²³⁵U (kg)</td>
<td>45.9</td>
<td>Total ²³⁵U (kg)</td>
</tr>
<tr>
<td>Percent Theoretical Density (% TD)</td>
<td>97</td>
<td>Percent Theoretical Density (% TD)</td>
</tr>
<tr>
<td>Clad Material</td>
<td>¹⁸⁴W</td>
<td>Clad Material</td>
</tr>
<tr>
<td>Clad Thickness (μm)</td>
<td>170</td>
<td>Clad Thickness (μm)</td>
</tr>
</tbody>
</table>

SCCTE is a 35,000 lbf thrust a LEU cermet NTP concept designed for a human Mars mission similar to the one described in [46]. TRIBLE is a 16,000 lbf thrust a LEU cermet NTP concept designed for a human Mars mission similar to the one described in [47].
2.4.1. Neutronics consideration in SCCTE and TRIBLE

SCCTE and TRIBLE have a degree of excess reactivity in their design. The excess reactivity was included to compensate for the uncertainty in the neutronic modeling and ensure that the point designs would still be critical as the design matured. In a clean core under normal operating conditions with control drums at 60 degrees from fully removed SCCTE has a keff of 1.01960 with a 1 sigma uncertainty of 0.00012 and TRIBLE has a keff of 1.03080 with a 1 sigma uncertainty of 0.00009.

Additional details of the neutronic characteristics of SCTTE and TRIBLE are presented in Table 3. The values in Table 3 were produced by MCNP 6.1 assuming clean core under normal operating conditions with control drums at 60 degrees from fully removed. It can be seen that TRIBLE with a lower Fuel to moderator can be seen to have a more thermal spectrum than SCCTE.
Table 3. Key SCCTE and TRIBLE neutronic parameters

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>SCCTE</th>
<th>TRIBLE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel Meat Average Power Density (MW/L)</td>
<td>13.4</td>
<td>15.0</td>
</tr>
<tr>
<td>Active Core Average Power Density (MW/L)</td>
<td>2.8</td>
<td>1.9</td>
</tr>
<tr>
<td>Fuel meat average thermal flux (&lt;0.625 ev) (cm&lt;sup&gt;2&lt;/sup&gt;s&lt;sup&gt;-1&lt;/sup&gt;)</td>
<td>5.3×10&lt;sup&gt;14&lt;/sup&gt;</td>
<td>5.9×10&lt;sup&gt;14&lt;/sup&gt;</td>
</tr>
<tr>
<td>Fuel meat average intermediate flux (0.625 eV - 100 keV) (cm&lt;sup&gt;2&lt;/sup&gt;s&lt;sup&gt;-1&lt;/sup&gt;)</td>
<td>3.8×10&lt;sup&gt;15&lt;/sup&gt;</td>
<td>2.1×10&lt;sup&gt;15&lt;/sup&gt;</td>
</tr>
<tr>
<td>Fuel meat average fast flux (&gt;100 keV) (cm&lt;sup&gt;2&lt;/sup&gt;s&lt;sup&gt;-1&lt;/sup&gt;)</td>
<td>5.8×10&lt;sup&gt;15&lt;/sup&gt;</td>
<td>3.4×10&lt;sup&gt;15&lt;/sup&gt;</td>
</tr>
<tr>
<td>% fissions caused by thermal energy neutrons (&lt;0.625 eV)</td>
<td>68.1</td>
<td>80.6</td>
</tr>
<tr>
<td>% fissions caused by intermediate energy neutron (0.625 eV - 100 keV)</td>
<td>26.0</td>
<td>15.9</td>
</tr>
<tr>
<td>% fissions caused by fast energy neutron (&gt;100 keV)</td>
<td>5.9</td>
<td>3.5</td>
</tr>
</tbody>
</table>

It is acknowledged that MCNP models used for SCCTE and TRIBLE are preliminary and, at the current fidelity, the MCNP models are likely missing a number of features that would remove reactivity. MCNP models for many “real hardware” programs are much more complicated and beyond the scope of this work. For example, the TREAT restart program MCNP models have material cards that are based on mass spectroscopy on real material samples. For the TREAT restart program both graphite and separately zircaloy have more than 200 isotopes in the material card [48].

The neutronic models of SCCTE and TRIBLE are of sufficient fidelity to enable fundamental research that supports LEU cermet NTP. They are the best available estimates for total flux, power density and spectrum available for LEU cermet NTP systems.

Some of the known limitations of the current MCNP models are listed below:
• Lack of evaluated or even published thermal scattering tables (known as $S(\alpha, \beta)$) for key components such as gaseous hydrogen, tungsten metal, ZrH$_{1.8}$ ($S(\alpha, \beta)$ for ZrH$_2$ is used), and ZrC.

• Unquantified isotopic makeup of non-$^{184}$W tungsten in the cermet

• Lack of coolant channels in the reflector. Initial work on this found that adding adequate coolant channels on a similar NTP system removed approximately 200 pcm of reactivity [26].

• Unquantified trace elements in all components.

• Hardware at the bottom of the fuel is undesigned and may add a large degree of neutron reflection.

As mentioned above, the SCCTE and TRIBLE design process assigns cross section based on an informed assumption about the power profile in the core. Preliminary work in [31] along with SCCTE specific analyses has been conducted that examines the impact of conducting iterative neutronic and thermal-hydraulic solutions, until the solution converges. This work used MCNP’s on-the-fly (OTF) cross section Doppler boarding with thermal scattering laws corrected with the “tmp” card or using the nearest $S(\alpha, \beta)$ table. It was found that after the first iteration that approximately 700 pcm of reactivity was lost when OTF cross sections were used, but more importantly, the power profile did not change appreciably. The power profile is key for calculating rocket performance figures of merit such as T/W and $I_{sp}$. 
2.4.2. Thermal Hydraulic consideration in SCCTE and TRIBLE

In an NTP system, it is advantageous to have the spatial power distribution flat radially and top peaked axially. A power distribution that is flat radially minimizes pressure drop in the core and lowers peak fuel power density. A fuel element that has a power distribution that is top peaked axially is capable of producing higher hydrogen outlet temperature (and therefore $I_{sp}$) at the same maximum fuel temperature.

A flatter radial power profile results in a lower pressure drop across the core, because each channel in the core must be orificed (flow restricted) to match flow to the power deposition in that channel. The larger the ratio between the power deposition in the hottest channel and the average channel, the larger the pressure drop from the required orificing. Channel by channel flow orificing was demonstrated during the ROVER/NERVA project for reactors with ~76,000 individual channels.

Figures 19 and 20 are the element by element power deposition in the SCCTE core and TRIBLE core, respectively. These element by element power depositions were produced with the control drums 60 degrees from all out. A combination of radial enrichment zoning and a combined lattice pattern of fuel elements and moderator elements was used to flatten the radial power profile. To flatten the radial power profile, moderator elements were moved to points in the core where the local power was lower and fuel elements where moved to locations in the core where the local power was high. SCCTE and TRIBLE are highly under moderated systems so adding moderation increases local power. Figure 21 shows the process of combining lattices to flatten the power profile in SCCTE.
To take into account the effects of power peaking and the subsequent flow orificing on pressure drop in the core, a “peaked channel factor” of 1.5 was used for SCCTE and TRIBLE. For core pressure drop calculations this peaked channel factor essentially models a coolant channel that receives 1.5 times the average coolant channel power, as well as 1.5 times the average coolant flow rate. A peaked channel factor of 1.5 is estimated to account conservatively for the effects of peaking in the core and in the fuel element. The core outlet pressures reported in Table 2 use a peaked channel factor of 1.5. All other thermal performance parameters in Table 2 are reported for an average channel.

Figure 19. The element by element power distribution in the SCCTE core
Figure 20. The element by element power distribution in the TIRBLE core.
Several additional seconds of I<sub>sp</sub> from a NTP system can be achieved by altering the axial power profile in the fuel elements so that more power is deposited nearer to the inlet (i.e. earlier in the coolant’s flow path) in the fuel element. Increasing I<sub>sp</sub> by shifting the power profile forward was first proposed in [49]. The underlying logic is that when the hydrogen is hot at the end of the fuel element, it is advantageous to have a lower power density. When the propellant is hot at the end of the fuel element, there is less possible difference in temperature to drive heat transfer between fuel centerline and the propellant, before the maximum allowable fuel temperature is met.

Figures 22 and 23 are the axial power profile of the SCCTE and TRIBLE cores, respectively. Power in these graphs is normalized by dividing by the power in the highest
power axial zone in the most power peaked fuel element (labeled “Max” in the figure). Two methods are used to alter the axial power profile in SCCTE and TRIBLE: Axial reflector (BeO) at the inlet of the fuel element and variable axial enrichment. Employing axial enrichment in a NTP systems is a trade between $I_{sp}$ and reactivity. To find promising trades between $I_{sp}$ and reactivity, several possible axial enrichments were run and compared. In SCCTE, an axial enrichment was chosen that produced 7.5 s of $I_{sp}$ for 570 pcm of reactivity, when compared to a constant enrichment. In Figure 24, the optimized axial enrichment used in SCCTE, with the resultant power profile, is compared to a constant enrichment and its resultant power profile.

![Normalized Power Deposition](image)

**Figure 22. The axial power in the SCCTE core**
Figure 23. The axial power in the TRIBLE core.

Figure 24. Constant enrichment (Unoptimized) axial enrichment vs variable axial enrichment (Optimized) and the resultant power profile.
Margin in the thermal calculations for SCCTE and TRIBLE is handled in a fashion similar to how the thermal margin was handled for the SNRE project during NERVA [1]. For SCCTE and TRIBLE, a maximum allowable fuel temperature of 2850 K is assumed based on historical work and the properties of cermet fuels. A 60 K thermal margin is added to this 2850 K limit and all thermal calculations are conducted assuming a maximum allowable temperature of 2790 K. A 60 K thermal margin is similar to what was used in the SNRE program.
Chapter 3: Modeling $^{135}\text{Xe}$ in LEU Cermet NTP Systems

LEU cermet NTP systems operate in a unique regime where $^{135}\text{Xe}$ has a pronounced effect on the performance of the system. Furthermore, modeling the behavior of $^{135}\text{Xe}$, in LEU cermet NTP systems, poses a set of novel challenges. This chapter details how $^{135}\text{Xe}$ was modeled in LEU cermet NTP systems, presents the worth of $^{135}\text{Xe}$ in SCCTE and TRIBLE during a representative human Mars mission and explains how $^{135}\text{Xe}$ interferes with the operation of LEU cermet NTP systems. $^{135m}\text{Xe}$ and its effect on xenon worth in LEU NTP systems is not discussed in this chapter but is the sole topic of Chapter 4.

The behavior of $^{135}\text{Xe}$ is well understood in traditional power or research reactors. $^{135}\text{Xe}$ is a fission product that is a strong neutron poison which builds in and decays during operation of a nuclear reactor. $^{135}\text{Xe}$ has one of the largest absorption cross selections of all nuclides. Figure 25 shows the relevant paths by which $^{135}\text{Xe}$ is created and decays in a nuclear reactor. In this graph, the precursors of $^{135}\text{I}$ are lumped into its fission yield.
Figure 25. Relevant paths which $^{135}\text{Xe}$ is created and decays in a nuclear reactor.

The operational regime for LEU cermet NTP systems is very different than traditional power or research reactors. Subsequently, the behavior of $^{135}\text{Xe}$ is different in LEU cermet NTP systems compared to traditional reactors. A few examples are listed below that highlight the differences in operational regime of LEU cermet NTP systems compared to traditional reactors:

- LEU cermet NTP systems have extremely high power densities. The high power density is necessary to keep total NTP system mass at a minimum.
- LEU cermet NTP systems operate in a thermal neutron spectrum. A thermal neutron spectrum is used because $^{184}\text{W}$ LEU $\text{UO}_2$ cermet fuel cannot be critical in a fast spectrum with currently attainable oxide loadings.
- Optimal operation of NTP systems for a Mars mission requires restarting the reactor 4 to 8 hour after full power operation. The 4 to 8 hour pause is included in the mission plan to optimize orbital dynamics.
LEU cermet NTP systems never operate with $^{135}\text{Xe}$ in steady state as orbital dynamics require NTP reactor operation in segments of approximately 30 minutes or less.

Furthermore, $^{135}\text{Xe}$ impacts the performance of a LEU cermet NTP differently than a traditional reactor. Below is a preliminary list of ways that $^{135}\text{Xe}$ impacts NTP performance that drove the initial investigation into $^{135}\text{Xe}$ in LEU cermet NTP systems. The effects of $^{135}\text{Xe}$ on LEU cermet NTP systems will be explained in more detail after the results of $^{135}\text{Xe}$ modeling are presented.

- Use of rotating control drums to compensate for reactivity loss caused by $^{135}\text{Xe}$ lowers the maximum $I_{sp}$ of the NTP system. Rotating the control drums lowers the maximum $I_{sp}$ because of changes to the radial power profile relative to the power profile that the system was orificed to. This phenomena is explained in more detail and quantified in later sections.
- The 4 to 8 hour pause in operation could result in $^{135}\text{Xe}$ building up enough negative reactivity such that the reactor could not be restarted.
- $^{135}\text{Xe}$ causes reactivity to change quickly over the course of a burn and understanding the rate that reactivity changes will help drive control system design.
- In general, NTP systems are high performance systems with minimal design margin and understanding the reactivity changes in the system is essential for
maximizing performance, while ensuring that the reactor does not operate outside of boundaries.

Understanding and being able to model $^{135}$Xe is important in this early stage of development for LEU cermet NTP systems. An early understanding of the role of $^{135}$Xe in LEU cermet NTP systems can help drive the design as the technology matures. In addition, $^{135}$Xe and its effects on performance may drive mission planning.

As mentioned previously, SCCTE and TRIBLE are initial point designs that were created, in part, for foundational research into LEU cermet NTP systems. For the purposes of modeling $^{135}$Xe, SCCTE and TRIBLE give the best available estimate of the neutron spectrums and power densities for LEU cermet NTP systems. Because of the representative LEU cermet NTP neutronic environments provided by SCCTE and TRIBLE, it is likely the trends and conclusions derived in this work can be applied to future LEU cermet NTP systems.

Modeling the evolution of $^{135}$Xe and its impact on reactivity in LEU cermet NTP systems was accomplished with the Monte Carlo reactors physics codes MCNP6.1.1 Beta [50] and Serpent 2.1.26[51] (hereafter referred to as “MCNP” and “Serpent”). Both of these codes have integrated burnup functionality and are well suited to model the evolution of $^{135}$Xe. Comparison and background of MCNP and Serpent is presented in section 3.2. “Infinite Lattice Studies”
3.1. A Human Mars Mission and the Operational Regime for NTP systems

It is necessary to understand the operational regime of NTP systems to model $^{135}$Xe. There are many ways for NTP systems to be utilized in a human Mars mission, but all possible operational regimes for the NTP systems are very different than most terrestrial reactors. NASA’s current baseline NTP human Mars mission calls for the NTP reactor to operate for less than 2 hours in 4 engine burns. “Engine burn” refers to nominal full power reactor operation. After less than 2 hours of operation, the reactor is disposed of in a nuclear safe orbit.

NASA’s current baseline NTP human Mars mission is derived from the Design Reference Architecture 5.0 (DRA 5.0) human Mars mission [46]. This human Mars mission is a conjunction class mission with a human crew of 6 and a total duration of 2 to 3 years. “Conjunction” here refers to when a spacecraft leaves Earth or Mars with Earth and Mars far apart. With Earth and Mars far apart, relatively low energy orbital transfers are possible between the planets. Figure 26 shows the path of the spacecraft during a conjunction class mission.
Figure 26. The path of the spacecraft during a conjunction class mission. This image is reprinted from [52].

A much shorter Mars missions, with a total mission duration as short as 400 days, is possible with an opposition class mission. “Opposition” here refers to when a spacecraft leaves Earth or Mars when the other planets are close together. Opposition class missions allow for a short mission duration, but require more energy to accomplish. Opposition class missions may also use a gravity assist from Venus. Figure 27 shows the path of the spacecraft during an opposition class mission with a gravity assist from Venus on the return to Earth.
Figure 27. The path of the spacecraft during a opposition class mission with a gravity assist from Venus on the return to Earth. This image is reprinted from [52].

Opposition class mission are not currently the focus of NASA’s Mars exploration goals. A central reason opposition class missions are not favored in comparison to conjunction class missions is the limited surface exploration time offered by opposition class Mars missions [46]. An opposition class mission allows for approximately 10 to 100 days of Martian surface exploration compared to approximately 400 to 600 days offered by a conjunction class mission. The science return is expected to be much larger for conjunction class missions. More so, as stated in the NASA DRA 5.0, the technology
development required for a 400 to 600 day mission will be “more supportive of the eventual longer term missions that would achieve sustained human presence.” [46].

The short total mission duration made possible by an opposition class mission is appealing for purposes of mitigating the dangers of deeps space such as radiation, the weakening of the human body in zero gravity, and psychological isolation of the crew. However, the short total mission duration made possible by an opposition mission would not be capable of completely mitigating the human health issues of deep space [52].

Conjunction class missions are the focus of this $^{135}$Xe modeling work as they are more relevant to NASA’s research agenda and are better documented. In addition, an opposition class mission would operate a NTP system in a similar manner to a conjunction class mission. An opposition class mission may require longer engine burns or more engine burns, but these would not be fundamentally different than for a Conjunction class mission. Much of this work could be applied to a NTP system in an opposition class mission.

Table 4 outlines NTP reactor operation during a representative conjunction class NASA DRA 5.0 style human Mars mission [46] [53]. The values in Table 4 are for a human Mars mission with 3 35,000 lbf NTP systems, but are representative for other thrust classes. The 200 day transit to Mars is an estimate to which $^{135}$Xe modeling is not sensitive. For a conjunction class human Mars mission with NTP systems with similar performance to SCCTE or TRIBLE, a transit to Mars can be expected to take between approximately 90 days to 250 days [50].
Table 4. A Representative Conjunction Class human Mars NTP mission outline. Information from [53].

<table>
<thead>
<tr>
<th>Part of the Mission</th>
<th>Reactor State</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trans Martian Injection 1 (TMI 1)</td>
<td>Full Power</td>
<td>25 Minutes</td>
</tr>
<tr>
<td>Waiting in an Elliptical Orbit around Earth</td>
<td>Off</td>
<td>5 Hours</td>
</tr>
<tr>
<td>Trans Martian Injection 2 (TMI 2)</td>
<td>Full Power</td>
<td>25 Minutes</td>
</tr>
<tr>
<td>Transit to Mars</td>
<td>Off</td>
<td>200 Days</td>
</tr>
<tr>
<td>Martian Orbital Injection (MOI)</td>
<td>Full Power</td>
<td>12 Minutes</td>
</tr>
<tr>
<td>Surface Operations on Mars</td>
<td>Off</td>
<td>500 Days</td>
</tr>
<tr>
<td>Trans Earth Injection (TEI)</td>
<td>Full Power</td>
<td>9 Minutes</td>
</tr>
<tr>
<td>Transit to Earth and disposal of NTP System</td>
<td>Off</td>
<td>200 Days</td>
</tr>
</tbody>
</table>

A notable feature of the representative conjunction class mission in Table 4 is the 5 hour pause in operation between Trans-Martian Injection 1 (TMI 1) and Trans-Martian Injection 2 (TMI 2). Two engine burns are used for the injection into the Trans-Martian trajectory, because a two engine burn Trans-Martian injection minimizes gravity losses and uses propellant more efficiently. Gravity losses are the losses in rocket performance that occur when a spacecraft accelerates against a gravity field. Gravity losses can be conceptualized of as the penalty for holding a rocket up in a gravity field. A two burn Trans-Martian injection minimizes gravity losses by maximizing the time that a NTP system accelerates tangential to Earth’s gravity field and not against it. Further details on
the orbital mechanics and gravity loss savings of a two burn Trans-Martian injection, can be found at [54].

A two burn Trans-Martian injection is problematic from the standpoint of $^{135}\text{Xe}$ and will be explored in more detail in later sections. The rational from a mission planning perspective, for a two burn Trans-Martian injection with 4 to 8 hours between the first and second burn, is as follows:

- A one burn Trans-Martian Injection burn would have more gravity losses and use propellant more inefficiently.
- Waiting longer between TMI 1 and TMI 2 for $^{135}\text{Xe}$ and $^{135}\text{I}$ to decay away, would require orbiting the Earth multiple times and would result in many more trips through the radiation intensive Van Allen belts. Adding several more passes through the Van Allen belts is undesirable for crew health and may impact the reliability of electronics.
3.2. Infinite Lattice Studies

A series of burnup calculations on an infinite lattice were conducted to determine the approach that would later be taken for the full core burnup calculations. Infinite lattice calculations are much less computationally intensive than full core calculations. The computational affordability of infinite lattice studies made them an effective tool to gain confidence and understanding, before time and computational resources were committed to producing full core calculations. Furthermore, infinite lattice calculations are better suited for isolating reactor physics phenomena than full core calculations, as the input files for infinite lattice calculations are much simpler and neutron leakage is not a factor.

The infinite lattice produced three central findings that later determined the approach of the full core calculations in the next section. These finding were:

1. Serpent predicts reactivity changes that are in agreement with MCNP.
2. Spatial self-shielding in the fuel element does not necessitate burnup cell meshing across the width of the fuel element.
3. $^{135m}$Xe has an appreciable affect on the reactivity of LEU cermet NTP systems.

The first finding (that Serpent and MCNP agree), is important because Serpent has been shown to be a factor of 58 times computationally faster than MCNP [55]. High fidelity full core burnup calculations are computationally intensive even with high
performance computer resources. Furthermore, adding $^{135m}$Xe to the burnup calculation is only possible with Serpent, which was found to be an important part of this work.

Serpent is a modern Monte Carlo reactor analysis and design code that is being developed by a team at the VTT Technical Research Centre of Finland. Serpent is significantly faster than MCNP, because it utilizes a more efficient particle tracking method and because Serpent also uses an internal unionized energy grid for all nuclides which allows for faster look up of cross section data.

The second finding is important, because adding burn cell meshing along the width of individual meshing would significantly increase number of burnup cells needed for a full core burnup calculation. In addition, radial fuel element burnup cell meshing would be very complex to implement for full core burnup calculations with NTP fuel geometry.

The third finding is a unique feature of moderated NTP systems and is the sole topic of chapter 4. In brief, $^{135m}$Xe is a strong neutron poison that can often be neglected in traditional reactors. $^{135m}$Xe may play an important role in NTP systems and it merits further study.

3.2.1. Infinite Lattice Study Approach Methodology

The infinite lattice MCNP and Serpent input files were produced with WORPH (Well Organized Reactor Physics). WORPH is an open source MATLAB code produced by the author for infinite lattice studies for common NTP reactor geometries [56] [57]. WORPH generates inputs for MCNP and Serpent based on a user produced input file and allows for easy modifications of key reactor parameters. The parameters that can be changed
include fuel geometry, fuel type, fuel to moderator ratio, tie tube, geometry, moderator type, and cross section selection.

The core configuration of SCCTE and TRIBLE cannot be exactly represented with a repeating infinite lattice structure, so average representative lattice structures were made for the SCCTE and TRIBLE core. SCCTE has 151 fuel elements and 150 moderator elements, which is approximately a 1:1 ratio of fuel to moderator elements. TRIBLE has 64 fuel elements, and 135 moderator elements, which is approximately a 1:2 ratio of fuel to moderator elements. The representative 1:1 unit cell that is used for SCCTEs infinite lattice calculations is presented in Figure 28 and the representative 1:2 unit cell ratio that is used for TRIBLEs infinite lattice calculations is presented in Figure 29. The unit cells in Figures 28 and 29 have periodic boundary conditions on all sides, including the length of the fuel element (in and out of the paper).

SCCTE and TRIBLE employ axial and radial variable enrichment zoning, so a volumetric average of the full core’s enrichment was used, in the representative unit cell. For the infinite lattice approximation, the average fuel meat power density in the infinite lattice was set equal to the core averaged fuel meat power density in the full core. SCCTE has a core averaged fuel meat power density of 13.4 GW/m$^3$ and TRIBLE has a core averaged fuel meat power density of 15.0 GW/m$^3$. The reactor operation and burn times come from the representative human Mars mission in Table 4. It is assumed that the NTP reactor reaches full power with a step function. This approximates reality, as it is desirable to have a NTP system reach full power very quickly to maximize performance. An approximant core averaged temperature of 1200 K was assumed for the fuel cross
sections and $S(\alpha,\beta)$ data. All tie tube components, including moderator, were given an 300 K cross sections and $S(\alpha,\beta)$ data.

Figure 28. The 1:1 fuel to moderator unit cell used for SCCTE’s infinite lattice calculations.
Figure 29. The 1:2 fuel to moderator unit cell used for TRIBLE’s infinite lattice calculations.

In this chapter, 4 infinite lattice cases were run for both SCCTE and TRIBLE (a total of 8 cases) to examine the effect of using MCNP versus Serpent and the effects of using burnup cell meshing across the fuel element versus no burnup cell meshing across the fuel element.

Producing input files for MCNP versus Serpent comparison was straightforward as WORPH can produce inputs for either code by changing a single parameter in a WORPH input file. In addition, MCNP and Serpent also have similar input files.

The primary goal of the comparison of MCNP versus Serpent was to verify the implementation of both codes and understand any differences that arose in the solution produced by the codes. As will be discussed in the results, MCNP and Serpent handle
some aspects of neutron transport differently and it would be expected that some solutions would differ slightly.

Examining effect of using burnup cell meshing across the width of the fuel element versus no burnup cell meshing across the fuel element was simplified with the use of WORPH. WORPH has the capability of producing burnup cells on a whole fuel element bases or on a channel by channel bases. A SCCTE or TRIBLE fuel element with a whole fuel element burnup cell, will have 1 burn cell; and the same fuel element, with channel by channel bases burnup cell meshing, will have 61 burnup cells. This is depicted in Figure 30, where on the left each hexagon (or pentagon on the periphery) is a different material and burnup cell and on the right all the fuel is the same color and lumped into 1 burn up cell.

![Diagram](image)

**Figure 30.** Cell by cell burnup meshing (Left) versus whole element burnup cell meshing (right).
It is necessary to investigate burnup cell meshing across the width of the fuel elements, because LEU cermet fuel elements have a large amount of spatial self-shielding and more fissions occur on the outside of the fuel element than on the inside on a per uranium atom basis. Because more fissions happen on the outside of the fuel element than on the inside of the fuel element, more $^{135}$Xe is created on the outside of the fuel elements than the inside of the fuel elements. The purpose of this infinite lattice study was to investigate whether or not burnup cell meshing across the width of the fuel elements was necessary to account for the self-shielding and to produce accurate estimations of $^{135}$Xe worth.

LEU cermet fuel has a large amount of spatial self-shielding, because thermal neutrons have a short path length in LEU cermet fuel. Furthermore, the fuel elements are large with a flat-to-flat dimension of about 3 cm compared to a pressurized water reactor fuel pin which is about 1 cm in diameter. The short neutron path length in LEU cermet fuel arises from the fact that the fuel has a high uranium oxide loading (~60% by volume) and the tungsten component of the fuel has a non-negligible cross section, even when tungsten is isotopically purified with a high percentage of $^{184}$W.

The spatial self-shielding was investigated and quantified for SCCTE, before the burnup calculations were run. The results of this investigation were the impetus for examining whether or not spatial self-shielding affected $^{135}$Xe worth calculations. The self-shielding was investigated using MCNP tallies to examine the spatial distribution of neutron flux and fission density in the fuel element. The tally cells match the channel by
channel burn up cells presented in Figure 30. For additional clarity, Figure 31 presents a section of SCCTE’s infinite lattice, with a fuel element with channel by channel tallies.

Figure 31. The SCCTE infinite lattice used to produce the results in Figure 32 and 33.

Figure 32 presents the spatial fission density distribution in the SCCTE fuel element and Figure 33 presents the neutron flux distribution in the SCCTE fuel element. The Figures illustrate that the neutrons that thermalize in the tie tubes do not make it very far into the fuel element and cause the fission density to peak where the fuel element is in contact with the tie tubes. Interestingly, the fast flux peaks where the fuel element is in contact with another fuel element, but the fast flux contributes only a small portion of the fissions.
Figure 32. The spatial fission density distribution in the SCCTE fuel element.

Figure 33. The spatial distribution of different neutron flux energy groups in the SCCTE fuel element.

MCNP and Serpent burnup calculations produce estimations of keff after burnup steps. The keff after each burn up step is converted to a reactivity change with Equation 65.
3. As MCNP and Serpent are Monte Carlo codes, the keff estimations they calculate has an uncertainty. The uncertainty on the change in reactivity can be calculated using Equation 4. Equation 4 is a common equation for propagating uncertainty that assumes the uncertainties in \( keff_1 \) and \( keff_x \) are random and uncorrelated. The simplified solution to Equation 4 is presented in Equation 5.

\[
\Delta \rho = \frac{keff_x - keff_1}{keff_1 \cdot keff_x} \times 10^5
\]  

\[
\sigma \Delta \rho = \sqrt{\left(\frac{\delta \rho}{\delta keff_1}\right)^2 \cdot \sigma keff_1^2 + \left(\frac{\delta \rho}{\delta keff_x}\right)^2 \cdot \sigma keff_x^2}
\]  

\[
\sigma \Delta \rho = \sqrt{\frac{\sigma keff_1^2}{keff_1^4} + \frac{\sigma keff_x^2}{keff_x^4}} \times 10^5
\]

where

\( keff_1 \) = keff at the beginning of the burnup calculation with a clean core at operational temperature.

\( keff_x \) = keff at burnup step x

\( \sigma keff \) = Standard deviation on a keff calculation

\( \Delta \rho \) = Change of reactivity from \( keff_1 \) to \( keff_x \) in units of pcm

\( \sigma \Delta \rho \) = Standard deviation of the change in reactivity from \( keff_1 \) to \( keff_x \) in units of pcm
3.2.2. Infinite Lattice Study Results

Figure 33 presents initial infinite lattice burnup results for SCCTE and TRIBLE so that the underlying physical processes of $^{135}$Xe can be discussed before the comparisons of burnup modeling strategies. A number of phenomena can be seen in Figure 33. During full power operation there are two factors that result in the reduction of reactivity, which consequently requires the rotation of the control drums to maintain a critical reactor: fissile material depletion ($^{235}$U) and fission product production (notably the powerful neutron poison fission products $^{135}$Xe). The combination of these two results in the noticeable reduction in reactivity during the full power burns. The most noticeable feature in Figure 33, however, is the large negative reactivity insertion between TMI1 and TMI2 and the resulting reactivity surge during TMI2. This is caused by the fission product $^{135}$I, which then decays (6.6 hour Half-life) into $^{135}$Xe (9.1 hour Half-life) causing the $^{135}$Xe to buildup and producing the large negative reactivity insertion. Furthermore, the sharp rise in reactivity seen in TMI2 is caused by the rapid burn out of $^{135}$Xe.

It can be seen that TRIBLE loses more reactivity during operation than SCCTE. This is expected as TRIBLE is a more moderated system with a slightly higher power density. The difference between TRIBLE and SCCTE is sharpest at the beginning of TMI 2.
Figure 34. The change in Reactivity in the SCCTE and TRIBLE infinite lattice burn up calculations. These results were produced MCNP burnup with channel by channel burn up cells.

Figure 35 is the change of reactivity for SCCTE infinite lattice as modeled with MCNP and Serpent and with and without channel by channel burnup cells to account for spatial self-shielding effects. In this Figure CBC refers to channel by channel burnup cells. Figure 36 is the difference in the predicted reactivity for the various burnup models compared to MCNP with channel by channel burn up cells. Figures 36 and 37 are the same as Figures 35 and 36, respectively, but for the TRIBLE infinite lattice calculations. Error bars are omitted for clarity purposes but the one sigma uncertainty on any Serpent point in Figures 35 or 37 is approximately 6 to 7 pcm and the one sigma uncertainty on any MCNP point is 11 to 13 pcm.
Figure 35. Reactivity change in the SCCTE infinite lattice calculation with different burnup models.

Figure 36. The difference in the reactivity change in the SCCTE infinite lattice calculation with different burnup models.
Figure 37. Reactivity change in the TRIBLE infinite lattice calculation with different burnup models.

Figure 38. The difference in the reactivity change in the TRIBLE infinite lattice calculation with different burnup models.
Figures 35 through 38 show that all the burnup models produced very close results. There is some disagreement at the beginning of TMI 2, but the fractional difference between the burnup models at TMI 2 is very small. Furthermore, as will be discussed in later sections, it is likely impossible to operate a NTP reactor at the start of TMI 2, so modeling reactivity at that point is less important. With these results, it can be concluded that Serpent, with whole fuel element burnup cell meshing, is sufficient to predict reactivity changes for the full core calculations for the purposes of this work.

It should be noted that the data points with whole burnup cell meshing in Figure 36 and 38 are more than 2 sigma different from the channel by channel burn cell meshing at the beginning of TMI 2. This trend is expected as spatial self-shielding with channel by channel meshing should result in a larger reactivity loss than modeling the fuel element as a whole with one burn cell. Although, as can be seen in Figure 35 and 37, the fractional impact of accounting for spatial self-shielding is negligible.

The initial keff values predicted by MCNP and Serpent were also in close agreement with a small expected difference. Serpent predicted an initial keff about 100 pcm lower than MCNP. The likely reason for the difference between the codes is that the Serpent has the option to employ “Doppler-Broadening Rejection Correction” which handles resonance scattering in heavy nuclei more accurately than MCNP and usually produces a lower prediction of keff [51]. The Doppler-Broadening Rejection Correction option was used in the Serpent input files, as the correction did not greatly affect the prediction of the reactivity changes and the use of the correction better represents reality. Tables 5 and 6 have the initial keffs for SCCTE and TRIBLE, respectively.
Table 5. Initial keffs for SCCTE.

<table>
<thead>
<tr>
<th>Case</th>
<th>Keff</th>
<th>1 sigma uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>SCCTE MCNP CBC</td>
<td>1.1600</td>
<td>1e-4</td>
</tr>
<tr>
<td>SCCTE MCNP Whole</td>
<td>1.1600</td>
<td>1e-4</td>
</tr>
<tr>
<td>SCCTE Serpent CBC</td>
<td>1.15896</td>
<td>7e-05</td>
</tr>
<tr>
<td>SCCTE MCNP Whole</td>
<td>1.15891</td>
<td>8e-05</td>
</tr>
</tbody>
</table>

Table 6. Initial keffs for TRIBLE.

<table>
<thead>
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<th>Case</th>
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<th>1 sigma uncertainty</th>
</tr>
</thead>
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<td>2e-04</td>
</tr>
<tr>
<td>TRIBLE MCNP Whole</td>
<td>1.2994</td>
<td>2e-04</td>
</tr>
<tr>
<td>TRIBLE Serpent CBC</td>
<td>1.29845</td>
<td>8e-05</td>
</tr>
<tr>
<td>TRIBLE MCNP Whole</td>
<td>1.29837</td>
<td>7e-05</td>
</tr>
</tbody>
</table>

3.3. Full Core Burnup Calculation

Based on the findings of the infinite lattice study, the full core burnup calculations were undertaken with Serpent and without burnup cell meshing across the fuel element. This approach saved enormous amounts of computational time and greatly simplified the processing of the results.

As, will be discussed in Chapter 4, $^{135m}$Xe was not included in these full burnup as its inclusion in burnup calculations is largely unpredicted the best estimate of its cross section is computability based. It should be noted though adding $^{135m}$Xe is only possible with Serpent.

The full core calculations assumed that the control drums were at a 60 degree angle (with 0 being all out for maximum reactivity). Temperature corrected cross sections that were based on temperatures during normal operation were used. The total core power for
both SCCTE and TRIBLE come from their thermal hydraulic calculations, which are discussed in Chapter 2. The burnup cells in SCCTE and TRIBLE were split into 10 axial divisions and into the radial divisions shown in Figure 39.

![Figure 39. The radial burn up cells in the SCCTE (right) and TRIBLE (Left). Each color represents fuel elements lumped into a burn volume. Gray is tie tube. Not to Scale.](image)

3.3.3. Full core Burnup Results and Discussion

Figure 40 presents the results of the full core burnup calculation for the SCCTE and TRIBLE reactors. Figure 40 is very similar to infinite lattice burnup calculations in Figure 34, but with a larger magnitude of reactivity changes. This is expected, as infinite lattice calculations often have a harder spectrum than full core calculations, and therefore underestimate the impact of neutron absorbers on reactivity. In addition, infinite lattice calculations do not capture the effects of power peaking in the core, which causes $^{135}$Xe to have more of an impact on reactivity. In a full core, fuel elements exposed to a higher
flux will produce more $^{135}$Xe, and, subsequently, $^{135}$Xe in places of higher flux in the core will have a larger impact on reactivity.

Figure 40. Reactivity change in the SCCTE and TRIBLE full core calculations.

Figure 41 presents the reactivity change in the SCCTE and TRIBLE, if the reactor were to wait after first burn (TMI 1) for the $^{135}$Xe to decay away. It can be seen that negative reactivity peaks at about 10 hours and asymptotes to zero after about 80 hours. This is similar to traditional reactors. Waiting 80 hours for the $^{135}$Xe to decay away would result in several more trips through the radiation intense Van Allen belt.
3.4. The Impact of $^{135}$Xe on LEU cermet NTP systems

The changes in reactivity presented in Figure 40 will degrade the performance of the NTP system and make the system difficult to control, if mitigation strategies are not implemented. The central issue is not keeping the core critical, as the current control drum design has more than enough reactivity swing to make up for any change in reactivity seen in Figure 40. The issue instead is maintaining the performance and controllability of the NTP system. Here, performance refers to thrust and $I_{sp}$ and controllability refers to ensuring the NTP system is within operating boundaries, such as maximum allowable fuel temperature.
In existing NTP designs, the reactivity changes noted in Figure 40 are resolved by rotating the radial control drums. This, however, introduces a number of issues. First of all there is a loss of $I_{sp}$ associated with circumferential control drum movement from their as designed nominal position. The $I_{sp}$ loss stems from the need for each coolant channel in a NTP reactor to be orificed to the power deposited in that channel in order to achieve the desired coolant exit temperature. Not orificing each channel would result in a significant decrease in performance, as there is a power gradient across the fuel elements.

When the circumferential control drums rotate, the radial power deposition changes rendering the channel orificing ineffective because the orificing no longer aligns with the radial power deposition. The change in radial power deposition results in some channels receiving more power than the orificed flow can take away. The as designed nominal position of the control drums is referred to as the “orifice angle”, as it is the control drum angle, and resultant spatial power distribution, that was used to determine the orificing for each channel.

To prevent the fuel temperature from rising above the maximum allowable fuel temperature, in the channels that receive more power when the radial power deposition changes, the total power reactor power must be lowered or the total core mass flow rate of $H_2$ must be increased.

Any combination of lowering core power or core mass flow will reduce performance of the NTP system and result in a combination of lower thrust or $I_{sp}$. In order to simplify mission planning and reactor control, the likely mitigation is to attempt to keep reactor power constant and alter the mass flow rate to the core. This mitigation strategy keeps
thrust constant, but lowers the $I_{sp}$ of the NTP system. The next section further explains and mathematically quantifies the $I_{sp}$ loss associated with control drum rotation.

Not turning the control drums would degrade performance and complicate control of the reactor. All major components of the LEU cermet NTP system have a negative temperature feed coefficient of reactivity, so it can be inferred that the NTP reactor would become critical at a lower temperature. A detailed examination of scenarios where the control drums were not turned to account for reactivity losses is a complex problem that is a part of future work. This problem is complex due to the multiple interconnected systems in a LEU cermet NTP system that impact reactivity, such as the turbopump, tie tubes, and the fuel elements. An integrated reactor systems simulation code will be required to examine transient NTP core behavior.

Beyond losing $I_{sp}$, actively turning control drums during operation is complicated. A nested closed loop control system, with control drums and rocket power cycle, would likely be enormously complex. The NTP system is a high performance reactor with minimal design margin and a small mistake in turning could put the reactor outside of its operating parameters. Furthermore, actively turning control drums introduces a failure mechanism since control drums may get stuck or over insert reactivity. Because of the difficulties of controlling NTP systems, it is important to understand how $^{135}$Xe affects reactivity and identify mitigation strategies.

Controlling an NTP system with the rapid burn out of $^{135}$Xe in TMI 2 is extremely difficult. TMI 2 is 25 minutes long and SCCTE has a reactivity insertion of about 1400 pcm and TRIBLE has a reactivity insertion of about 2000 pcm. To operate a NTP system
in this regime, there will need to be extensive development of control systems or mitigation strategies will need to be implemented.

Figures 42 through 47 display the power per element normalized by dividing by the power per element at the orifice angle. These figures show how the normalized power per element profile changes when the control drum turn in and out from the orifice angle. The orifice angle for these graphs is 90 degree meaning the control drum is halfway out. Figures 42 and 45 are for SCCTE and TRIBLE, respectively, with the control drums at the 90 degree orifice angle. It can be seen that every fuel element has the same normalized power per element because this is the radial power distribution that the orificing was designed to. As the control drums rotate out, letting more neutrons be reflected back into the core, as shown in Figures 43 and 46, the fuel elements on the periphery get a larger fraction of the power than they received at the orifice angle. As the control drums rotate in, letting less neutrons be reflected back into the core, as shown on in Figures 44 and 47, the fuel elements on the periphery get a smaller fraction of the power than they received at the orifice angle. An assumption, in Figures 42 through 47, is that the core remains at the same total power.

This analysis only quantifies the change in power profile from moving the control drums. The effects of burnup and $^{135}$Xe on the power profile are expected to be small and were not included in this analysis.
Figure 42. Power distribution in SCCTE with control drums at 90 degrees.

Figure 43. Power distribution in SCCTE with control drums at 30 degrees.
Figure 44. Power distribution in SCCTE with control drums at 150 degrees.

Figure 45. Power distribution in TRIBLE with control drums at 90 degrees.
Figure 46. Power distribution in TRIBLE with control drums at 30 degrees.

Figure 47. Power distribution in TRIBLE with control drums at 150 degrees.
3.4.4. Quantifying $I_{sp}$ Loss

A preliminary estimation of the loss of $I_{sp}$ as a function of control drum angle was formulated using neutronic power deposition calculations (using codes such as MCNP) and a number of simplifying assumptions. Solving for the $I_{sp}$ as a function of control drum angle explicitly with the 1-D thermal solver in SPOC would be enormously complex and would require many iterations over 9000 fuel channels. With a number of simplifying assumptions, the $I_{sp}$ loss associated with control drum movement away from the orifice angle can be estimated with much easier implementation and much less computation.

This estimate is preliminary and likely underestimates the $I_{sp}$ loss. Furthermore, it does not consider if the turbopump is capable of driving the required increases in flow or if the flow chokes in the fuel channel.

The following assumptions were used to estimate $I_{sp}$ as a function of control drum angle:

1. Thrust is kept constant and flow rate is increased to compensate for a lower $I_{sp}$. This may be the desired mode of operation of a NTP system, as maintaining a constant thrust level can simplify orbital maneuvers.

2. Each channel is orificed based on the power deposited in that fuel channel to maximize performance. The orificing is conducted in a manner so that the fuel in every channel achieves the maximum allowable fuel temperature somewhere along its axial length.

3. The temperature of the hydrogen, as it leaves the fuel, is directly proportional to the energy the hydrogen received from the fuel, while it was in the fuel element. This assumption is not entirely accurate, as it requires hydrogen to have a constant
specific heat. Hydrogen does not have a constant specific heat but for a preliminary estimate, it can be treated as such.

4. $I_{sp}$ is a linear function of temperature of the hydrogen leaving the reactor. This is a good assumption in the regime of operation and can be seen by reexamining Figure 5 in Chapter 1.

5. Power and flow rate in a fuel channel must be increased by the same fraction or the temperature difference, between the bulk hydrogen and fuel max (centerline) will rise. This can be accomplished with a heat transfer coefficient, between the fuel and bulk hydrogen, that is a linear function of flow rate. This assumption underestimates the loss of $I_{sp}$, as the heat transfer coefficient is sub-linear as a function of flow rate in a channel. The Nusselt number for hydrogen in a channel is a function of Reynolds number to the power of 0.8. This assumption also underestimates the loss of $I_{sp}$, because it does not consider the conductive heat transfer which will require a larger temperature difference to drive as power increases. Although, the conductive heat transfer temperature difference is small in LEU cermet NTP systems.

6. The shape of the power gradients across the fuel elements does not change as a function of control drum angle. This assumption will slightly underestimate the loss of $I_{sp}$, but it is not expected that the flux shape would change sharply over the volume of a fuel elements with rotation of the control drums.

With these assumptions, it can be concluded that power during operation stays constant regardless of the control drum angle and that $I_{sp}$ is linearly proportional to only
mass flow rate of hydrogen in the reactor. The logic of this is explained with Equations 6 - 10.

Equations 6 is simply assumption 4 restated, where \( I_{sp} \) is directly proportional to the temperature of the hydrogen leaving the reactor. Equations 7 restates assumption 5 (that the power of the reactor divided by the mass flow rate is proportional to the temperature of the hydrogen leaving the fuel). Equations 8 is the definition of \( I_{sp} \) stated as a proportionality. Equation 9 combines Equations 6 and Equations 8.

\[
T_{out}(\theta) \propto I_{sp}(\theta) \quad (6)
\]

\[
\frac{P}{F_{core}(\theta)} \propto T_{out}(\theta) \quad (7)
\]

\[
I_{sp}(\theta) * F_{core}(\theta) \propto Th \quad (8)
\]

\[
T_{out}(\theta) * F_{core}(\theta) \propto Th \quad (9)
\]

where

\( \theta \) = Control drum angle

\( T_{out} \) = Temperature of the hydrogen leaving the reactor

\( P \) = Power of the NTP systems reactor

\( F_{core} \) = Flow rate in the NTP system’s core

\( I_{sp} \) = Specific impulse

\( Th \) = Thrust of the NTP system
Given Equations 7 and 9, it can be shown that power and thrust are directly proportional to each other given the assumptions. Equation 10 demonstrates this logic by combining Equations 7 and 9.

\[
\frac{P}{F_{core}(\theta)} \cdot F_{core}(\theta) \propto Th \rightarrow P \propto Th \tag{10}
\]

As it is assumed that thrust is held constant (assumption 1), it can be concluded that power will also be held constant during normal operation. With power being held constant, the power term in Equation 7 can be set to 1, corresponding to 100% full power, to give Equation 11. Equation 11 shows that given the assumptions \( I_{sp} \) is inversely proportional to the flow rate of hydrogen in the reactor.

\[
\frac{1}{F_{core}(\theta)} \propto I_{sp}(\theta) \tag{11}
\]

As stated before, turning the control drums lowers \( I_{sp} \), because flow must be increased to ensure that no fuel element violates its maximum allowable temperature. Given assumption 5 and assumption 3, an increase of power in a fuel element over its orifice angle power requires a proportional increase in flow or the temperature of the maximum fuel element will rise. The relationship between changing power in an individual fuel element and the minimum flow required not to violate the maximum temperature in the fuel element is given by Equation 12.

\[
F_i(\theta) = \frac{P_i(\theta)}{P_i(\theta_o)} \cdot F_i(\theta_o) \tag{12}
\]

where

\( F_i \)=Flow rate in fuel element i
\( P_i \) = Power of fuel element i calculated with MCNP or Serpent.

\( \theta_o \) = Angle of the control drums.

\( \theta_o \) = The orifice angle of the control drums (Assumed to be 90 degrees here).

The \( \frac{P_i(\theta)}{P_i(\theta_o)} \) was produced with MCNP or Serpent and is what is presented in Figures 42 through 47.

Because the orificing is static, flow must be increased to the entire NTP core, when flow is increased to a single fuel element. A mechanism to increase the flow to a single fuel element during NTP operation would require complicated active valving. Because flow cannot be adjusted to a single fuel element, the flow rate to the entire core is determined by the maximum ratio of \( \frac{P_i(\theta)}{P_i(\theta_o)} \) for all of the fuel elements in the NTP systems core. This is shown in Equation 13.

\[
F_{core}(\theta) = \text{Max}_i \left( \frac{P_i(\theta)}{P_i(\theta_o)} \right) \ast F_{core}(\theta_o) \tag{13}
\]

where

\( \text{Max}_i() \) = A function that finds the maximum ratio of \( \frac{P_i(\theta)}{P_i(\theta_o)} \) for all fuel elements in a core.

Equation 11 and Equation 13 can be combined to form the relationship for the \( I_{sp} \) at a control drum angle that is written in Equation 14. Simple algebraic manipulation leads to the estimation of \( I_{sp} \) that is written in Equation 15.

\[
I_{sp}(\theta) = I_{sp}(\theta_o) \ast \left( \text{Max} \left( \frac{P_i(\theta)}{P_i(\theta_o)} \right) \right)^{-1} \tag{14}
\]
\[ \Delta I_{sp}(\theta) = I_{sp}(\theta_o) - I_{sp}(\theta) \ast \left( \text{Max} \left( \frac{P_t(\theta)}{P_t(\theta_o)} \right) \right)^{-1} \]  

(15)

where

\[ \Delta I_{sp}(\theta) = \text{loss of } I_{sp} \text{ as a function of } \theta \]

Figure 48 uses Equation 15 and multiple MCNP runs to quantify the \( I_{sp} \) loss for SCCTE and TRIBLE assuming an orifice angle of 90 degrees (control drums half way out).

Figure 48. Control drum angle verse \( I_{sp} \) loss in SCCTE and TRIBLE.
A relationship between control drum reactivity insertion and $I_{sp}$ loss can be made with a reactivity worth curve of the control drums. Figure 49 is the reactivity worth curve of the control drums in SCCTE and TRIBLE. Figure 50 combines Figures 48 and 49 to make curves of control drum reactivity insertion versus $I_{sp}$ loss.

Figure 49. Control drum worth curve for SCCTE and TRIBLE.
3.5. $^{135}$Xe in other NTP systems

$^{135}$Xe is not a unique issue to LEU cermet NTP systems. Any moderated NTP system with a similar core geometry would be similarly impacted by $^{135}$Xe. The findings and approaches in this work can be applied to a number of other NTP concepts.

The original NERVA era reactors had an appreciable amount reactivity loss to $^{135}$Xe [56] but $^{135}$Xe’s impact on the reactor was not well quantified. Recent research has identified $^{135}$Xe as impacting the performance of NERVA style HEU graphite composite fueled NTP systems [57]. Other recent research, supported by the author, conducted a similar analysis to this work on LEU graphite composite fueled NTP systems [58]. This work on LEU graphite composite fueled NTP systems found the
impact of $^{135}$Xe to be larger in LEU graphite composite fueled NTP systems than in LEU cermet NTP systems.
Chapter 4: The Metastable State of $^{135}\text{Xe}$

LEU cermet NTP systems operate in a regime where the metastable state of $^{135}\text{Xe}$ ($^{135m}\text{Xe}$) may have a notable impact on reactivity. This chapter gives background on $^{135m}\text{Xe}$, explains how $^{135m}\text{Xe}$ was included in the burn up calculations for SCCTE and TRIBLE and presents the results of including $^{135m}\text{Xe}$ in burn up calculations for SCCTE and TRIBLE.

Typical reactor burnup calculations exert significant effort to take into account the effects of $^{135}\text{Xe}$, one the biggest and most important contributors to reactivity loss during reactor operation in thermal reactors. However, despite the importance of $^{135}\text{Xe}$ in these calculations, typically only the ground state is considered and given credit during burnup. In addition to the ground state, there exists the metastable state of $^{135}\text{Xe}$. $^{135m}\text{Xe}$ is given a 0 barn cross section by default in many burn up calculations. However, recent nuclear data models in the TENDL nuclear data library indicate $^{135m}\text{Xe}$ has a (n, $\gamma$) cross section that is approximately 4 times larger than $^{135}\text{Xe}$ at thermal energies [59].

The effect of $^{135m}\text{Xe}$ on reactor operation has only recently been broached as a topic of research. For most reactors, $^{135m}\text{Xe}$ has little effect on steady state xenon worth even with $^{135m}\text{Xe}$’s larger cross section. This work has identified LEU cermet NTP reactors as one of the unique reactors for which $^{135m}\text{Xe}$ can have a notable effect on reactivity.
This work highlights the need for basic nuclear data experiments for $^{135m}$Xe. No experimental cross section measurements exist for $^{135m}$Xe. The cross sections produced with physics models for $^{135m}$Xe in the TENDL libraries are an indication that $^{135m}$Xe may have an impact on the operation of NTP systems. To have greater confidence in modeling NTP systems, experimentally produced cross sections for $^{135m}$Xe are needed.

4.1. Nuclear data for $^{135m}$Xe

No validated cross sections exist for $^{135m}$Xe, so the $^{135m}$Xe cross section in the TENDL nuclear data libraries was used. The TENDL nuclear data libraries are made through the use of the TALYS nuclear model code system which is known for its ability to build cross-section libraries entirely with nuclear models that are then enhanced with experimental data. This allows the production of nuclear cross section data of important nuclides for which there is limited experimental data, such as $^{135m}$Xe. The TENDL nuclear data library currently provides the best available estimation for $^{135m}$Xe’s cross section.

The relevant paths by which $^{135m}$Xe is generated and decays in a $^{235}$U system are presented in Figure 51, along with the thermal (n, $\gamma$) cross-sections. All data in Figure 51 is from the ENDF/B-VII.1 nuclear library, except for the (n, $\gamma$) cross-section for $^{135m}$Xe, which comes from TENDL-2015 nuclear library. The fission yields of precursors to $^{135}$I are lumped into the fission yield of $^{135}$I.
The $^{135\text{m}}\text{Xe}$ (n, $\gamma$) cross section has varied over the various releases of the TENDL nuclear data libraries. Figure 52 compares TENDL $^{135\text{m}}\text{Xe}$ (n, $\gamma$) from 2009 to 2015 against the ENDF/B-VII.1 $^{135}\text{Xe}$ (n, $\gamma$). With the exception of TENDL-2012, the $^{135\text{m}}\text{Xe}$ (n, $\gamma$) is larger than the $^{135}\text{Xe}$ (n, $\gamma$) cross section for all years of the TENDL nuclear data libraries.
Figure 52. TENDL $^{135m}$Xe (n, $\gamma$) (called z, y in the title) from 2009 to 2015 compared against ENDF/B-VII.1 $^{135}$Xe (n, $\gamma$). Note: TENDL-2015, TENDL-2014 TENDL-2013 are almost completely the same except in the resonance region.

4.2. Why $^{135m}$Xe has a notable effect in LEU cermet NTP systems

The reactivity of LEU cermet NTP systems is impacted by $^{135m}$Xe because LEU cermet NTP systems operate in a unique regime where prompt xenon ($^{135m}$Xe and $^{135}$Xe directly from fission) makes up a substantial amount of negative reactivity. The ratio of $^{135m}$Xe to $^{135}$Xe is much higher for prompt xenon than for xenon that accumulates from...
the decay of $^{135}$I. It can be seen in Figure 51 that $^{135m}$Xe, makes up the majority of prompt xenon, but a small portion of the total xenon, which is dominated by the decay of $^{135}$I.

LEU cermet NTP have a significant prompt xenon worth, because LEU cermet NTP systems have extremely high power densities, with a thermal neutron spectrum, and operate on the order of the half-life of $^{135m}$Xe (15.3 minutes). Furthermore, NTP systems operate with a rapid start up to full power to maximize propellant usage efficiency. The rapid startup, on the order of tens of seconds, prevents xenon building up from the decay of $^{135}$I. Startup of a traditional power reactor may take hours and would allow $^{135}$I build up and decay, thus diluting the ratio of $^{135m}$Xe to $^{135}$Xe.

High power density, fast start up and operation on the order of 15 minutes are needed for $^{135m}$Xe to have a notable impact on reactivity. The reactivity of a traditional reactor operating at steady state is not impacted notably by $^{135m}$Xe, because the ratio of $^{135m}$Xe to $^{135}$Xe is much lower. At steady state operation of a traditional reactor, most of the xenon in the core comes from the decay of $^{135}$I, which mostly decays to $^{135}$Xe. Furthermore, in a traditional reactor operating in steady state, $^{135m}$Xe cannot accumulate, because the half-life of $^{135m}$Xe is shorter than the half-life of $^{135}$Xe by factor of approximately 36.

4.2.1. Explanation of $^{135m}$Xe with a 0-D Model

A simplified 0-D model was created to better understand and explain the effect of $^{135m}$Xe in thermal spectrum nuclear reactors. This will aid in understanding the Serpent burnup results with $^{135m}$Xe presented in later sections. The governing differential equations for the 0-D model, with one neutron energy group, are presented in Equations 16-18. These equations describe the evolution of $^{135}$I, $^{135}$Xe and $^{135m}$Xe in the 0-D model.
Analytical solutions for the time dependent concentrations of $^{135}$I, $^{135}$Xe and $^{135m}$Xe can be readily produced with commercial computer algebra system software. The time dependent analytical solution is omitted for readability purposes as it is quite lengthy.

A number of assumptions were made to simplify the solution. The 0.03% decay branch from $^{135m}$Xe directly to $^{135}$Cs is ignored, and $^{135m}$Xe is assumed to decay entirely to $^{135}$Xe. Similarly, the independent fission yields (fission yield directly from a fission) of precursors to $^{135}$I are lumped into the independent fission yield for $^{135}$I. Neutron absorption in Iodine was ignored as $^{135}$I has a neutron absorption cross section several orders of magnitude smaller than $^{135}$Xe. An initial condition of zero concentrations of $^{135}$I, $^{135}$Xe, and $^{135m}$Xe is assumed.

$$b_{Xe} l(t) \lambda_I + \phi \Sigma_f \gamma_{Xe} - \phi Xe(t) \sigma_{a,Xe} - Xe(t) \lambda_{Xe} + Xem(t) \lambda_{Xem} = \frac{\partial Xe}{\partial t} \tag{16}$$

$$b_{Xem} l(t) \lambda_I + \phi \Sigma_f \gamma_{Xem} - \phi Xem(t) \sigma_{a,Xem} - Xem(t) \lambda_{Xem} = \frac{\partial Xem}{\partial t} \tag{17}$$

$$\phi \Sigma_f \gamma_I - I(t) \lambda_I = \frac{\partial I}{\partial t} \tag{18}$$

where

$I$ Concentration of $^{135}$I

$Xe$ Concentration of $^{135}$Xe

$Xem$ Concentration of $^{135m}$Xe

$b_{Xe}$ Decay branching ratio $^{135}$I $\rightarrow$ $^{135}$Xe

$b_{Xem}$ Decay branching ratio $^{135}$I $\rightarrow$ $^{135m}$Xe

$\gamma_I$ Lumped independent fission yield of $^{135}$I

$\gamma_{Xe}$ Independent fission yield of $^{135}$Xe
\( \gamma_{Xe} \) Independent fission yield of \(^{135m}\text{Xe} \)

\( \lambda_I \) Decay Constant of \(^{135}\text{I} \)

\( \lambda_{Xe} \) Decay Constant of \(^{135}\text{Xe} \)

\( \gamma_{Xe} \) Decay Constant of \(^{135m}\text{Xe} \)

\( \sigma_{a,Xe} \) Microscopic cross-Section of \(^{135}\text{Xe} \)

\( \sigma_{a,Xem} \) Microscopic cross-Section of \(^{135m}\text{Xe} \)

\( \phi \) One group thermal flux

\( \Sigma_f \) Macroscopic fission cross-section of fuel

For a reactor operating near critical that has a negligible amount of neutron leakage, the total amount of negative reactivity caused by the addition of a poison is given by \([60]\). This is a useful model for this preliminary work as the fuel’s macroscopic cross section cancels out in the final solution. Equation 19 is based on work in \([60]\) and shows the reactivity change (\( \Delta \rho \)) for thermal spectrum reactors, as a function of total inventory of \(^{135}\text{Xe} \) and \(^{135m}\text{Xe} \) in the core.

\[
\frac{Xe \sigma_{a,Xe} + Xem \sigma_{a,Xem}}{\Sigma_f \nu} = \Delta \rho
\]  

(19)

where

\( \Delta \rho \) Xenon Worth

\( \nu \) Neutrons per fission
Values of parameters for the sample case are presented in Table 7. The one group cross sections for $^{135}\text{Xe}$ and $^{135m}\text{Xe}$ were set equal to the 2200 m/s cross sections and ideal $1/v$ absorption is assumed. The thermal cross section for $^{135m}\text{Xe}$ was taken from the TENDL-2015 nuclear data library. All other nuclear data comes from the ENDF/B-VII.1 nuclear data library.

<table>
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<th>Parameter</th>
<th>Value</th>
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<tbody>
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<td>$\lambda_l$</td>
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<tr>
<td>$\lambda_{Xe}$</td>
<td>2.107e-5 s$^{-1}$</td>
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<tr>
<td>$\lambda_{Xem}$</td>
<td>7.557e-4 s$^{-1}$</td>
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<td>$\gamma_l$</td>
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<td>$\gamma_{Xem}$</td>
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The results of the simplified 0-D model are presented in Figures 53 through 56. These figures compare the xenon worth with and without $^{135m}\text{Xe}$ in the model. In the without $^{135m}\text{Xe}$ case, the cross section of $^{135m}\text{Xe}$ is set to zero. Figures 53 and 54 are on a linear time scale, over an hour of operation, to show the reactivity over a time scale similar to a NTP burn. Figures 55 and 56 are on a logarithmic time scale over 30 days of operation which is more representative of the time scale for the operation of a traditional power reactor.
Figure 53. The absolute difference in xenon worth with and without $^{135m}$Xe for different flux levels.

Figure 54. The ratio of xenon worth with and without $^{135m}$Xe for different flux levels.
Figure 55. The absolute difference in xenon worth with and without $^{135m}$Xe for different flux levels on a log time scale.

Figure 56. The ratio of xenon worth with and without $^{135m}$Xe for different flux levels on a log time scale.
LEU cermet NTP systems operate with a thermal flux in the $10^{14}$ to $10^{15}$ (n/cm$^2$s) range for a maximum time span of 25 minutes (1500 s) in the representative mission. Examining Figures 53 through 56, it can be seen that much of the operation of a LEU cermet NTP falls in a regime where $^{135m}$Xe has a noticeable absolute impact and fractional impact on reactivity.

Traditional light water reactors that are used for power generation have a thermal flux in the $10^{13}$ to $10^{14}$ (n/cm$^2$s) range and have much longer periods of operation than NTP systems. Figures 53 through 56 demonstrate that much of the operation of traditional light water reactors falls in a regime where $^{135m}$Xe has a very small fractional impact on xenon worth and a small impact on the absolute xenon worth. Furthermore, traditional light water reactors change power very slowly. The step increase in power, assumed in this model, while representative of a NTP system, overstates the impact of $^{135m}$Xe early in the operation of traditional light water reactors.

4.3. Other research into the effects of $^{135m}$Xe on reactor operations.

The potential for $^{135m}$Xe to affect reactor operation was first identified in CANDU reactors. It was discovered that including $^{135m}$Xe within the xenon reactivity worth slightly increased the steady-state xenon worth and could possibly affect transient behavior [61]. A more thorough evaluation of CANDU reactors by the same researchers later showed that $^{135m}$Xe could impact the power coefficient of reactivity [62].
Other research by the author found that $^{135m}\text{Xe}$ can have a substantial impact on steady state xenon worth for thermal spectrum molten salt reactors with on-line removal of xenon [63]. In this work it was found that the steady state xenon worth increases by up to a factor of 2, when $^{135m}\text{Xe}$, with TENDL-2015’s cross sections, were included in the xenon worth calculations.

### 4.4. Modeling $^{135m}\text{Xe}$ in LEU cermet NTP systems

$^{135m}\text{Xe}$ was added to the nuclear data libraries in Serpent and infinite lattice calculations were conducted to assess the effect of $^{135m}\text{Xe}$ on reactivity on SCCTE and TRIBLE. Nuclear data from the TENDL-2014 was used for $^{135m}\text{Xe}$. These infinite lattice calculations were conducted in the same manner as the infinite lattice calculations conducted in Chapter 3. For the infinite lattice approximation, the average fuel meat power density in the infinite lattice was set equal to the core averaged fuel meat power density in the full core. SCCTE has a core averaged fuel meat power density of 13.4 GW/m$^3$ and TRIBLE has a core averaged fuel meat power density of 15.0 GW/m$^3$. An approximant core averaged temperature of 1200 K was assumed for the fuel cross sections and $S(\alpha,\beta)$ data. All tie tube components, including moderator, were given a 300 K cross sections and $S(\alpha,\beta)$ data. The infinite lattice calculations presented here use a channel by channel burn cell mesh.

Serpent is a modern, highly flexible, Monte Carlo reactor physics code and adding cross section data, decay paths and fission yield data can be accomplished with relative ease. Adding $^{135m}\text{Xe}$ to burnup in MCNP would have been a substantial effort that was
not undertaken, because Serpent was verified to produce very close results with MCNP in Chapter 3 and in other cross code verifications [51].

Figure 57 presents the reactivity change in the SCCTE infinite lattice burnup, with and without $^{135m}$Xe over the representative human Mars mission. Figure 58 presents the fractional difference in xenon reactivity between the burn up model with and without $^{135m}$Xe for SCCTE. Figure 59 and 60 repeat Figures 57 and 58 for the TRIBLE infinite lattice burnup calculations. Error bars represent a 95% confidence interval and horizontal portions of the error bar are removed for clarity in later burns.

![Figure 57. Burnup profile for the SCCTE infinite lattice showing the burnup profile with and without $^{135m}$Xe.](image-url)
Figure 58. Fractional difference in reactivity for the SCCTE infinite lattice with and without $^{135m}$Xe.

Figure 59. Burnup profile for the TRIBE infinite lattice showing the burnup profile with and without $^{135m}$Xe.
Figure 60. Fractional difference in reactivity for the TRIBLE infinite lattice with and without $^{135m}$Xe.

It can be seen that the Serpent burnup model with $^{135m}$Xe show a larger reduction in reactivity than burnup models without $^{135m}$Xe during operation. For SCCTE, the maximum absolute difference is 43 pcm and the maximum fractional difference is 1.68. For TRIBLE, the maximum absolute difference is 64 pcm and the maximum fractional difference is 1.98. This is the expected result because prompt xenon is a large source of negative reactivity during the operation of a high power density thermal spectrum reactor that operates on a time scale much shorter than the half-life of $^{135}$I.

Another phenomenon caused by $^{135m}$Xe can be seen at the beginning of the TMI2 burn. Xenon builds in during the five hours while the NTP reactor is in orbit around earth between the TMI1 burn and the TMI2 burn, from the decay of $^{135}$I. The burn up model
with $^{135m}$Xe predicts a total negative reactivity that is slightly less than the burn up model without $^{135m}$Xe.

The reason the $^{135m}$Xe model predicts less xenon worth at the beginning of TMI 2 is that less prompt xenon survives the TMI 1 burn, because more prompt xenon is lost through the larger absorption cross section of $^{135m}$Xe than would otherwise occur. If $^{135m}$Xe were not included in the burnup model, the $^{135m}$Xe is given a 0 b cross section and is left to decay to $^{135}$Xe during the wait between TMI 1 and TMI 2. The depletion output file for SCCTE with $^{135m}$Xe indicates that the total inventory of xenon ($^{135m}$Xe and $^{135}$Xe) at the end of TMI 1 is reduced by a factor of 52.7%, when compared the inventory of xenon ($^{135m}$Xe and $^{135}$Xe) at the end of TMI 1, in the burn up model without $^{135m}$Xe.

4.5. Possible impact of $^{135m}$Xe on Operation and Design

These initial results indicate that $^{135m}$Xe can have a notable impact on thermal NTP systems like LEU cermet NTP systems. It is important to be able to quantify reactivity changes in a NTP system so that control systems can be designed to accommodate the changes in reactivity. As stated before, LEU cermet NTP systems will likely have little design margin and understanding the mechanisms that cause reactivity to change in these systems is important for their development.

Furthermore, as will be discussed in more detail in the next chapter, understanding how reactivity changes during operation is important for the development of burnable neutron poisons to contradict the changes in reactivity during operation. If the reactivity is poorly quantified, the development of the burnable poison would be difficult.
It should be noted that there is a need for basic nuclear data experiments for $^{135m}\text{Xe}$ and the work presented here uses model based estimations for the cross section of $^{135m}\text{Xe}$. Producing an evaluated cross section for $^{135m}\text{Xe}$, based on measured nuclear data, will help better model and develop LEU cermet NTP systems.
Chapter 5: Possible $^{135}$Xe Mitigation and Future Work

It was demonstrated in Chapter 3 that $^{135}$Xe will impact the operation of a LEU cermet NTP system. The reactivity loss due to the buildup of $^{135}$Xe and other fission products during operation is difficult to account for with rotating control drums. The use of rotating control drums results in a loss of $I_{sp}$. In order for LEU cermet NTP systems to be used, to their fullest potential, for a human Mars mission, the impact of $^{135}$Xe must be mitigated.

This chapter proposes mitigation strategies that minimize the impact of $^{135}$Xe on LEU NTP systems. In addition, this chapter suggests future work that will lead to a better understanding of $^{135}$Xe in NTP systems and will help to further develop $^{135}$Xe mitigation strategies.

5.1. Proposed Mitigation Strategies

A partial solution to mitigate $^{135}$Xe in NTP systems has been identified, as a part of collaborative work, with the author and another researcher in [58]. The work in [58] is applied to LEU graphite composite systems and it is extended to LEU cermet system here. This mitigation strategy is capable of maintaining the control drums at a constant position for the majority of the burns. This mitigation strategy does not solve the rapid burn out of xenon during TMI2, but that will be discussed in more detail later.
Central to this mitigation strategy is employing two complimentary systems to keep radial control drums at the same position during operation. The two systems are:

- Burnable neutron poisons to contradict reactivity changes during burns
- Modifying hydrogen density in the H\textsubscript{2} in the tie tubes to contradict reactivity changes between burns

A burnable neutron poison can add reactivity at approximately the same rate that reactivity is removed during operation by $^{135}$Xe build up, uranium depletion, and other mechanisms. The end result with a well-designed burnable poison is that there is no or little reactivity change during a burn. The smaller the change in reactivity there is during a burn, the more likely feedback effects in the core can compensate for burnup without degrading performance or needing to rotate the control drums.

The burnable poison solution identified in [58] is named BORGalloy (Burnable-poison Operating a Reactor with Gadolinium alloy) and consist of approximately 50 to 200 ppm concentrations of natural or enriched gadolinium in the outer tie tube structural material. The outer tie tube structural material is made of a metal like Inconel or Zircaloy. In SCCTE and TRIBLE the outer tie tube structural material is made of Zircaloy. Figure 61 is a diagram of the tie tube with the location of BORGalloy labeled.
The $^{157}$Gd in natural gadolinium has the largest absorption cross section of any stable isotope and rapidly burns out during operation. Because of its large absorption cross section, only small amounts are needed to contradict the change in reactivity during operation in a LEU cermet NTP system. Figure 62 varies the gadolinium content in BORGalloy for a full core SCCTE burn. This burnup calculation was conducted in Serpent in a similar way to the full core burnup calculations in Chapter 3. The BORGalloy was separated into burn cells with 10 axial sections and 4 radial sections.
It can be seen that with about 150 ppm of Gadolinium in BORGalloy, the change in reactivity over TMI1, MOI and TEI is small. At concentrations below 150 ppm of Gadolinium, it can be seen the reactivity gained from the burnable poison is not enough to counteract the reactivity loss during operation. At concentrations above 150 ppm of Gadolinium, the reactivity rises during the burn. This is undesirable and could lead the core to rise in power and violate the maximum allowable temperature. For this reason, it is important to be able to quantify the reactivity changes during a burn.

A draw back to the use of burnable poisons in this manner is that there is a reactivity penalty that must be compensated for in the design. 150 ppm of Gadolinium in

Figure 62. SCCTE burnup with BORGalloy using different gadolinium loadings.
BORGalloy removes a considerable 9800 pcm of reactivity. While this is a large amount of reactivity, current excess reactivity in the SCCTE design allows for reactivity decreasing design features like BORGalloy to be incorporated. Furthermore designing more reactivity into the NTP system is not difficult and does not have a significant mass penalty. The added simplicity of not needing to turn control drums during TMI1, MOI and TEI likely makes burnable poisons an appealing solution.

It can also be seen in Figure 62 that with 150 ppm of Gadolinium in BORGalloy, the reactivity at the start of MOI and TEI is higher than for TMI1 as the burnable poison burns out. This is undesirable, because the rise in reactivity requires control drum movement to counteract. The solution to the rising reactivity that happens between burns with BORGalloy, is to change the hydrogen pressure in the tie tubes for each burn. For the purposes of this work this strategy is called “pressure correction”. The reactivity of LEU cermet NTP systems is sensitive to the hydrogen density in the tie tubes with approximately 1% increase in pressure resulting in 5 pcm of added reactivity. By increasing the hydrogen density in the tie tubes in a uniform fashion throughout the core, the change in power profile will be less than it would be with control drums. Control drums cause power to change sharply at the periphery of the core. By maintaining a constant radial power profile, the NTP system can operate at its maximum I_sp as discussed in Chapter 3 section 3.4. “The Impact of $^{135}$Xe on LEU cermet NTP systems”.

Figure 63 presents a burnup profile of the SCCTE system with 150 ppm of Gadolinium in the BORGalloy and pressure correction in the tie tubes to ensure that the starting reactivity of the TMI1, MOI and TEI burns is nearly the same. Nominal average
pressure in the SCCTE tie tubes is approximately 11.06 MPa. For the pressure correction seen in Figures 63 to be implemented, TMI1 requires an average pressure of 16.93 MPa in the tie tubes, MOI requires an average pressure of 11.96 MPa in the tie tubes, and TEI requires an average pressure of 11.06 MPa in the tie tubes. Less pressure correction is needed if a lower concentration of Gadolinium is used and a larger change in reactivity is accepted during a burn.

Figure 63. SCCTE burnup with optimized Gd loading in the BORGalloy and hydrogen pressure correction to have a consistent initial reactivity for MOI and TEI. Note: TMI and TMI2 have the same reactivity profile with and without pressure correction.

The issue of the large amount of xenon worth at the beginning of TMI 2 is not corrected by burnable poisons or pressure correction. No convenient or novel solutions
were found for mitigating the $^{135}$Xe at the beginning of TMI2. Possible solutions, with notable drawbacks, to handling the $^{135}$Xe at the beginning of TMI2 include:

- Developing a control system that can manage the rapid burn out of $^{135}$Xe at the beginning of TMI2
- Waiting longer between TMI1 and TMI2 to let $^{135}$Xe decay and finding solutions protect crew and electronics from the added radiation associated with passing through the Van Allen Belts many more times.
- Conduct a single burn trans-Martian injection and develop mission architectures that minimize and compensate for gravity losses.

The BORGalloy and pressure correction approach pairs very well with a single burn trans-Martian injection, or waiting longer between TMI1 and TMI2. Figure 64 is the reference mission with 48 hours between TMI1 and TMI2. It can be seen that BORGalloy and pressure correction are very effective at minimizing reactivity changes for this longer wait approach. Figure 65 assumes an arbitrary 60 minute single trans-Martian injection burn and it once more can be seen that BORGalloy and pressure correction strategy effectively reduce reactivity changes during operation.
Figure 64. SCCTE burnup with optimized Gd loading in the BORGalloy, hydrogen pressure correction and a 48 hour wait between TMI1 and TMI2. Note: TMI1 and TMI2 have the same reactivity profile with and without pressure correction.
It should be noted, no combination of hardening the core’s spectrum or lowering the power density of the NTP system was found that could significantly lower xenon worth, without drastically lowering the performance of the NTP system. Hardening the core’s spectrum, or lowering the power density, required an unacceptable increase in core mass. Furthermore, as stated in Chapter 2, an unmoderated LEU cermet NTP system is subcritical and would require a significant increase over currently achievable uranium loadings for criticality to be attainable.
5.2. Future Work

LEU cermet NTP systems and other NTP systems are early in their development and much work must be completed before these systems can take humans to destinations such as Mars. The work and ideas presented here will only be completely validated when a LEU cermet NTP system is built and tested. For this reason, the discussion of future work is kept to possible near term goals that will assist in modeling $^{135}$Xe and developing mitigation strategies for $^{135}$Xe.

There is a need for further development and higher fidelity modeling of LEU cermet design points. As discussed in Chapter 2 section 2.4.1. “Neutronics consideration in SCCTE and TRIBLE” there are many neutronic assumptions and simplifications made in the current models for SCCTE and TRIBLE. By building higher fidelity neutronic models, it will better be possible to capture and quantify neutronic phenomena in these systems. In addition, SCCTE and TRIBLE are very preliminary designs and further mechanical and thermal development will likely change the neutronic environment.

An integrated reactor systems code is needed for analyzing transient behavior and better understand the effects of $^{135}$Xe on LEU cermet NTP systems. An integrated reactor systems code would be able to better assess what happens to the core, when reactivity changes and the control drums do not move to counteract the change and temperature feedback comes into play. This integrated reactor systems code would need to include the power cycle/turbopump, temperature feedback from the numerous components, and burnup effects, among many other phenomena. RELAP 7 and the MOOSE is a potential framework for producing this integrated reactor systems code.
This work has identified the benefits of waiting longer between TMI1 and TMI2 or unitizing single burn trans-Martian injection in mitigating the effects of $^{135}\text{Xe}$ on operation. Further work, from mission planners and spacecraft designers, is needed to quantify how these alternative approaches to the trans-Martian injection would affect the spacecraft and mission architecture.

Chapter 4 identified the possible impact of $^{135\text{m}}\text{Xe}$ on LEU cermet systems, but the model based TENDL cross sections were used, because they are the best available estimation of $^{135\text{m}}\text{Xe}$'s cross section. No experimental data exists for the $^{135\text{m}}\text{Xe}$'s cross section. If the cross section of $^{135}\text{Xe}$ is larger than the cross section of $^{135}\text{Xe}$, as is indicated by the TENDL-2015 nuclear data library, then it will be important to have evaluated cross sections for $^{135\text{m}}\text{Xe}$ validated by nuclear experiments.
Chapter 6: Summary

The work presented here, represents an increase in the understanding for LEU cermet NTP systems regarding how they are effected by $^{135}$Xe. NASA has the goal of sending humans to Mars and NTP is an appealing technology to make this goal a reality. This work assists the goal of human exploration of Mars by investigating a promising subset of the NTP system design space, and investing a highly important issue in this subset of NTP systems. The knowledge gained in this work will aid in the development of LEU cermet NTP systems and other NTP technologies.

In Chapter 2, the SCCTE and TRIBLE LEU cermet design points were introduced. These design points were created with SPOC and were produced through extensive “brute force optimization”. They were created in part to serve as a reference design for foundational NTP research and have been used as such by other researchers. In this work, they were used as the reference designs for burnup calculations.

In Chapter 3, the reactivity changes during operation of SCCTE and TRIBLE were quantified using MCNP and Serpent. Infinite lattices were first used to verify methods and approaches before more computationally intense full core burn calculations were undertaken. WORPH was used for the creation of the infinite lattice MCNP and Serpent input files. The infinite lattice calculations indicated that MCNP 6.1.1 Beta and Serpent
produced very similar results and that burnup cells across the fuel element were not needed to capture spatial shelf shielding effects.

The infinite lattice results were used to inform the approach undertaken for the full core burnup calculations. Full core burnup calculations were conducted with Serpent and without burnup cell meshing across the width of the fuel element. Full core burnup calculations in SCCTE and TRIBLE indicate that the maximum reactivity loss during 25 minutes of operation is approximately 165 pcm for both reactors. Reactivity loss during shutdown after 25 minutes of operation, peaks at about 2650 pcm in SCCTE and 3550 pcm in TRIBLE, at approximately 10 hours after the reactor shuts down.

In addition, in Chapter 3 the potential effect of $^{135}$Xe on NTP performance and controllability is discussed. The rapid burnout of $^{135}$Xe during TMI2 is identified as posing some serious challenges for control. Furthermore, a relationship to estimate $I_{sp}$ loss as a function of control drum angle or reactivity is derived and presented.

In Chapter 4, the potential impact of $^{135m}$Xe on the reactivity in LEU cermet NTP systems was identified. The model based TENDL-2015 nuclear data library indicates that $^{135m}$Xe has an absorption cross section about 4 times larger than the absorption cross section of the ground state of $^{135}$Xe. Including the TENDL-2015 $^{135m}$Xe cross section in the burnup calculations led to a notable increase in xenon worth during operation. Model based TENDL cross sections were used because no experimentally determined cross sections are available for $^{135m}$Xe. This work identifies a need for basic nuclear data experiments to measure the cross section of $^{135m}$Xe instead of relying on models.
In Chapter 5, mitigation strategies were proposed to counteract the effects of $^{135}$Xe on LEU cermet NTP systems. These proposed mitigation strategies show great promise for eliminating the need for turning control drums during operation of LEU cermet NTP systems, although they pose some drawbacks which must be considered. Future work was suggested that would aid in understanding $^{135}$Xe in LEU cermet NTP systems and developing mitigation strategies to mitigate its effects. Central facets of the suggested future work include developing an integrated reactor systems code and acquiring experimentally validated $^{135m}$Xe cross sections.
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