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INITIAL FUEL POSSIBILITIES FOR THE THORIUM
MOLTEN SALT REACTOR

by

DUSTIN GAGE GREEN

A THESIS

Presented to the Faculty of the Graduate School of the
MISSOURI UNIVERSITY OF SCIENCE AND TECHNOLOGY

In Partial Fulfillment of the Requirements for the Degree

MASTER OF SCIENCE IN NUCLEAR ENGINEERING

2015

Approved by

Ayodeji Alajo, Advisor
Xin Liu
Gary Mueller

ABSTRACT

The Generation IV International Forum placed six reactors as priority for research and development to compensate for the world's increasing energy demands. Among the six were Molten Salt Reactors (MSRs). These reactors utilize the Th/²³³U fuel cycle using molten fluoride or chloride salts as coolants. MSRs also have the possibility to use other fissile fuels especially with the first fleet of reactors given the low amount of Uranium-233 available commercially.

With the possibility of diverting from using ²³³U initially, the research presented here will benchmark ²³³U as a main fuel for MSRs using the Thorium Molten Salt Reactor (TMSR) designed by Billebaud Annick and her team at the Laboratory for Subatomic Particles and Cosmology in France. Uranium-235 and Plutonium-239 will then be tested as suitable initial fuels for the first fleet of TMSRs. These fuels will be compared to the reference data based on neutron flux spectra and breeding capabilities.

ACKNOWLEDGMENTS

A big thanks to Dr. Alajo and the Nuclear Engineering Department at Missouri S&T. Thank you to the Nuclear Regulatory Commission for funding the research. I would like to also thank Dr. Mueller and Dr. Liu for accepting the positions to be on my committee.

Also, a huge chunk of gratitude goes to my lovely wife for putting up with me and my schooling for three extra semesters.

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1. INTRODUCTION

Molten Salt Reactors (MSRs) have a certain flexibility when it comes to how they are operated and managed. Molten salt reactors have the capability of operating in the thermal, epithermal, and fast neutron spectra and can also use different nuclear fuels to produce fission. Figure 1.1 displays a simplified Molten Salt Reactor system. MSRs can be operated utilizing the Th/ ^{233}U fuel cycle using molten fluoride or chloride salts. These types of MSRs are called Thorium Molten Salt Reactors (TMSRs) and rely on a thorium blanket to breed ^{233}U as seen in Equation 1. Using an onsite chemical processing system,

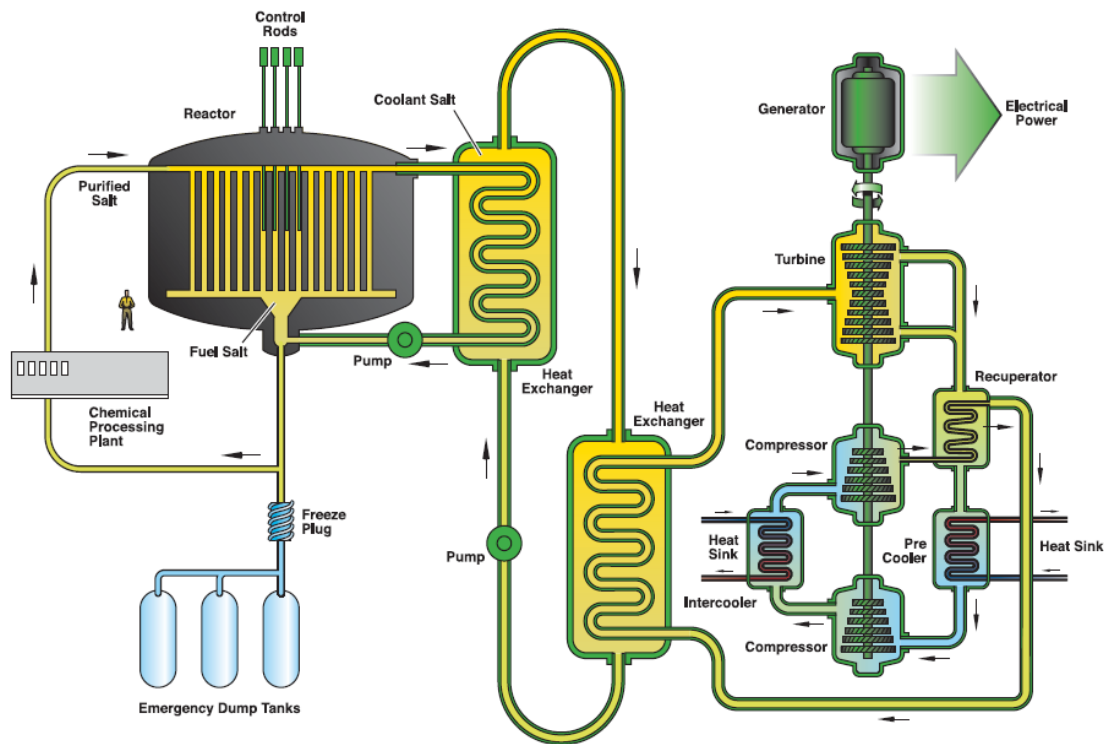
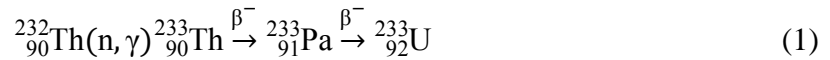


Figure 1.1. Simplified Molten Salt Reactor schematic (A Technology Roadmap for Generation IV Nuclear Energy Systems, 2002)

any fission products along with the $^{233}_{91}\text{Pa}$ produced from the thorium are extracted. $^{233}_{91}\text{Pa}$ has a 27 day half-life before it decays to $^{233}_{92}\text{U}$ and can be reinserted into the core. With this



chemical processing system, TMSRs fulfil the criteria of the Generation IV International Forum for nonproliferation concerns and a closed nuclear fuel cycle.

For the research presented here, using MCNP, a Thorium Molten Salt Reactor using $^{233}_{92}\text{U}$ for the initial and operating fuel will be benchmarked based on the data presented by Billebaud Annick and her team at the Laboratory for Subatomic Particles and Cosmology in France. Comparison of average neutron flux as a function of neutron energy will be the main basis of benchmarking. Two additional nuclear fuels will be compared with $^{233}_{92}\text{U}$. These fuels are $^{235}_{92}\text{U}$ and $^{239}_{94}\text{Pu}$ which have been chosen due to nonproliferation concerns. During the cold war era, the U.S. and former Soviet Union stockpiled nuclear weapons made from $^{235}_{92}\text{U}$ and $^{239}_{94}\text{Pu}$. After the dissolution of the Soviet Union, disarmament measures in U.S. and Russia provided the opportunity to use these fissile materials as nuclear fuel. When used for nuclear weapons, these two metals are enriched to over 90 weight%, however, through fluorination, the metal can easily be dissolved into a salt for use in MSR (Military Warheads as a Source of Nuclear Fuel, 2014). Along with aiding in the reduction of nuclear warhead stockpiles, incorporating ^{235}U and ^{239}Pu into the first fleet of TMSRs will allow for the reactors to power up without an initial fuel of ^{233}U . The two major aspects looked at will be how well these

fuels breed $^{233}_{92}\text{U}$ in the blanket and their fluxes across the system. Ultimately, this thesis will document whether TMSRs can be initially fueled with these alternate fuels.

2. THORIUM MOLTEN SALT REACTOR CONCEPT

The base design for this project comes from the Thorium Molten Salt Reactor that is being designed by Billebaud Annick and her team at the Laboratory for Subatomic Particles and Cosmology in France as seen in Figure 2.1. The design is a $3000\text{MW}_{\text{th}}$ reactor that operates on the $\text{Th}/^{233}\text{U}$ fuel cycle with a mean fuel temperature of 750°C .

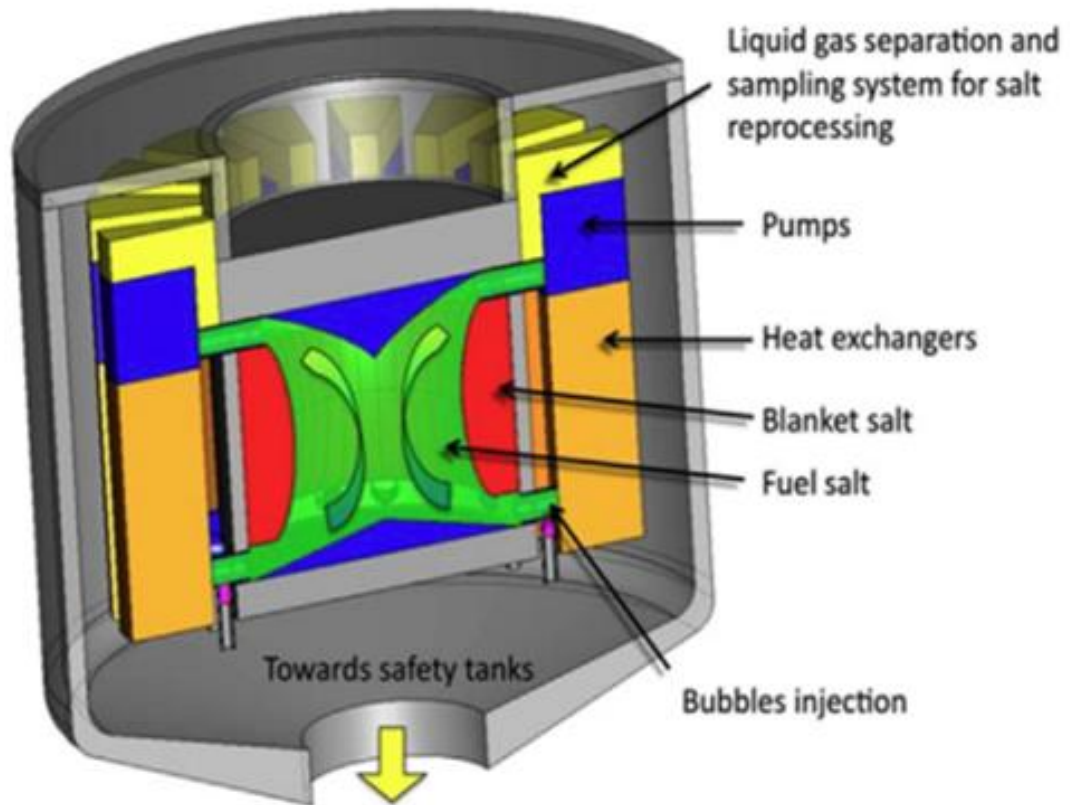


Figure 2.1. Concept design with basic components shown of the TMSR (Serp, et al., 2014)

The central salt channel (green) consists of a LiF, ThF₄, and UF₄ salt mixture set at a eutectic point corresponding to a melting temperature of 565°C as seen in Figure 2.2. The total fuel salt volume is set at 18m³ with a distribution of half in-core and half out-of-core (Merle-Lucotte, Heuer, Allibert, Doligez, & Ghetta, Minimizing the Fissile Inventory of the Molten Salt Fast Reactor, 2009). The system utilizes a chemical processing system to remove unwanted fission products (FPs) from the fuel and blanket salt. The fuel salt reprocessing rate is set at 40L per day in order to provide a constant k_{eff} value of one (Merle-Lucotte, Heuer, Allibert, Doligez, & Ghetta, Minimizing the Fissile Inventory of the Molten Salt Fast Reactor, 2009). Figure 2.3 provides an overview of the chemical processing system.

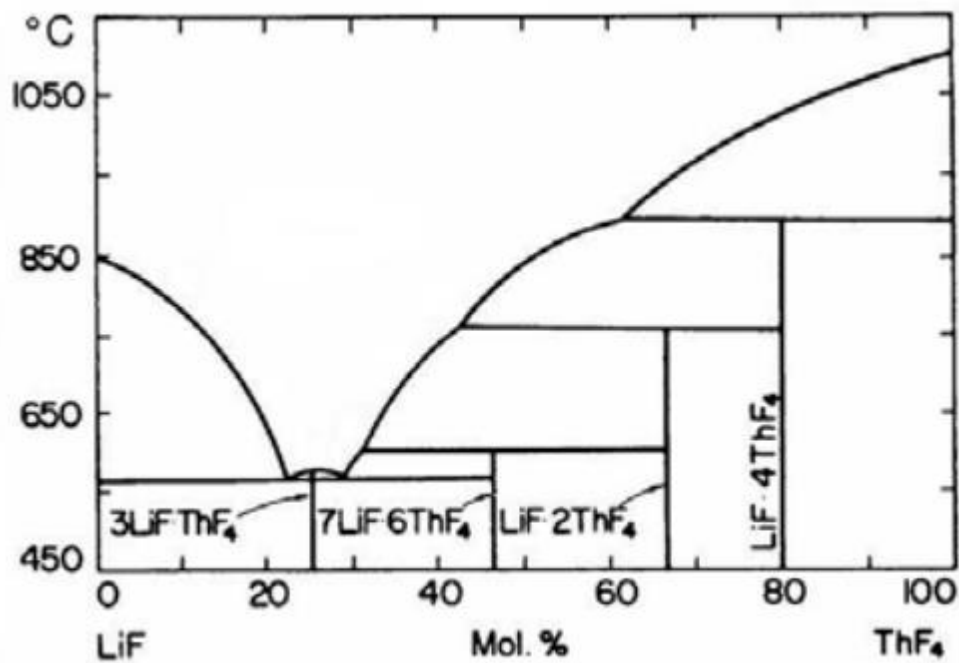


Figure 2.2. LiF-ThF₄ phase diagram (Merle-Lucotte, et al., The Non-Moderated TMSR, An Efficient Actinide Burner and a Very Promising Thorium-Based Breeder, 2007)

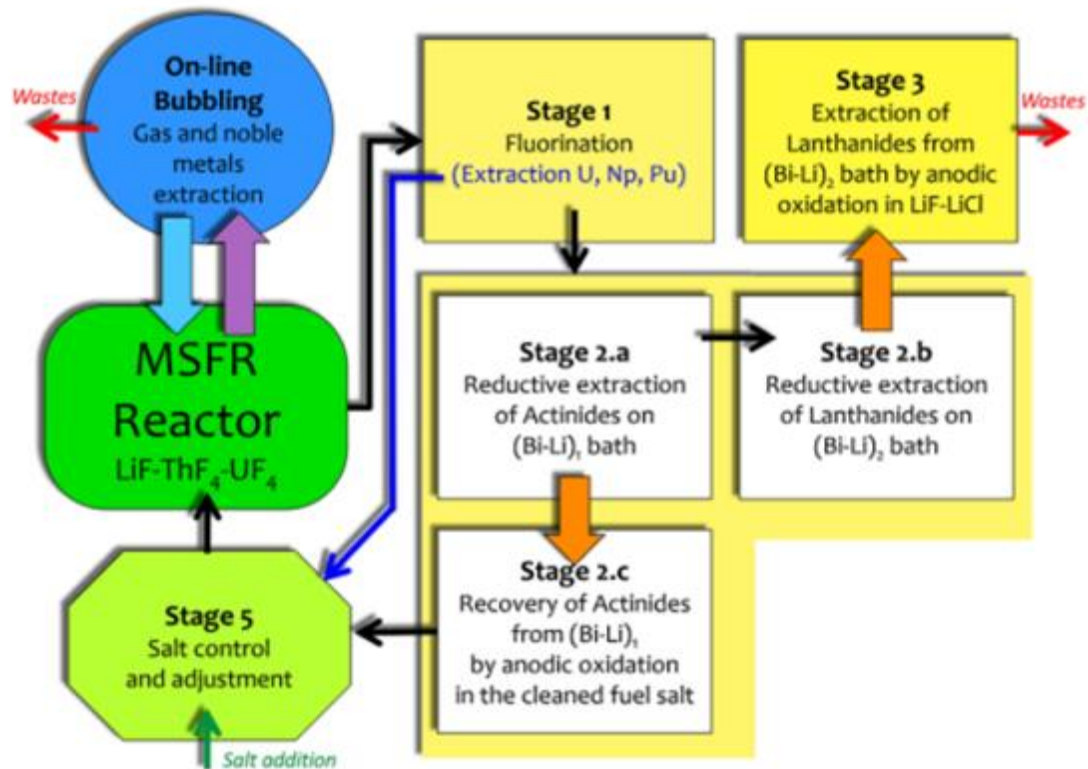


Figure 2.3. Basic overview of the chemical processing system used to purify the fuel and blanket salt (Rubiolo, et al., January 2013)

The blanket salt (red) consists only of LiF and ThF_4 and set at the same eutectic point. Within the blanket, thorium absorbs neutrons to eventually decay into ^{233}U (see Equation 1). Every six months, the blanket salt is fully reprocessed through the chemical reprocessing system to remove the protactinium and uranium and reset it back to its original composition.

Above and below the core reside thick nickel hastelloy reflectors. The same alloy surrounds the heat exchangers and core externals. The reflectors along with the boron carbide radial reflector that surrounds the blanket salt are capable of blocking over 99% of the escaping neutrons (Rouch, et al., 2014). This allows for a reactor operation time of 133 years to produce 100 dpa (displacements per atom) in the most irradiated section of

the axial reflector (Merle-Lucotte, Heuer, Allibert, Doligez, & Ghetta, Minimizing the Fissile Inventory of the Molten Salt Fast Reactor, 2009).

The structural materials surrounding the core have to bear a high neutron flux coupled with high temperatures. For these components nickel hastelloy is used. This Ni-based alloy contains W and Cr and is detailed in Table 2.1. For the simulations used in the literature and in the research presented here, all materials radially outside of the boron carbide reflector and axially outside of the fuel salt channel are composed of nickel hastelloy.

Table 2.1. Composition (at%) of nickel hastelloy used in the reference TMSR (Merle-Lucotte, Heuer, Allibert, Doligez, & Ghetta, Minimizing the Fissile Inventory of the Molten Salt Fast Reactor, 2009)

Ni	W	Cr	Mo	Fe	Ti	C
79.432	9.976	8.014	0.736	0.632	0.295	0.294
Mn	Si	Al	B	P	S	
0.257	0.252	0.052	0.033	0.023	0.004	

2.1. GEOMETRY

The main salt channel of the TMSR is a single cylinder measuring 2.25m high by 2.25m in diameter with a volume of about 9m³. The blanket that surrounds the main salt channel is 50cm thick. The boron carbide reflector on the perimeter of the blanket salt is 20cm thick. The two axial reflectors on the top and bottom of the core measure 50cm in height and have a diameter of 2.95m. Figure 2.4 represents a vertical cross-cut of the TMSR.

2.2. SALT PROPERTIES

The initial fuel salt is composed of $\text{LiF-ThF}_4\text{-}^{233}\text{UF}_4$ and maintains 77.5 mole % LiF throughout operation with a 99.999 mole % of ^7Li . As seen in Figure 2.2, the heavy nuclei proportion is set at 22.5 mole % which is the eutectic point corresponding to a melting temperature of 565°C . The fraction of $^{233}\text{UF}_4$ is set to remain at 2.7 mole % throughout operation of the reactor in order to maintain an exactly critical reactivity level. The remaining molar percentage consists of ThF_4 . For the radial blanket, an equivalent salt of 77.5 LiF – 22.5 ThF_4 is used. The physicochemical properties for the TMSR fuel salt are tabulated in Table 2.2 along with the values used for the MCNP simulations.

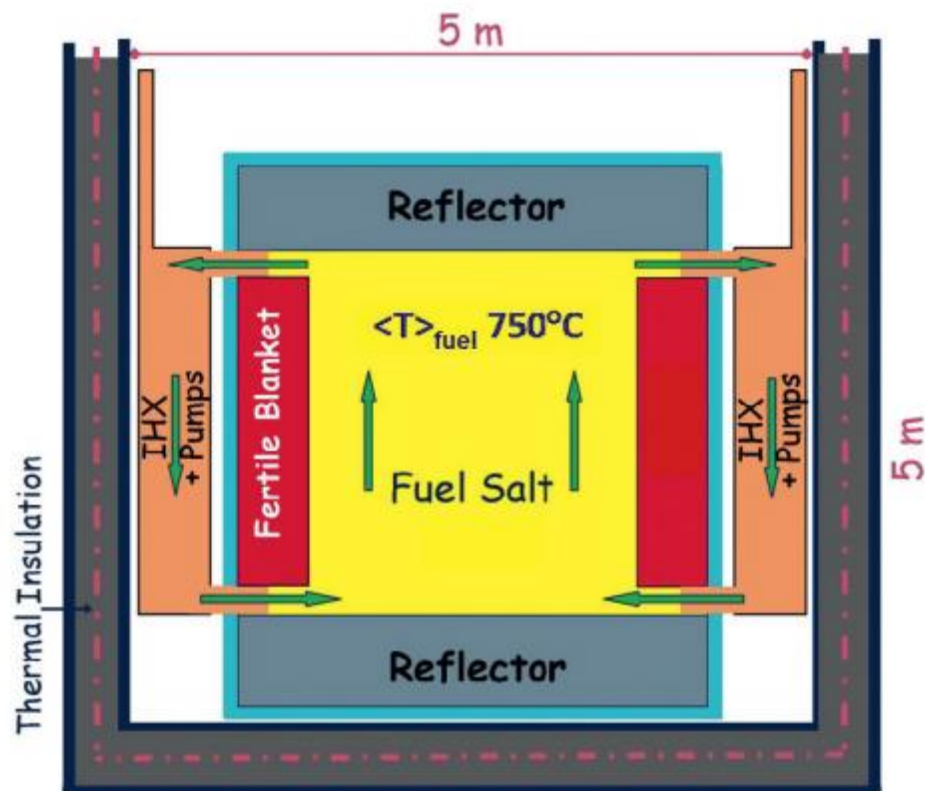


Figure 2.4. Vertical, to-scale cross-cut of the TMSR (Rouch, et al., 2014)

Table 2.2. Physicochemical properties used for the salts at a mean temperature of 775°C (Merle-Lucotte, Heuer, Allibert, Doligez, & Ghetta, Minimizing the Fissile Inventory of the Molten Salt Fast Reactor, 2009)

	Formula	Value at 775°C	Value at 630°C
Density ρ (g/cm ³)	$4.632 - 7.526 \cdot 10^{-4} \cdot T(^{\circ}\text{C})$	4.05	4.16
Dynamic Viscosity μ (Pa.s)	$0.39943 \cdot 10^{-3} \cdot \exp(2812.9/T(\text{K}))$	$5.85 \cdot 10^{-3}$	$8.996 \cdot 10^{-3}$
Thermal Conductivity λ (W/m/K)	$0.16016 + 5 \cdot 10^{-4} \cdot T(^{\circ}\text{C})$	0.548	0.475
Caloric Capacity c (J/kg/K)	—	1045	—

3. MCNP

Monte Carlo N-Particle Transport Code (MCNP) is a general purpose software developed by Los Alamos National Laboratory. This code can be used for transport calculations of neutrons, photons, electrons, or any combination of the three. The primary use of the code involves the simulation of nuclear processes such as fission, but it has the capability of applications in areas such as, but not limited to, radiation protection and shielding, radiography, medical physics, detector design, and fusion (X-5 Monte Carlo Team, 2003).

3.1. MCNP MODEL, CORE SPECIFICATIONS AND ASSUMPTIONS

MCNP input files were developed in accordance with the specifications of the Thorium Molten Salt Reactor (TMSR) discussed in Chapter 2. Some specifications of the TMSR were not provided in current literature. In these cases, reasonable assumptions were made based on relative sizes and physical plausibility. MCNP version 5 was used for the neutronics simulations and MCNPx version 2.7 was used for burnup calculations.

A height of 185cm is assumed for the radial blanket. This assumption is deduced from Figure 2.4 which is a to-scale cross-cut of the TMSR core. This sets the volume of the blanket at 8m^3 . The ^{10}B atomic abundance has been shown to fluctuate between samples of boron (Baum, Ernesti, Knox, Miller, & Watson, 2009). Given this information, a ^{10}B atomic abundance of 19.9% is chosen which correlates to the most common abundance listed in *Nuclides and Isotopes: Chart of the Nuclides* (Baum, Ernesti, Knox, Miller, & Watson, 2009). As seen in Figure 3.1, a stainless steel cell (red)

outlines the perimeter of the reactor. Though not in the literature, this cell allows for an accounting of any neutrons that escape past the nickel hastelloy reflectors.

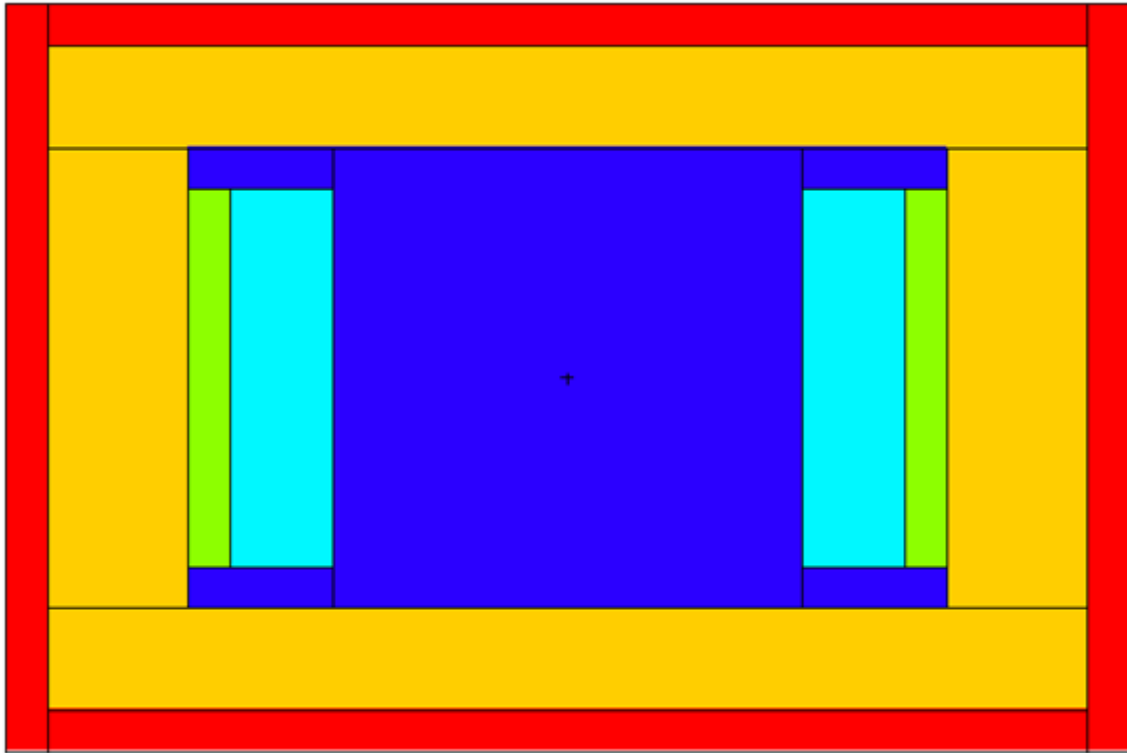


Figure 3.1. Vertical cross-cut of the simulated TMSR in MCNP. Dark blue is the fuel salt. Light blue is the blanket salt. Green is the boron carbide reflector. Yellow is the surrounding nickel hastelloy. Red is a stainless steel outer shell.

In order to first address the neutron flux of the system, the tally ‘f4:n’ is used.

This tally calculates the average neutron flux within the specified cell. In this case the cell is the central fuel salt channel as seen in Figure 3.1. An energy mesh is also used in order to obtain neutron fluxes at each energy level. This energy range begins at 1.00E-9 MeV and extends to 100 MeV and is broken into 442 bins.

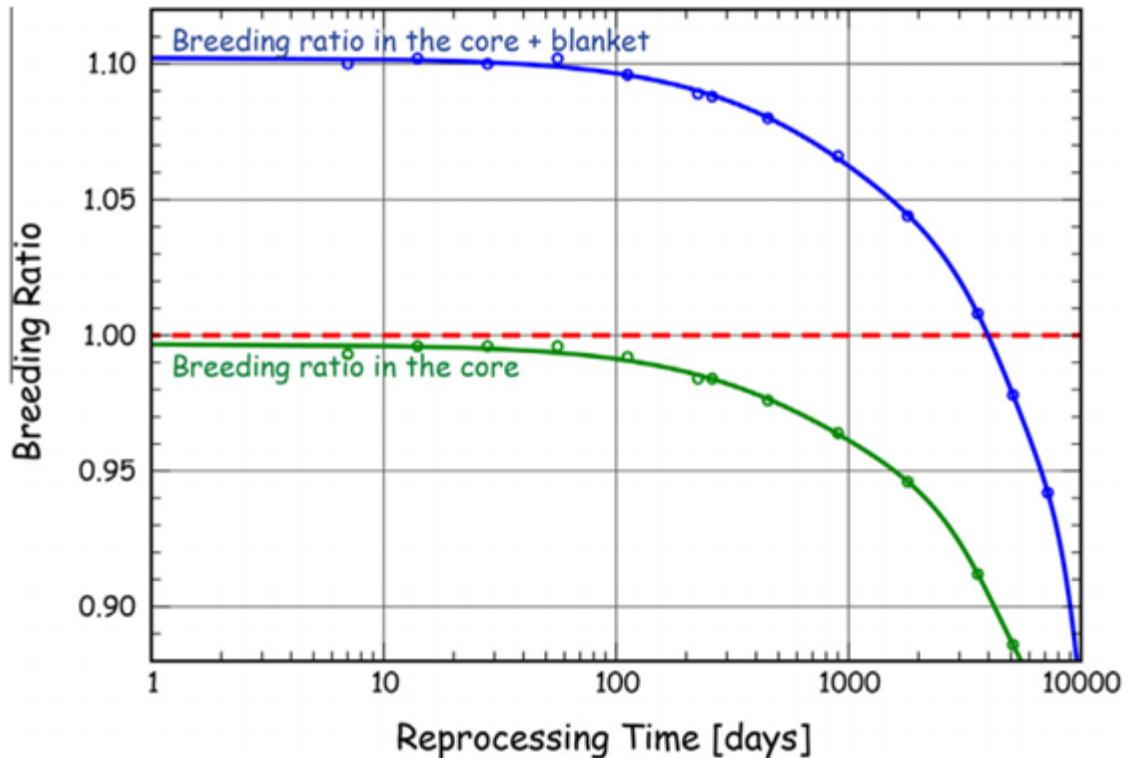


Figure 3.2. Breeding ratio of the reference TMSR as a function of the reprocessing rate (Heuer, et al., 2014)

For the criticality calculations, the command ‘kcode’ is used. 20,000 initial particles per cycle are used. Using 300 active cycles yields a total of six million histories in the simulation. The total number of histories was sufficient to assure accurate results and reliable statistics.

In order to test how well each fuel salt performs with the blanket salt, MCNPX has to be used. Using MCNPX, the burnup within the blanket can be simulated. For this, a ‘BURN’ card is used within the data card section of the input code. For these burn calculations, the main fuel salt remains critical and no burn is performed on it. This is done because the fuel salt is reprocessed on a daily basis to maintain a critical reactivity value of one. As Figure 3.2 shows, reprocessing every day allows for a breeding ratio

within the core to be just under 1.00. This means that the bulk of the breeding comes from the blanket. Since the core is initially fueled to be barely critical and its ability to maintain criticality heavily relies on reprocessing, no burn is required since it can be assumed that the breeding rate of ^{233}U is an almost equal ratio to its fission rate. The burn time is set at six months with three intervals of 60 days each and is simulated at the specified power of $3000\text{MW}_{\text{th}}$.

3.2. URANIUM 233

The $^{233}\text{UF}_4$ concentration in the fuel salt is set at 2.7 mole %. This equates to about 7 weight % of ^{233}U . The goal is to benchmark the MCNP data against the data presented within the literature based on the neutron flux in the core and the amount of ^{233}U bred from the blanket. As seen in Figure 3.3, it is expected that a ^{233}U -started TMSR should be able to breed its initial fissile inventory within 55 years. This expectation coupled with a fast neutron spectrum (see Figure 3.4), will conclude whether the simulated data will be comparable to data presented in the literature.

3.3. URANIUM 235

The TMSR configuration fueled with ^{233}U was set as the reference for a version of the reactor fueled with ^{235}U . It is found that a reactor fueled by ^{235}U requires 4.3 mole % of $^{235}\text{UF}_4$ in order to maintain a constant criticality of one. This equates to 11.3 weight % of ^{235}U . The neutronic characteristics of the ^{235}U fueled reactor will be compared with those of the ^{233}U -based configuration.

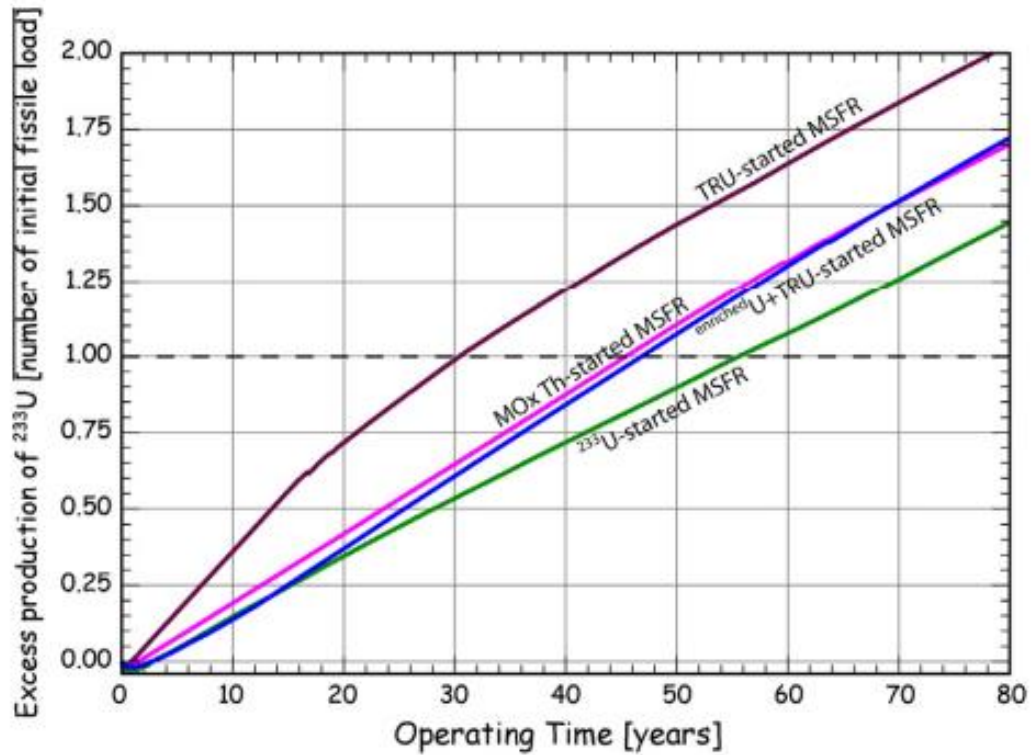


Figure 3.3. Excess production of ^{233}U as a function of time.

3.4. PLUTONIUM 239

For the final simulation, a Plutonium-239 fuel salt will be compared to the aforementioned fuel compositions. For this reactor, 11.56 weight % of ^{239}Pu allows for a maintained criticality value of one. As in the two previous simulations, the neutron flux along with the amount of fissile inventory produced by the blanket will be compared to the other simulations and the reference TMSR.

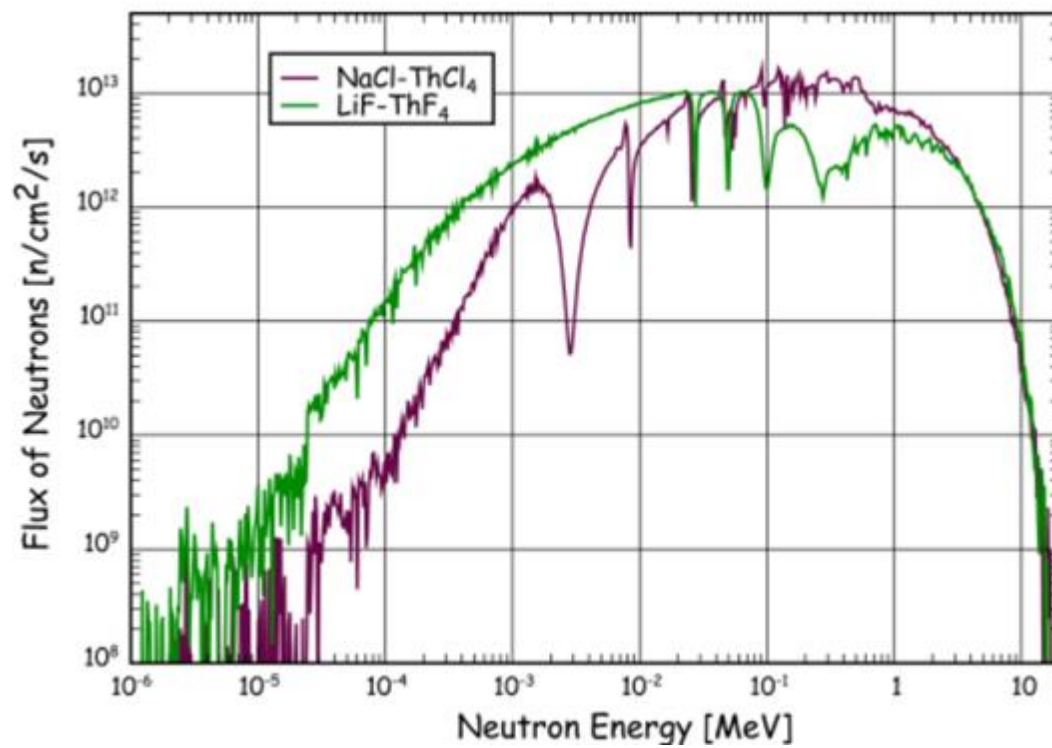


Figure 3.4. Neutron spectra for a chloride salt (purple) and a fluoride salt (green) (Rubiolo, et al., January 2013)

4. RESULTS

4.1. URANIUM 233

Figure 4.1 illustrates the average neutron flux for the fuel salt and the blanket salt in the ^{233}U -operated TMSR. When the green graph in Figure 4.1 is compared to the green graph in Figure 3.4, it can be seen that the core flux spectrum are similar. The flux peak from both Figures are in the same order of magnitude. The flux depressions seen between 10 keV and 1 MeV are due to parasitic absorption at resonance energies of ^{19}F , which is

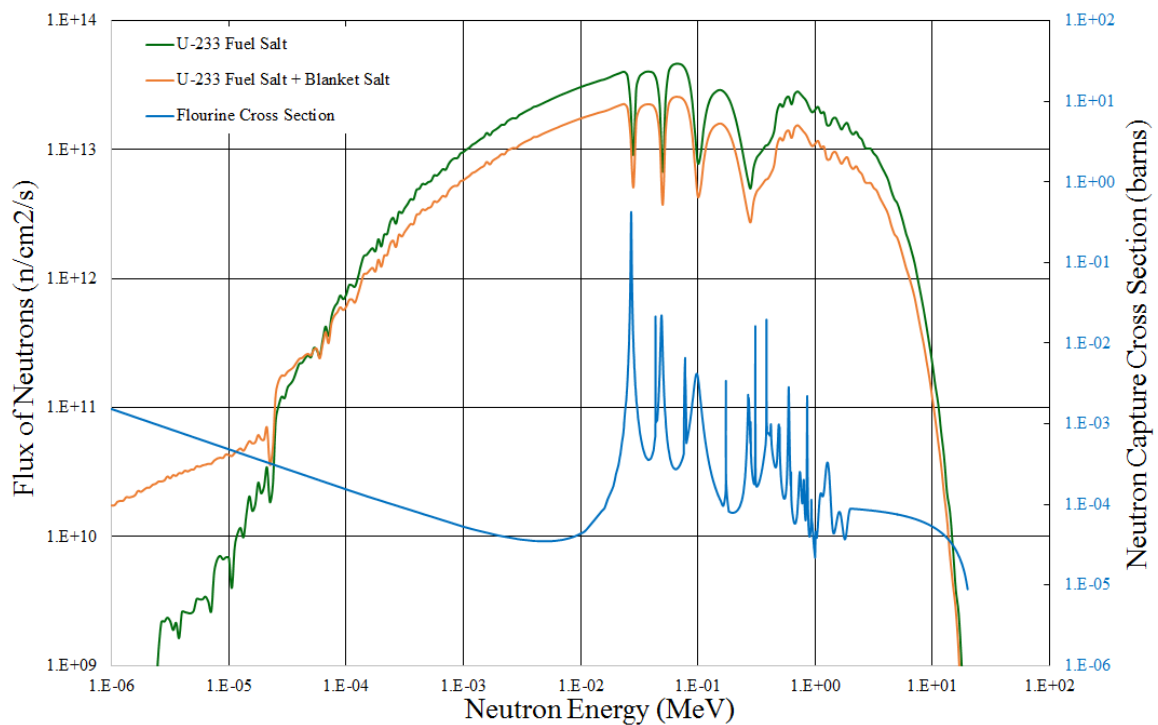


Figure 4.1. Neutron flux spectrum of the ^{233}U -operated TMSR shown with the cross section values of Fluorine-19 (Blue). The fuel salt flux is depicted in green whereas a union of the fuel salt and blanket salt is depicted in orange.

abundant in the driver fuel and blanket (see Figs. 4.1, 4.3 and 4.5). However, the results from the calculations performed indicates flux of a higher magnitude than the result from Rubiolo, et al. It should be noted that the flux spectrum averaged over the active core and blanket region results in similar spectral magnitude to Figure 3.4. Also, as discussed in further detail in Section 4.4, the use of an in-house code by the researchers could lead to a more refined neutron flux. Since this is an evaluation of the fuel salt and how it performs, the blanket salt is kept separate in the calculations to produce more accurate results pertaining to the fuel salt.

In order to determine the amount of fissile inventory that is bred from the blanket salt of $\text{ThF}_4\text{-LiF}$, the data is extrapolated based on a six month burn of the system. Since the blanket salt is reset every six months through the chemical reprocessing system, it can be concluded that the data produced from the simulation will provide an excellent estimation for the amount of fissile fuel produced within the blanket. Figure 4.2 illustrates the doubling time of the reactor, which is the estimated time in order to breed enough fissile inventory to replace the initial core and fuel a second TMSR. With an initial ^{233}U inventory of 5,268kg, it will take about 45 years to reach this criteria. This estimate varies by 10 years when compared to Figure 3.3. This variation can be attributed to the overall higher neutron flux exhibited by the MCNP simulation. A higher neutron rate per area within the blanket allows for more neutrons to be absorbed and thus a faster doubling time of the reactor. Overall, it can be concluded that the MCNP simulations presented here are valid given the successful benchmarking to the ^{233}U reference TMSR.

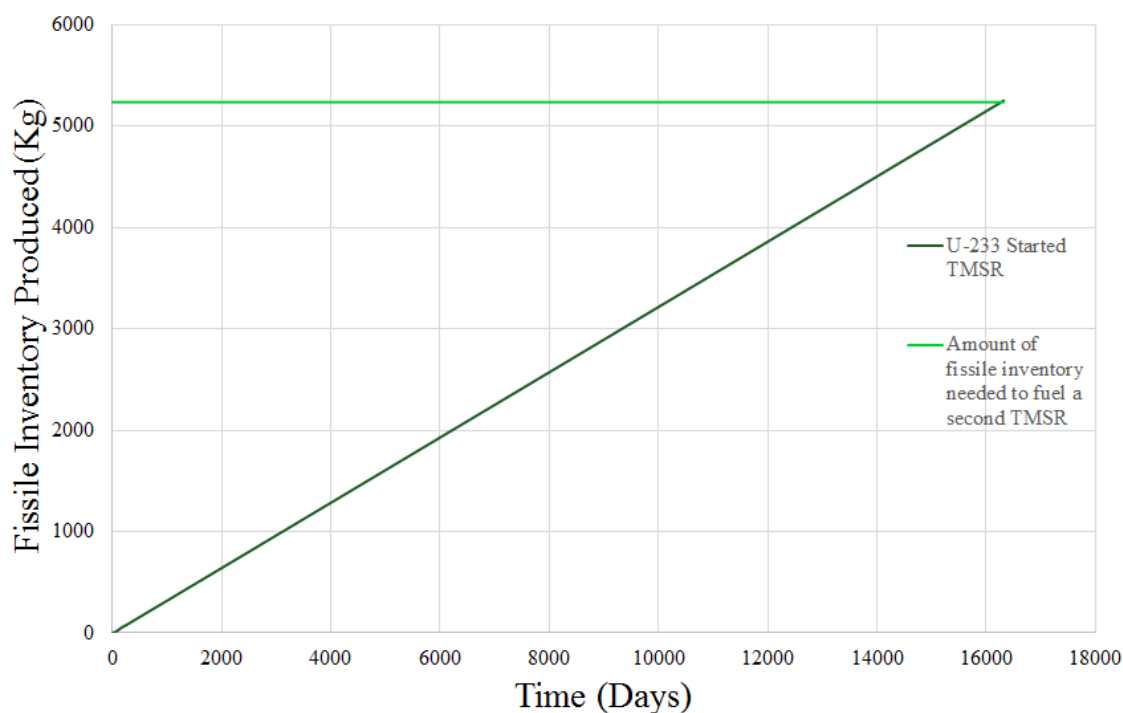


Figure 4.2. Estimation of the doubling time for the ^{233}U -operated TMSR

4.2. URANIUM 235

The average neutron flux spectra for the ^{235}U -fueled TMSR is illustrated in Figure 4.3. This spectra has very little variation when compared to the ^{233}U model and yields an average relative error of 2.2%. The blanket salt neutron flux is included in Figure 4.3 to indicate that a coupling of the two salts' neutron flux spectra would produce a slightly lower average neutron flux spectrum.

The doubling time for the $^{235}\text{UF}_4$ fueled TMSR can be seen in Figure 4.4. As in the previous section, the data is based on one six month burn of the blanket salt with the

fuel salt channel maintaining a criticality value of one for the duration of the burn. With an initial fissile inventory of 8,452kg, the doubling time for the reactor is 76 years. This is almost double the required time for a ^{233}U -started TMSR. This longer doubling time is due to the larger fissile inventory needed to maintain a critical reactor.

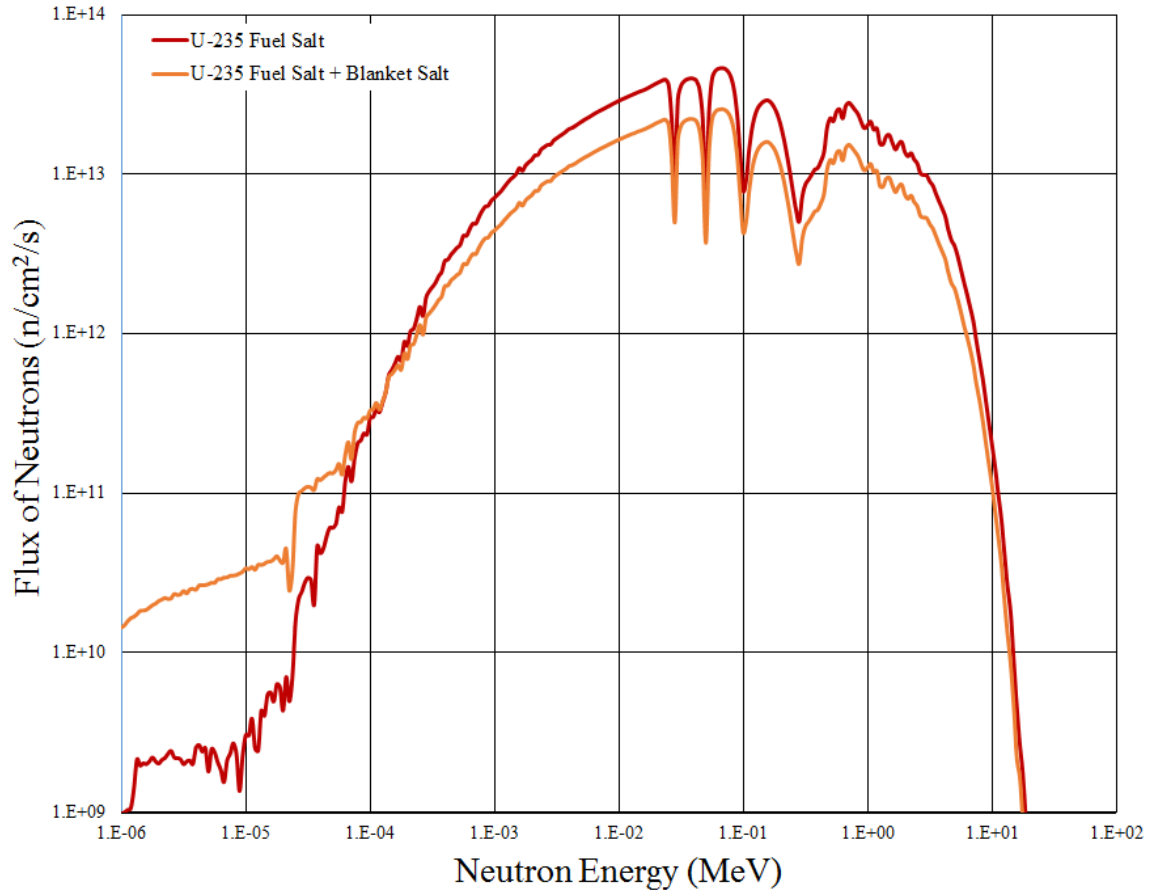


Figure 5.3. Neutron flux spectrum of the ^{235}U -operated TMSR. The fuel salt flux is depicted in red, whereas the union of the fuel salt and blanket salt is depicted in orange.

4.3. PLUTONIUM 239

The neutron flux spectrum for the ^{239}Pu -operated TMSR is shown in Figure 4.5. The neutron flux spectra follows the same trend as the previous two fuel salts and yields an average relative error of 1.9%. As with the previous figures, the fuel salt and blanket

salt are separated to emphasize that coupling the two salts together for an average flux spectrum will yield lower fluxes and lead to wrong interpretation of the fuel salt and how it performs.

Figure 4.6 shows that the estimated doubling time for a TMSR fueled with ^{239}Pu is 78 years to replace the initial inventory of 8,580kg needed to maintain a criticality value of one within the fuel salt channel. This is longer than either of the previous reactors and is due to the higher amount of initial inventory that the blanket must replace.

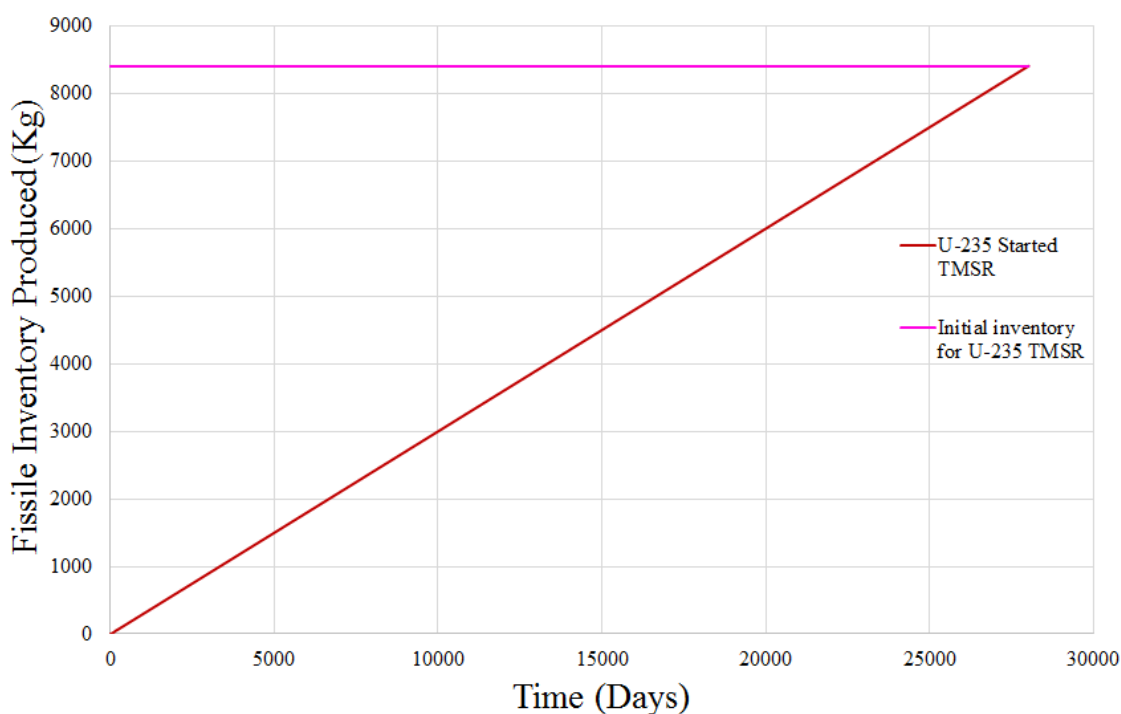


Figure 4.4. Estimation of the doubling time for the ^{235}U -operated TMSR

4.4. DISCUSSION

As seen in Figures 4.1, 4.3, and 4.5, the average neutron flux spectrum is slightly higher than that of the reference TMSR. Along with making the assumption that the reference data is based on a neutron flux of the fuel and blanket salt, it can also be

deduced that the in-house code, which the researchers coupled with MCNP, produced a more accurate neutron energy spectra. With these statements, it can be seen from Section 4.1 that the MCNP simulation reasonably agrees with the reference TMSR and allows for a good comparison of the ^{235}U and ^{239}Pu TMSRs with the ^{233}U TMSR.

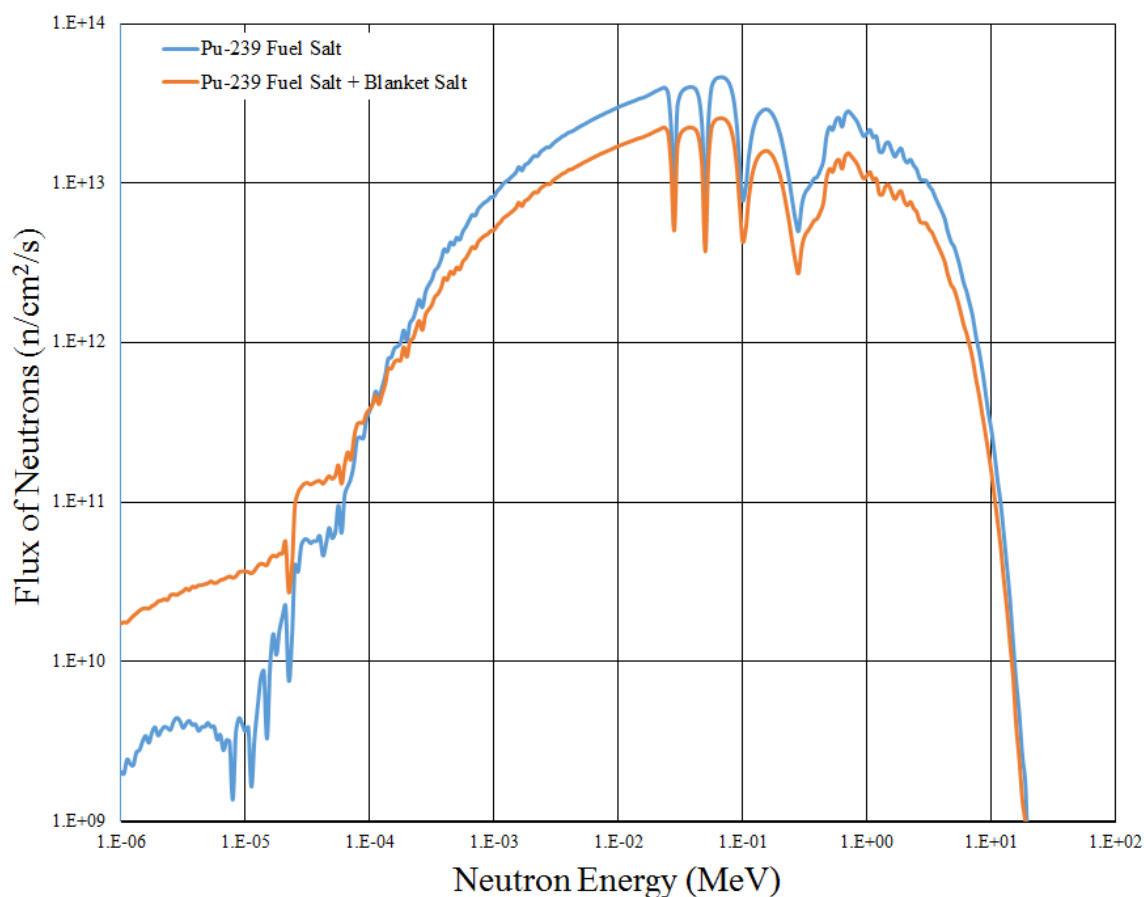


Figure 4.5. Neutron flux spectrum of the ^{239}Pu -operated TMSR. The fuel salt flux is depicted in blue, whereas a union of the fuel salt and blanket salt is depicted in orange.

From the simulations, it can be concluded that a ^{233}U -fueled TMSR would be the most efficient in terms of breeding more fuel for future TMSRs. However, Figure 3.3 shows that this is the opposite. It shows that the reference TMSR has the longest excess

production time and that a TRU-started TMSR would have the shortest. This is due to the fact that the data is based on the amount of excess ^{233}U produced in the blanket salt in reference to how much ^{233}U has already been used. Since the TRU and MOx fuels do not require an initial ^{233}U inventory, their excess production of ^{233}U increases more rapidly than that of the reference TMSR. Since the reference TMSR must breed enough fuel to replace its initial inventory before it can show excess production, its breeding times are longer. If one compares the breeding times of the ^{235}U and ^{239}Pu reactors based on this criteria, it can be concluded that a ^{239}Pu -operated TMSR would breed 5,200kg of ^{233}U in just 47.8 years, and a ^{235}U -operated TMSR would breed the same amount in 48 years.

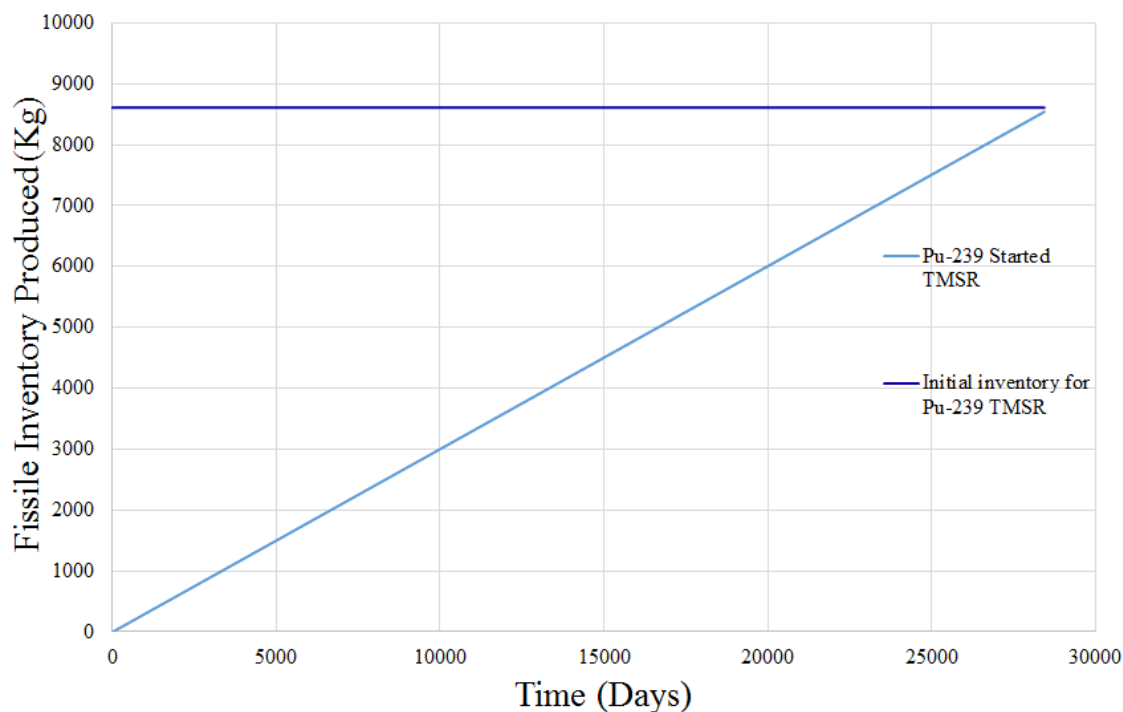


Figure 4.6. Estimation of the doubling time for the ^{239}Pu -operated TMSR

5. CONCLUSION

A thesis of a Thorium Molten Salt Reactor has been presented that benchmarks the reference TMSR and compares it to two alternate starter fuels maintaining criticality at an equal eutectic point to the reference data. With ^{235}U and ^{239}Pu readily available within nuclear weapons, these fuels can be used to start the first generation of MSR and breed ^{233}U for future generations. It can also be determined from Figures 4.4 and 4.6 that despite the long doubling times for ^{235}U and ^{239}Pu , both fissile fuels still breed ^{233}U at a similar rate to that of a ^{233}U -operated reactor thus concluding that both could be initial fuels in order to breed more fuel for future TMSRs.

APPENDIX A.

MCNP URANIUM 233 INPUT CODE

TMSR 2.7% U-233

c

c

c

c Cell Cards

c

1	100	-4.16	-101	103	-102	imp:n=1	VOL=8946175.95
2	200	-4.16	-201	101	-202	203	imp:n=1 VOL=7991426.31
3	300	-2.52	-301	201	-202	203	imp:n=1 VOL=4010243.02
4	400	-8.89	-401	301	-202	203	imp:n=1
5	400	-8.89	-402	401	-102	103	imp:n=1
6	400	-8.89	-403	102	-402		imp:n=1
7	400	-8.89	-103	404	-402		imp:n=1
8	500	-7.9	-501	402	-502	503	imp:n=1
9	500	-7.9	-402	403	-502		imp:n=1
10	500	-7.9	-402	503	-404		imp:n=1
11	100	-4.16	-401	202	-102	101	imp:n=1 VOL=1297477.77
12	100	-4.16	-401	103	-203	101	imp:n=1 VOL=1297477.77
13	0		-503:502:501				imp:n=0

c Surface Cards

c Central Salt Channel

101 cz 112.5

102 pz 112.5

103 pz -112.5

c

c Radial Blanket

c Use 101 as the inner radius

201 cz 162.5

202 pz 92.5

203 pz -92.5

c

c Boron Carbide Reflector

301 cz 182.5

c Use 201 as the inner radius

c Use 202 & 203 for top and bottom

c

c Ni-Alloy

401 cz 195

402 cz 250

c Use 102 and 103 for the top and bottom

403 pz 162.5

404 pz -162.5

c

c Stainless Steel

501 cz 270

502 pz 182.5

503 pz -182.5

c Data Cards

mode n

kcode 20000 1.0 50 400

ksrc 0 0 0

0 0 50

0 0 -50

BURN TIME = 60 60 60 \$ 6 months

MAT = 200 300

POWER = 3000

PFRAC = 1 2r

OMIT = 200 8 6014 7016 8018 8019 9018 10021 10022 91230

300 7 6014 7016 8018 8019 9018 10021 10022

AFMIN = 1.0E-10 5r

BOPT = 1.0 -14 -1

MATVOL = 7991426.31 4010243.02

c Fuel Salt LiF-ThF4-U233F4

m100 9019.72c -0.355802

3006.72c -0.00000060146 \$ 0.001mol% Li6

3007.72c -0.0601453985 \$ 99.999mol% Li7

90232.72c -0.5136998 \$ 22.5mol% of ThF4-U233F4

92233.72c -0.070352 \$ 2.7mol% U233F4

c Blanket Salt LiF-ThF4

m200 90232.72c -0.583926 \$ 22.5mol% of ThF4

9019.72c -0.355909

3006.72c -0.000060164

3007.72c -0.0601633984

c Boron Carbide Radial Reflector

m300 5010.72c -0.15574343 \$ I used atomic abundance of 19.9% for B10

5011.72c -0.62688687 \$ B10 concentrations can vary from

6000.72c -0.21736970 \$ 19.5% to 21.5%

c Nickel Hastelloy

c Ni-66.04 wt%

m400 28058.72c -0.449579848

28060.72c -0.173177352

28061.72c -0.0075278996

28062.72c -0.024002238

28064.72c -0.0061126624

c W-25.98 wt%

74182.72c -0.06915876

74183.72c -0.03717738

74184.72c -0.07960272

74186.72c -0.07386114

c Cr-5.90 wt%

	24050.72c	-0.00256355
	24052.72c	-0.04943551
	24053.72c	-0.00501559
	24054.72c	-0.139535
c	Mo-1.00 wt%	
	42092.72c	-0.001477
	42094.72c	-0.000923
	42095.72c	-0.001590
	42096.72c	-0.001668
	42097.72c	-0.000956
	42098.72c	-0.002419
	42100.72c	-0.000967
c	Fe-0.5 wt%	
	26054.72c	-0.00029225
	26056.72c	-0.0045877
	26057.72c	-0.00010595
	26058.72c	-0.0000141
c	Ti-0.20 wt%	
	22046.72c	-0.000165
	22047.72c	-0.0001488
	22048.72c	-0.0014744
	22049.72c	-0.0001082
	22050.72c	-0.0001036
c	C-0.05 wt%	
	6000.72c	-0.0005
c	Mn-0.20 wt%	
	25055.72c	-0.0020
c	Si-0.10 wt%	
	14028.72c	-0.00092223
	14029.72c	-0.00004685
	14030.72c	-0.00003092
c	Al-0.02 wt%	
	13027.72c	-0.0002
c	B-0.01 wt%	
	5010.72c	-0.0000199
	5011.72c	-0.0000801
c	P-0.01 wt%	
	15031.72c	-0.0001
c	SS 316	
c	.18 Cr	
m500	24050.72c	-0.007512282
	24052.72c	-0.150659658
	24053.72c	-0.01741212
	24054.72c	-0.00441594
c	.14 Ni	
	28058.72c	-0.0940758

28060.72c -0.0374878
 28061.72c -0.0016562
 28062.72c -0.005369
 28064.72c -0.0014112
 c .03 Mo
 42092.72c -0.0042438
 42094.72c -0.0027405
 42095.72c -0.0047187
 42096.72c -0.0050022
 42097.72c -0.002868
 42098.72c -0.0074058
 42100.72c -0.003021
 c .0008 C
 6000.72c -0.0008
 25055.72c -0.02
 15031.72c -0.00045
 c .0003 S
 16032.72c -0.000284145
 16033.72c -0.000002313
 16034.72c -0.000013506
 16036.72c -0.000000036
 c .0075 Si
 14028.72c -0.00688995
 14029.72c -0.000362475
 14030.72c -0.0002475
 c .001 N
 7014.72c -0.0009961
 7015.72c -0.0000039
 c .64995 Fe
 26054.72c -0.036722175
 26056.72c -0.59730405
 26057.72c -0.01403892
 26058.72c -0.001884855
 c
 f4:n 1 2
 e4 1.05000e-10 &
 1.00000e-9 1.05925e-9 1.12202e-9 1.18850e-9 1.25893e-9 &
 1.33352e-9 1.41254e-9 1.49624e-9 1.58489e-9 1.67880e-9 &
 1.77828e-9 1.88365e-9 1.99526e-9 2.11349e-9 2.23872e-9 &
 2.37137e-9 2.51189e-9 2.66073e-9 2.81838e-9 2.98538e-9 &
 3.16228e-9 3.34965e-9 3.54813e-9 3.75837e-9 3.98107e-9 &
 4.21697e-9 4.46684e-9 4.73151e-9 5.01187e-9 5.30884e-9 &
 5.62341e-9 5.95662e-9 6.30957e-9 6.68344e-9 7.07946e-9 &
 7.49894e-9 7.94328e-9 8.41395e-9 8.91251e-9 9.44061e-9 &
 1.00000e-8 1.05925e-8 1.12202e-8 1.18850e-8 1.25893e-8 &
 1.33352e-8 1.41254e-8 1.49624e-8 1.58489e-8 1.67880e-8 &

1.77828e-8 1.88365e-8 1.99526e-8 2.11349e-8 2.23872e-8 &
2.37137e-8 2.51189e-8 2.66073e-8 2.81838e-8 2.98538e-8 &
3.16228e-8 3.34965e-8 3.54813e-8 3.75837e-8 3.98107e-8 &
4.21697e-8 4.46684e-8 4.73151e-8 5.01187e-8 5.30884e-8 &
5.62341e-8 5.95662e-8 6.30957e-8 6.68344e-8 7.07946e-8 &
7.49894e-8 7.94328e-8 8.41395e-8 8.91251e-8 9.44061e-8 &
1.00000e-7 1.05925e-7 1.12202e-7 1.18850e-7 1.25893e-7 &
1.33352e-7 1.41254e-7 1.49624e-7 1.58489e-7 1.67880e-7 &
1.77828e-7 1.88365e-7 1.99526e-7 2.11349e-7 2.23872e-7 &
2.37137e-7 2.51189e-7 2.66073e-7 2.81838e-7 2.98538e-7 &
3.16228e-7 3.34965e-7 3.54813e-7 3.75837e-7 3.98107e-7 &
4.21697e-7 4.46684e-7 4.73151e-7 5.01187e-7 5.30884e-7 &
5.62341e-7 5.95662e-7 6.30957e-7 6.68344e-7 7.07946e-7 &
7.49894e-7 7.94328e-7 8.41395e-7 8.91251e-7 9.44061e-7 &
1.00000e-6 1.05925e-6 1.12202e-6 1.18850e-6 1.25893e-6 &
1.33352e-6 1.41254e-6 1.49624e-6 1.58489e-6 1.67880e-6 &
1.77828e-6 1.88365e-6 1.99526e-6 2.11349e-6 2.23872e-6 &
2.37137e-6 2.51189e-6 2.66073e-6 2.81838e-6 2.98538e-6 &
3.16228e-6 3.34965e-6 3.54813e-6 3.75837e-6 3.98107e-6 &
4.21697e-6 4.46684e-6 4.73151e-6 5.01187e-6 5.30884e-6 &
5.62341e-6 5.95662e-6 6.30957e-6 6.68344e-6 7.07946e-6 &
7.49894e-6 7.94328e-6 8.41395e-6 8.91251e-6 9.44061e-6 &
1.00000e-5 1.05925e-5 1.12202e-5 1.18850e-5 1.25893e-5 &
1.33352e-5 1.41254e-5 1.49624e-5 1.58489e-5 1.67880e-5 &
1.77828e-5 1.88365e-5 1.99526e-5 2.11349e-5 2.23872e-5 &
2.37137e-5 2.51189e-5 2.66073e-5 2.81838e-5 2.98538e-5 &
3.16228e-5 3.34965e-5 3.54813e-5 3.75837e-5 3.98107e-5 &
4.21697e-5 4.46684e-5 4.73151e-5 5.01187e-5 5.30884e-5 &
5.62341e-5 5.95662e-5 6.30957e-5 6.68344e-5 7.07946e-5 &
7.49894e-5 7.94328e-5 8.41395e-5 8.91251e-5 9.44061e-5 &
1.00000e-4 1.05925e-4 1.12202e-4 1.18850e-4 1.25893e-4 &
1.33352e-4 1.41254e-4 1.49624e-4 1.58489e-4 1.67880e-4 &
1.77828e-4 1.88365e-4 1.99526e-4 2.11349e-4 2.23872e-4 &
2.37137e-4 2.51189e-4 2.66073e-4 2.81838e-4 2.98538e-4 &
3.16228e-4 3.34965e-4 3.54813e-4 3.75837e-4 3.98107e-4 &
4.21697e-4 4.46684e-4 4.73151e-4 5.01187e-4 5.30884e-4 &
5.62341e-4 5.95662e-4 6.30957e-4 6.68344e-4 7.07946e-4 &
7.49894e-4 7.94328e-4 8.41395e-4 8.91251e-4 9.44061e-4 &
1.00000e-3 1.05925e-3 1.12202e-3 1.18850e-3 1.25893e-3 &
1.33352e-3 1.41254e-3 1.49624e-3 1.58489e-3 1.67880e-3 &
1.77828e-3 1.88365e-3 1.99526e-3 2.11349e-3 2.23872e-3 &
2.37137e-3 2.51189e-3 2.66073e-3 2.81838e-3 2.98538e-3 &
3.16228e-3 3.34965e-3 3.54813e-3 3.75837e-3 3.98107e-3 &
4.21697e-3 4.46684e-3 4.73151e-3 5.01187e-3 5.30884e-3 &
5.62341e-3 5.95662e-3 6.30957e-3 6.68344e-3 7.07946e-3 &
7.49894e-3 7.94328e-3 8.41395e-3 8.91251e-3 9.44061e-3 &

1.00000e-2 1.05925e-2 1.12202e-2 1.18850e-2 1.25893e-2 &
 1.33352e-2 1.41254e-2 1.49624e-2 1.58489e-2 1.67880e-2 &
 1.77828e-2 1.88365e-2 1.99526e-2 2.11349e-2 2.23872e-2 &
 2.37137e-2 2.51189e-2 2.66073e-2 2.81838e-2 2.98538e-2 &
 3.16228e-2 3.34965e-2 3.54813e-2 3.75837e-2 3.98107e-2 &
 4.21697e-2 4.46684e-2 4.73151e-2 5.01187e-2 5.30884e-2 &
 5.62341e-2 5.95662e-2 6.30957e-2 6.68344e-2 7.07946e-2 &
 7.49894e-2 7.94328e-2 8.41395e-2 8.91251e-2 9.44061e-2 &
 1.00000e-1 1.05925e-1 1.12202e-1 1.18850e-1 1.25893e-1 &
 1.33352e-1 1.41254e-1 1.49624e-1 1.58489e-1 1.67880e-1 &
 1.77828e-1 1.88365e-1 1.99526e-1 2.11349e-1 2.23872e-1 &
 2.37137e-1 2.51189e-1 2.66073e-1 2.81838e-1 2.98538e-1 &
 3.16228e-1 3.34965e-1 3.54813e-1 3.75837e-1 3.98107e-1 &
 4.21697e-1 4.46684e-1 4.73151e-1 5.01187e-1 5.30884e-1 &
 5.62341e-1 5.95662e-1 6.30957e-1 6.68344e-1 7.07946e-1 &
 7.49894e-1 7.94328e-1 8.41395e-1 8.91251e-1 9.44061e-1 &
 1.00000e+0 1.05925e+0 1.12202e+0 1.18850e+0 1.25893e+0 &
 1.33352e+0 1.41254e+0 1.49624e+0 1.58489e+0 1.67880e+0 &
 1.77828e+0 1.88365e+0 1.99526e+0 2.11349e+0 2.23872e+0 &
 2.37137e+0 2.51189e+0 2.66073e+0 2.81838e+0 2.98538e+0 &
 3.16228e+0 3.34965e+0 3.54813e+0 3.75837e+0 3.98107e+0 &
 4.21697e+0 4.46684e+0 4.73151e+0 5.01187e+0 5.30884e+0 &
 5.62341e+0 5.95662e+0 6.30957e+0 6.68344e+0 7.07946e+0 &
 7.49894e+0 7.94328e+0 8.41395e+0 8.91251e+0 9.44061e+0 &
 1.00000e+1 1.05925e+1 1.12202e+1 1.18850e+1 1.25893e+1 &
 1.33352e+1 1.41254e+1 1.49624e+1 1.58489e+1 1.67880e+1 &
 1.77828e+1 1.88365e+1 1.99526e+1 2.11349e+1 2.23872e+1 &
 2.37137e+1 2.51189e+1 2.66073e+1 2.81838e+1 2.98538e+1 &
 3.16228e+1 3.34965e+1 3.54813e+1 3.75837e+1 3.98107e+1 &
 4.21697e+1 4.46684e+1 4.73151e+1 5.01187e+1 5.30884e+1 &
 5.62341e+1 5.95662e+1 6.30957e+1 6.68344e+1 7.07946e+1 &
 7.49894e+1 7.94328e+1 8.41395e+1 8.91251e+1 9.44061e+1 &
 1.00000e+2
 fm4 2.324E+20

APPENDIX B.

MCNP URANIUM 235 INPUT CODE

TMSR 4.3% U-235

c

c

c

c Cell Cards

c

c Cell Cards

c

1	100	-4.16	-101	103	-102	imp:n=1	VOL=8946175.95
2	200	-4.16	-201	101	-202	203	imp:n=1 VOL=7991426.31
3	300	-2.52	-301	201	-202	203	imp:n=1 VOL=4010243.02
4	400	-8.89	-401	301	-202	203	imp:n=1
5	400	-8.89	-402	401	-102	103	imp:n=1
6	400	-8.89	-403	102	-402		imp:n=1
7	400	-8.89	-103	404	-402		imp:n=1
8	500	-7.9	-501	402	-502	503	imp:n=1
9	500	-7.9	-402	403	-502		imp:n=1
10	500	-7.9	-402	503	-404		imp:n=1
11	100	-4.16	-401	202	-102	101	imp:n=1 VOL=1297477.77
12	100	-4.16	-401	103	-203	101	imp:n=1 VOL=1297477.77
13	0		-503:502:501				imp:n=0

c Surface Cards

c Central Salt Channel

101 cz 112.5

102 pz 112.5

103 pz -112.5

c

c Radial Blanket

c Use 101 as the inner radius

201 cz 162.5

202 pz 92.5

203 pz -92.5

c

c Boron Carbide Reflector

301 cz 182.5

c Use 201 as the inner radius

c Use 202 & 203 for top and bottom

c

c Ni-Alloy

401 cz 195

402 cz 250

c Use 102 and 103 for the top and bottom

403 pz 162.5

404 pz -162.5

c

c Stainless Steel

501 cz 270

502 pz 182.5

503 pz -182.5

c Data Cards

mode n

kcode 20000 1.0 50 400

ksrc 0 0 0

0 0 50

0 0 -50

BURN TIME = 60 60 60

\$ 6 months

MAT = 200 300

POWER = 3000

PFRAC = 1 2r

OMIT = 200 8 6014 7016 8018 8019 9018 10021 10022 91230

300 7 6014 7016 8018 8019 9018 10021 10022

AFMIN = 1.0E-10 5r

BOPT = 1.0 -14 -1

MATVOL = 7991426.31 4010243.02

c Fuel Salt LiF-ThF4-U233F4

m100 9019.72c -0.355395

3006.72c -0.00000060078 \$ 0.001mol% Li6

3007.72c -0.0600773992 \$ 99.999mol% Li7

90232.72c -0.4716497 \$ 18.2mol% of ThF4-U235F4

92235.72c -0.112877 \$ 4.3mol% U235F4

c Blanket Salt LiF-ThF4

m200 90232.72c -0.583926 \$ 22.5mol% of ThF4

9019.72c -0.355909

3006.72c -0.000060164

3007.72c -0.0601633984

c Boron Carbide Radial Reflector

m300 5010.72c -0.15574343 \$ I used atomic abundance of 19.9% for B10

5011.72c -0.62688687 \$ B10 concentrations can vary from

6000.72c -0.21736970 \$ 19.5% to 21.5%

c Nickel Hastelloy

c Ni-66.04 wt%

m400 28058.72c -0.449579848

28060.72c -0.173177352

28061.72c -0.0075278996

28062.72c -0.024002238

28064.72c -0.0061126624

c W-25.98 wt%

74182.72c -0.06915876

74183.72c -0.03717738

74184.72c -0.07960272

74186.72c -0.07386114
c Cr-5.90 wt%
24050.72c -0.00256355
24052.72c -0.04943551
24053.72c -0.00501559
24054.72c -0.139535
c Mo-1.00 wt%
42092.72c -0.001477
42094.72c -0.000923
42095.72c -0.001590
42096.72c -0.001668
42097.72c -0.000956
42098.72c -0.002419
42100.72c -0.000967
c Fe-0.5 wt%
26054.72c -0.00029225
26056.72c -0.0045877
26057.72c -0.00010595
26058.72c -0.0000141
c Ti-0.20 wt%
22046.72c -0.000165
22047.72c -0.0001488
22048.72c -0.0014744
22049.72c -0.0001082
22050.72c -0.0001036
c C-0.05 wt%
6000.72c -0.0005
c Mn-0.20 wt%
25055.72c -0.0020
c Si-0.10 wt%
14028.72c -0.00092223
14029.72c -0.00004685
14030.72c -0.00003092
c Al-0.02 wt%
13027.72c -0.0002
c B-0.01 wt%
5010.72c -0.0000199
5011.72c -0.0000801
c P-0.01 wt%
15031.72c -0.0001
c SS 316
c .18 Cr
m500 24050.72c -0.007512282
24052.72c -0.150659658
24053.72c -0.01741212
24054.72c -0.00441594

c .14 Ni
 28058.72c -0.0940758
 28060.72c -0.0374878
 28061.72c -0.0016562
 28062.72c -0.005369
 28064.72c -0.0014112
 c .03 Mo
 42092.72c -0.0042438
 42094.72c -0.0027405
 42095.72c -0.0047187
 42096.72c -0.0050022
 42097.72c -0.002868
 42098.72c -0.0074058
 42100.72c -0.003021
 c .0008 C
 6000.72c -0.0008
 25055.72c -0.02
 15031.72c -0.00045
 c .0003 S
 16032.72c -0.000284145
 16033.72c -0.000002313
 16034.72c -0.000013506
 16036.72c -0.000000036
 c .0075 Si
 14028.72c -0.00688995
 14029.72c -0.000362475
 14030.72c -0.0002475
 c .001 N
 7014.72c -0.0009961
 7015.72c -0.0000039
 c .64995 Fe
 26054.72c -0.036722175
 26056.72c -0.59730405
 26057.72c -0.01403892
 26058.72c -0.001884855
 f4:n 1 2
 e4 1.05000e-10 &
 1.00000e-9 1.05925e-9 1.12202e-9 1.18850e-9 1.25893e-9 &
 1.33352e-9 1.41254e-9 1.49624e-9 1.58489e-9 1.67880e-9 &
 1.77828e-9 1.88365e-9 1.99526e-9 2.11349e-9 2.23872e-9 &
 2.37137e-9 2.51189e-9 2.66073e-9 2.81838e-9 2.98538e-9 &
 3.16228e-9 3.34965e-9 3.54813e-9 3.75837e-9 3.98107e-9 &
 4.21697e-9 4.46684e-9 4.73151e-9 5.01187e-9 5.30884e-9 &
 5.62341e-9 5.95662e-9 6.30957e-9 6.68344e-9 7.07946e-9 &
 7.49894e-9 7.94328e-9 8.41395e-9 8.91251e-9 9.44061e-9 &
 1.00000e-8 1.05925e-8 1.12202e-8 1.18850e-8 1.25893e-8 &

1.33352e-8 1.41254e-8 1.49624e-8 1.58489e-8 1.67880e-8 &
1.77828e-8 1.88365e-8 1.99526e-8 2.11349e-8 2.23872e-8 &
2.37137e-8 2.51189e-8 2.66073e-8 2.81838e-8 2.98538e-8 &
3.16228e-8 3.34965e-8 3.54813e-8 3.75837e-8 3.98107e-8 &
4.21697e-8 4.46684e-8 4.73151e-8 5.01187e-8 5.30884e-8 &
5.62341e-8 5.95662e-8 6.30957e-8 6.68344e-8 7.07946e-8 &
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5.62341e+1 5.95662e+1 6.30957e+1 6.68344e+1 7.07946e+1 &
7.49894e+1 7.94328e+1 8.41395e+1 8.91251e+1 9.44061e+1 &
1.00000e+2

fm4 2.321E+20

APPENDIX C.

MCNP PLUTONIUM 239 INPUT CODE

TMSR 4.3% Pu-239

c

c

c

c Cell Cards

c

1 100 -4.16 -101 103 -102 imp:n=1 VOL=8946175.95
 2 200 -4.16 -201 101 -202 203 imp:n=1 VOL=7991426.31
 3 300 -2.52 -301 201 -202 203 imp:n=1 VOL=4010243.02
 4 400 -8.89 -401 301 -202 203 imp:n=1
 5 400 -8.89 -402 401 -102 103 imp:n=1
 6 400 -8.89 -403 102 -402 imp:n=1
 7 400 -8.89 -103 404 -402 imp:n=1
 8 500 -7.9 -501 402 -502 503 imp:n=1
 9 500 -7.9 -402 403 -502 imp:n=1
 10 500 -7.9 -402 503 -404 imp:n=1
 11 100 -4.16 -401 202 -102 101 imp:n=1 VOL=1297477.77
 12 100 -4.16 -401 103 -203 101 imp:n=1 VOL=1297477.77
 13 0 -503:502:501 imp:n=0

c Surface Cards

c Central Salt Channel

101 cz 112.5

102 pz 112.5

103 pz -112.5

c

c Radial Blanket

c Use 101 as the inner radius

201 cz 162.5

202 pz 92.5

203 pz -92.5

c

c Boron Carbide Reflector

301 cz 182.5

c Use 201 as the inner radius

c Use 202 & 203 for top and bottom

c

c Ni-Alloy

401 cz 195

402 cz 250

c Use 102 and 103 for the top and bottom

403 pz 162.5

404 pz -162.5

c

c Stainless Steel

501 cz 270

502 pz 182.5

503 pz -182.5

c Data Cards

mode n

kcode 20000 1.0 50 400

ksrc 0 0 0

0 0 50

0 0 -50

BURN TIME = 60 60 60 \$ 6 months

MAT = 200 300

POWER = 3000

PFRAC = 1 2r

OMIT = 200 8 6014 7016 8018 8019 9018 10021 10022 91230

300 7 6014 7016 8018 8019 9018 10021 10022

AFMIN = 1.0E-10 5r

BOPT = 1.0 -14 -1

MATVOL = 7991426.31 4010243.02

c Fuel Salt LiF-ThF4-U233F4

m100 9019.72c -0.348783

3006.72c -0.000000605 \$ 0.001mol% Li6

3007.72c -0.060512395 \$ 99.999mol% Li7

90232.72c -0.4750696 \$ 18.20mol% of ThF4-Pu239F3

94239.72c -0.115635 \$ 4.3mol% Pu239F3

c Blanket Salt LiF-ThF4

m200 90232.72c -0.583926 \$ 22.5mol% of ThF4

9019.72c -0.355909

3006.72c -0.000060164

3007.72c -0.0601633984

c Boron Carbide Radial Reflector

m300 5010.72c -0.15574343 \$ I used atomic abundance of 19.9% for B10

5011.72c -0.62688687 \$ B10 concentrations can vary from

6000.72c -0.21736970 \$ 19.5% to 21.5%

c Nickel Hastelloy

c Ni-66.04 wt%

m400 28058.72c -0.449579848

28060.72c -0.173177352

28061.72c -0.0075278996

28062.72c -0.024002238

28064.72c -0.0061126624

c W-25.98 wt%

74182.72c -0.06915876

74183.72c -0.03717738

74184.72c -0.07960272

74186.72c -0.07386114

c Cr-5.90 wt%

24050.72c	-0.00256355
24052.72c	-0.04943551
24053.72c	-0.00501559
24054.72c	-0.139535
c Mo-1.00 wt%	
42092.72c	-0.001477
42094.72c	-0.000923
42095.72c	-0.001590
42096.72c	-0.001668
42097.72c	-0.000956
42098.72c	-0.002419
42100.72c	-0.000967
c Fe-0.5 wt%	
26054.72c	-0.00029225
26056.72c	-0.0045877
26057.72c	-0.00010595
26058.72c	-0.0000141
c Ti-0.20 wt%	
22046.72c	-0.000165
22047.72c	-0.0001488
22048.72c	-0.0014744
22049.72c	-0.0001082
22050.72c	-0.0001036
c C-0.05 wt%	
6000.72c	-0.0005
c Mn-0.20 wt%	
25055.72c	-0.0020
c Si-0.10 wt%	
14028.72c	-0.00092223
14029.72c	-0.00004685
14030.72c	-0.00003092
c Al-0.02 wt%	
13027.72c	-0.0002
c B-0.01 wt%	
5010.72c	-0.0000199
5011.72c	-0.0000801
c P-0.01 wt%	
15031.72c	-0.0001
c SS 316	
c .18 Cr	
m500 24050.72c	-0.007512282
24052.72c	-0.150659658
24053.72c	-0.01741212
24054.72c	-0.00441594
c .14 Ni	
28058.72c	-0.0940758

28060.72c -0.0374878
 28061.72c -0.0016562
 28062.72c -0.005369
 28064.72c -0.0014112
 c .03 Mo
 42092.72c -0.0042438
 42094.72c -0.0027405
 42095.72c -0.0047187
 42096.72c -0.0050022
 42097.72c -0.002868
 42098.72c -0.0074058
 42100.72c -0.003021
 c .0008 C
 6000.72c -0.0008
 25055.72c -0.02
 15031.72c -0.00045
 c .0003 S
 16032.72c -0.000284145
 16033.72c -0.000002313
 16034.72c -0.000013506
 16036.72c -0.000000036
 c .0075 Si
 14028.72c -0.00688995
 14029.72c -0.000362475
 14030.72c -0.0002475
 c .001 N
 7014.72c -0.0009961
 7015.72c -0.0000039
 c .64995 Fe
 26054.72c -0.036722175
 26056.72c -0.59730405
 26057.72c -0.01403892
 26058.72c -0.001884855
 f4:n 1 2
 e4 1.05000e-10 &
 1.00000e-9 1.05925e-9 1.12202e-9 1.18850e-9 1.25893e-9 &
 1.33352e-9 1.41254e-9 1.49624e-9 1.58489e-9 1.67880e-9 &
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 1.77828e+1 1.88365e+1 1.99526e+1 2.11349e+1 2.23872e+1 &
 2.37137e+1 2.51189e+1 2.66073e+1 2.81838e+1 2.98538e+1 &
 3.16228e+1 3.34965e+1 3.54813e+1 3.75837e+1 3.98107e+1 &
 4.21697e+1 4.46684e+1 4.73151e+1 5.01187e+1 5.30884e+1 &
 5.62341e+1 5.95662e+1 6.30957e+1 6.68344e+1 7.07946e+1 &
 7.49894e+1 7.94328e+1 8.41395e+1 8.91251e+1 9.44061e+1 &
 1.00000e+2
 fm4 2.332E+20

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