Analysis of Multi-recycle Thorium Fuel Cycles in Comparison with Once-through Fuel Cycles

A Thesis
Presented to
The Academic Faculty

by

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In Partial Fulfillment
of the Requirements for the Degree
Master of Science in the
Nuclear and Radiological Engineering Program
School of Mechanical Engineering

Georgia Institute of Technology
May 2013

Analysis of Multi-recycle Thorium Fuel Cycles in Comparison with Once-through Fuel Cycles

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Date Approved: 03/29/2013

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ACKNOWLEDGEMENTS

I express my deepest gratitude to Dr. Bojan Petrovic, my faculty advisor, for his guidance and patience in helping me to reach my goals. It is with his advice that this thesis was made possible. I would also like to thank Dr. Fausto Franceschini and the rest of the researchers at Westinghouse Electric Co. who collaborated in a research project that helped fund this research.

I am thankful for a loving mother and father who made my education possible through immense emotional and monetary support. I give thanks to all of my family and friends who are caring and supportive of my endeavors.

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SUMMARY

Depletion of nuclear fuel in fission reactors produces transuranic waste products which have long half-lives. Minor actinides (MAs) comprise all of the transuranic elements except for plutonium. These MAs would burden the repository with long term heat and radio-toxicity, possibly up to one million years or more. Current policy dictates that a repository should be designed to safely contain the waste for a million years. However, the uncertainty is extremely high over such a long time period. It may not be possible to account for every event that could occur over 1 million years. It is therefore desirable to reduce the amount of long lived waste products as much as possible so that an unexpected release of stored materials would have reduced/acceptable consequences.

The purpose of this research is to develop a methodology for a thorium fuel recycling analysis that provides results for isotopics and radiotoxicity evaluation and analysis. This research is motivated by the need to reduce the long term radiological hazard in spent nuclear fuel, which mitigates the mixing hazard (radio-toxicity and chemical toxicity) and decay heat load on the repository. The first part of the thesis presents comparison of several once-through cases with uranium and thorium fuels to show how transuranics build up as fuel is depleted. The once-through analysis is performed for the following pairs of comparison cases: low enriched uranium dioxide (UOX) vs. thorium dioxide with ^{233}UOX (^{233}U-ThOX), natural uranium dioxide mixed with transuranic oxides (U-TRUOX) vs. thorium dioxide mixed with transuranic oxides (Th-TRUOX), natural uranium dioxide mixed with weapons grade plutonium dioxide (U-WGPuOX) vs. thorium dioxide mixed with weapons grade plutonium dioxide (Th-WGPuOX), natural uranium dioxide mixed with reactor grade plutonium dioxide (U-RGPuOX) vs. thorium mixed with reactor grade plutonium dioxide (Th-RGPuOX). The second part of the research

evaluates the thorium fuel equilibrium cycle in a pressurized water reactor (PWR) and compares several recycling cases with different partitioning schemes. Radio-toxicity results of the once-through cycle and multi-recycle calculations demonstrate advantages for thorium fuel and reprocessing with respect to long term nuclear waste management.

INTRODUCTION

Fuel Cycle Background

The current fuel cycle employed in commercial reactors in the United States is a once-through fuel cycle with low-enriched uranium fuel depleted in light water reactors. Several steps of this fuel cycle are described in this section; however the focus is on the back end of the fuel cycle. The fuel cycle starts when uranium ore is mined from the ground. Then the uranium is converted into uranium hexafluoride and sent to be enriched. After enrichment the fuel pellets are fabricated and irradiated in a light water reactor (LWR). When the reactor is refueled the irradiated fuel is placed into a cooling pool for several years until the more active fission products decay away. Finally, the irradiated fuel is placed into temporary storage casks at the reactor site[1]. The next step in the once-through fuel cycle is still being debated. Some suggest that the spent fuel should be put in a permanent underground repository. However, it is well known fact that spent fuel is not really spent fuel. Spent fuel still contains 95% uranium[2]. The current fuel cycle only utilizes a tiny fraction of the energy in the fuel. Spent fuel can be reprocessed in order to further utilize stored energy[1]. In addition to improved utilization of fuel, reprocessing would reduce the time HLW radio-toxicity requires to decrease to acceptable levels.

Most reprocessing in the US has only been demonstrated on a small scale for several test reactors with fuel forms that differed from oxide pellets bound in Zircaloy 4 with the exception of West Valley Reprocessing Facility. The West Valley Reprocessing Facility used PUREX to reprocess nearly 650 metric tons of spent fuel from 1966-1972. Types of fuel that the West Valley Facility processed include metallic fuel from the weapons plutonium program, uranium oxide fuels, and even thorium oxide fuels. The West Valley Facility was shut down due to difficulties properly monitoring worker's dosage and due to evolving regulations requiring costly

upgrades to protect against earthquakes and other natural disasters[3]. Examples of reprocessing for test reactor include pyroprocessing at Argonne National Laboratory for EBR II's metallic fuel, and online reprocessing using molten fluoride salts for the molten salt reactor at Oak Ridge National Laboratory. Only PUREX has been used on a large scale to separate plutonium for producing weapons in the US. Further development and adaptation for the PUREX process for civilian use has been done in France, Russia, India, Japan, and the UK[4]. The PUREX process has some proliferation risks because it separates plutonium from uranium, hence why it was used for producing weapons[5]. More advanced aqueous reprocessing technologies seek to reduce the proliferation risk by keeping plutonium and uranium together. The UREX and UREX+ process under development offers more proliferation resistant separation capabilities for legacy nuclear waste[4]. The THOREX process could be used to separate fission products from thorium based fuels although this technology is not as developed as PUREX[4]. Some research has been done on using a combination of PUREX and THOREX to achieved desired separation of isotopes[6].

Regardless of whether spent nuclear fuel is reprocessed or not a permanent repository is necessary to store the leftover high level waste (HLW) products. Technical requirements under current policy are too stringent to be met unless separation and recycling of spent nuclear fuel is implemented in order to reduce to long term hazard of the fuel. An Advanced multi-recycle fuel cycle using improved fuel could greatly simplify the design of a permanent repository by reducing the time it takes for the long term radio-toxicity to decrease to a level that is equivalent to natural uranium ore[7].

Advantages and Disadvantages of the Thorium Fuel Cycle

Thorium fuel has potential for superior performance compared to uranium fuel, especially when the metric is the environmental impact of the spent fuel. It produces fewer transuranics

than uranium fuel because it is a lighter isotope and requires many more neutron captures in order to produce minor actinides. In a once-through cycle, uranium fuel depleted in a PWR produces around five orders of magnitude more MAs than thorium fuel mixed with ^{233}U. This also makes thorium fuel a better candidate for the incineration of weapons grade plutonium[8]. Thorium is about 3 to 4 times more abundant in the Earth's crust than uranium with significant deposits occurring in many different locations around the world, ensuring long term sustainability[9]. Thorium fuel with ^{233}U has better capabilities for breeding in a thermal spectrum than uranium and plutonium fuel. This is due to a higher capture cross-section in ^{232}Th, and because ^{233}U has an excellent fission to capture cross-section ratio in the thermal spectrum. Also, it is more chemically stable and has better thermal properties than uranium fuel. Fissile material bred in a thorium reactor is more proliferation resistant because ^{232}U, which emits high energy gamma radiation, is produced along with ^{233}U [10]. The fertile reaction chains for the thorium cycle and plutonium cycle are shown in figure 1.

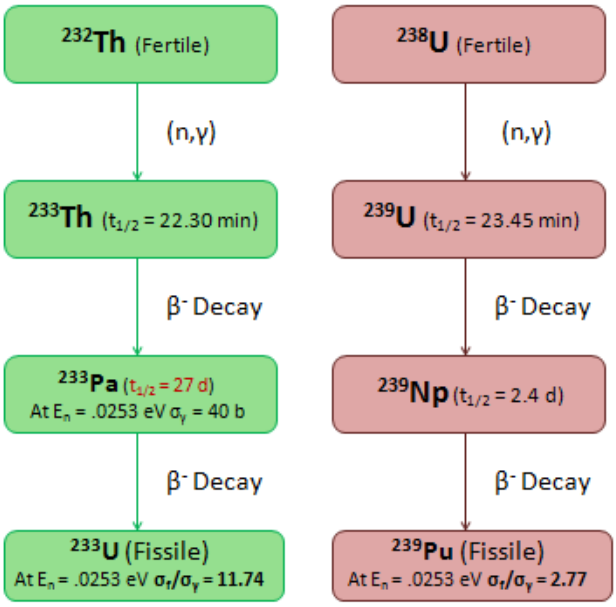

Figure 1. Fertile transmutation chains for thorium and uranium fuel cycles

^{232}Th is not a fuel itself, but a fertile isotope. Thorium must absorb a neutron in order to make ^{233}U, which is fissile. In order to get the most benefit from thorium fuel it must be reprocessed to make use of ^{233}U. Most difficulties with thorium arise during reprocessing. While the molecular stability of thorium dioxide is beneficial during irradiation, it can be challenging to reprocess. Thorium dioxide does not dissolve easily in aqueous separation processes and requires a longer time with more corrosive acids adding greater costs to the fuel cycle. Molten salt reactors may circumvent this difficulty, but current technological trends and political friction have stifled further development of this technology. In addition to hindering weapon production, ^{232}U makes reprocessing difficult because it produces harmful penetrating radiation. ^{232}U is produced through several different pathways. The most common pathway is through[11]:

$$^{232}_{90}Th \xrightarrow{n,2n} {}^{231}_{90}Th \xrightarrow{\beta^-} {}^{231}_{91}Pa \xrightarrow{n,\gamma} {}^{232}_{91}Pa \xrightarrow{\beta^-} {}^{232}_{92}U \qquad \textbf{Eq 1.1}$$

Additionally, an n,2n reaction with ^{233}U can produce ^{232}U. ^{232}U alpha decays to ^{228Th} which alpha decays with a half-life of 68.9 years. ^{232}U's decay chain produces ^{212}Bi and ^{208}Tl which emits 0.7–1.8 MeV and 2.6 MeV respectively. A reprocessing facility will require costly equipment and shielding for remote handling of irradiated thorium fuel due to the highly penetrating radiation. Since thorium fuel has a higher melting point than uranium fuel, it requires higher temperatures to sinter into pellets[10] .

The current once-through uranium fuel cycle costs much less than a closed thorium fuel cycle. However, a closed thorium fuel cycle has much better utilization of resources. A closed fuel cycle can produce hundreds of times more energy from the same amount of fuel than a once-through cycle. While a closed thorium cycle is seen as more expensive than once-through uranium fuel cycle, when considering the effects of the backend of the fuel cycle reprocessing can make a closed thorium fuel-cycle a cheaper way to utilize nuclear energy[7]. However, further

development of thorium based fuel reprocessing technologies is required for commercial implementation.

Thorium Fuel in a PWR

All current commercial reactors in the US are LWRs. The advantage of using thorium fuel in a LWR instead of an advanced reactor design is that there is more experience in the nuclear industry with LWRs. It is reported that tests using thorium-based fuels in LWRs have shown excellent performance with the (Th:U)O2 and (Th:Pu)O2 fuels. Burn-ups of up to about 60 000–80 000 MWd/tHM seem to be possible[12]. There have been several studies on thorium fuel cycles with limited recycling and closed fuel cycles in PWRs. These studies look at heterogeneous configurations in order to achieve a better conversion ratio. The two types of heterogeneous configurations include seed and blanket core and heterogeneous fuel assemblies. PWRs with thorium fuel require a heterogeneous reactor core configuration to achieve a sustainable breeding ratio, but the achievable discharge burnup is only around 20 GWd/tHM in currently operating reactors due to parasitic absorption in thorium. This is a very small discharge burnup compared to what current normal uranium fuel achieves. This technology was demonstrated at the Shippingport Reactor from 1977 to 1982[13].

Earlier research of thorium fuel in LWRs has demonstrated how thorium fuel generates less plutonium and minor actinides than uranium fuel. A previous study was done at Brookhaven National Laboratory compared once-through isotopic composition as a function of burnup between thorium and uranium fuels. The results showed uranium fuel producing three orders of magnitude more plutonium and five orders of magnitude more minor actinides than thorium fuel. Thorium fuel has much lower radioactivity and decay heat than uranium fuel

from 300 years to around 5000 years until the decay of the daughter isotopes of ^{232}U and ^{233}U dominate radioactivity[14].

A previous study done at Karlsruhe Institute of Technology performed analysis on a multi-recycling of thorium fuel mixed with enriched uranium. The results showed that using 73% thorium the minor actinides and plutonium production together was halved with a 25% reduction in minor actinides compared to normal enriched uranium fuel. The multi-recycling scheme in this study separates out fission products, plutonium, and minor actinides leaving only uranium and thorium oxide fuels[15].

Another study done at Delft University of Technology in the Netherlands did a similar study comparing different enrichments of uranium mixed with thorium fuel in a multi-recycle scenario. They compared low enriched uranium with no thorium, uranium at 20% enrichment with 75% thorium fuel and high enriched uranium with 95% thorium. The once-through results show that the fuel with higher thorium concentration has a lower radiotoxicity until about 20,000 years when daughters of ^{233}U dominate. The results show that if ^{233}U is not available for top up then highly enriched uranium is required for using thorium to reduce radiotoxicity in a multi-recycle scenario where minor actinides are removed and.1% to 1% is taken as losses each cycle depending on the isotope[16].

This work develops and implements a methodology for multi-recycling analysis with selective separation of actinides using the SCALE code package. It is motivated by the need for an approach which considers sustainability and long-term waste management as important factors for evaluating fuel cycles[17]. In contrast to the previous studies, not including Todosow, this thesis considers recycling thorium + ^{233}U fuel assumed with no bounds on pure ^{233}U and

^{232}Th makup instead of HEU. Also, the thorium fuel multi-recycle study in this thesis compares recycling back transuranics with strategic separation of specific actinides each cycle in order to reduce long term radio-toxicity, whereas the previous studies look at either separating all transuranics or not separating any of them. This thesis compares three recycling options: (i) recycling back all actinides; (ii) selectively removing Np in each recycle; and, (iii) removing Np and Pu each cycle. Also, the effect of separation efficiency will be analyzed since the capabilities of THOREX and other potential recycling processes are still fairly uncertain. Multi-recycle isotopics and radio-toxicity are evaluated for separation efficiencies of 100%, 95%, and 70%. Selectively removing actinides at the beginning of the plutonium absorption chain mitigates production of plutonium and minor actinides and may be more cost effective than recycling all actinides back. Figure 2 shows the actinide transmutation chains. The figure shows that the most likely absorption pathway to heavier minor actinides is through ^{242}Pu(n,γ)^{243}Pu where ^{243}Pu decays quickly beta decays to ^{243}Am which leads directly to higher minor actinides. ^{238}Pu is produced after ^{237}Np absorbs a neutron producing ^{238}Np which decays after approximately two days.

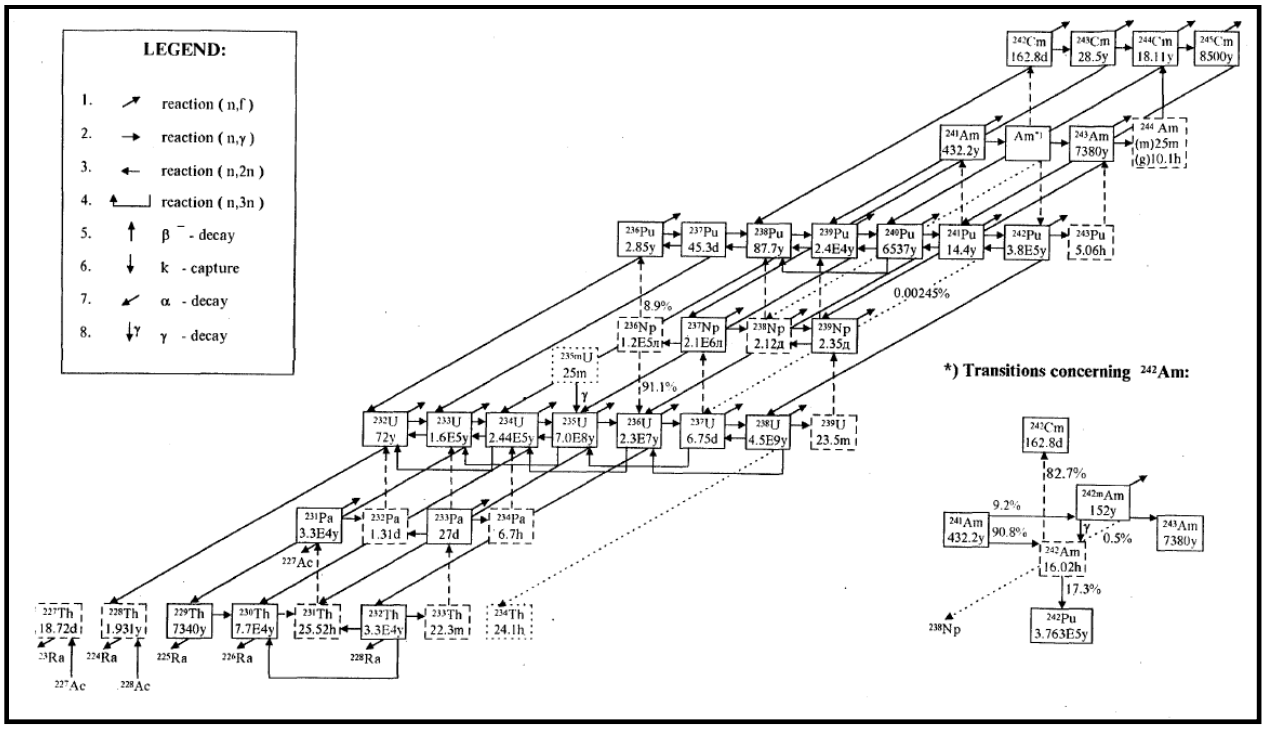

Figure 2. Actinide transmutation chain from thorium to curium[18].

In addition to the multi-recycle study, four pairs of once-through cycles compare thorium and uranium based fuels. The pairs of once-through cases include the two pairs of once through cases in Todosow in addition to uranium or thorium mixed with weapons grade plutonium and reactor grade plutonium.

The following chapters in this thesis include methodology, once-through cycle isotopics results, multi-recycle isotopics results, and radiotoxicity results. Chapter 2, methodology, describes modeling methods in SCALE6.0, once-through depletion calculations, multi-recycle separation scenario calculations, and radio-toxicity calculations. Chapter 3, once-through isotopic results, includes depletion results for the four pairs of uranium and thorium based fuels. Chapter 4, multi-recycle results, shows isotopics for the three different separation cases and the effect of changing separation efficiency on isotopics. Chapter 5, radio-toxicity results, compares

radio-toxicity of once-through cases and multi-recycle cases. Chapter 6 contains conclusions and recommendations for future work.

METHODOLOGY

A methodology was developed to perform simulations for the studies done in this thesis. This was necessary in order to evaluate once-through cycle scenarios with equivalent cycle lengths and to investigate thorium fuel multi-recycle scenarios. The first part of the methodology includes developing an iterative process to calculate fissile material concentration for the correct cycle length based on the linear reactivity approximation using SCALE6.0. The second part of the methodology was developing scripts that calculated the fissile material concentration, simulated separation of fission products, simulated partitioning of select transuranics, and calculated the needed makeup for each residence cycle. This chapter includes a description of how the SCALE6.0 depletion calculation is set up, the method for calculating fissile material concentration for correct cycle length, and the multi-recycle separation and partitioning methodology.

Depletion Calculations in SCALE6.0

SCALE6.0 is a nuclear physics simulation code package that has several control sequences to be selected by the user depending on the desired type of calculation. Control sequences include TRITON used for depletion, CSAS used for criticality safety, TSUNAMI used for sensitivity studies, and MAVRIC for shielding calculations. Each control sequence calls upon several of the many specialized modular codes to complete a task and then pass its result to the next module until the calculation is completed. Depletion calculations in this study used the TRITON sequence in the SCALE6.0 package. Figure 3 shows the order the codes are called by TRITON to perform a 2D deterministic depletion calculation.

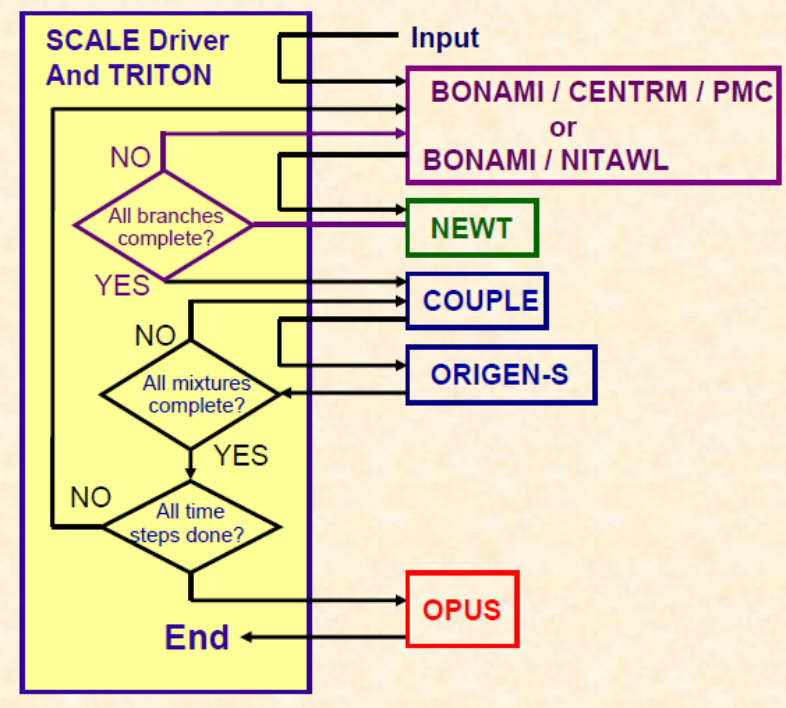

Figure 3. TRITON 2D deterministic depletion sequence[19]

Included, but not shown above are the Crawdad and Worker modules. Crawdad reads the input and generates problem specific data sets for the BONAMI and NEWT codes. Worker reads the cross-section data libraries in preparation for CENTRM and PMC which calculate problem dependent cross-sections. Worker is then called again to take the problem dependent cross-sections and prepare them for NEWT, which is a 2D discrete-ordinates transport code. COUPLE then takes flux weighted cross-sections from NEWT and prepares them for ORIGEN-S, which is the depletion code. This sequence is repeated for each time step for the length of the fuel cycle[18].

Once-Through Cycle Calculations

To allow consistent comparison among the considered cases, as well as the previous results, all of the once-through depletion calculations are modeled as a three batch fuel cycle[14]. Each cycle lasts for 18 months with 486 full power days (FPD) and a 54 day down time to

account for refueling and maintenance. In total each batch is depleted for 1458 FPD. The capacity factor is 90%. Instead of full 3-D core analysis, depletion calculations are performed on the quarter fuel assembly level. The correct fissile isotope concentrations for each fuel type must be solved for to give the required cycle length in order to compare different fuels. This is achieved using the linear reactivity approximation and solving for where the second batch's K-inf is equal to K_o. A K-inf of K_o is solved for in order to account for assumed $(K_o-1)/K_o$ representative core leakage because the depletion calculation is for a quarter fuel assembly with reflective boundary conditions. In this study K_o is assumed to be 1.03 to represent 3% core leakage. Two initial fissile isotope concentration guesses are made in order to solve for the amount of fissile material that gives the required cycle length. The cycle lengths of the initial guesses are calculated in SCALE6.0. A linear interpolation is used to solve for the correct fissile concentration. The fissile concentration is represented by x and K-inf is represented by f(x). The two initial concentration guesses are represented by x_a and x_b. Equation 2.1 shows how the linear interpolation is done.

$$x_1 = \frac{K_o - f(x_b) - \left(\frac{f(x_b)-f(x_a)}{x_b-x_a}\right)x_b}{\frac{f(x_b)-f(x_a)}{x_b-x_a}} \qquad \textbf{Eq. 2.1}$$

If the new fissile concentration still does not give the correct cycle length then another linear interpolation is done using x_1 and x_b to find x_2. This is repeated until to K-inf at 972 FPD converges to 1.03, typically requiring about two to four iterations to converge within 100 pcm. Once the correct fissile concentration is calculated the density and specific power must be recalculated. The weight fraction of each isotope is converted to atom fractions. The atom fraction is used to weight the partial densities which are summed to get the new mixture's density.

Multi-recycle Calculation

Multi-recycle isotopics are calculated for several thorium fuel recycling scenarios. Depletion is modeled in SCALE6.0. After each cycle, the output from SCALE6.0 is used to generate a new input for the next cycle. Figures 4-7 shows the mass flow diagrams for several closed thorium fuel cycle scenarios.

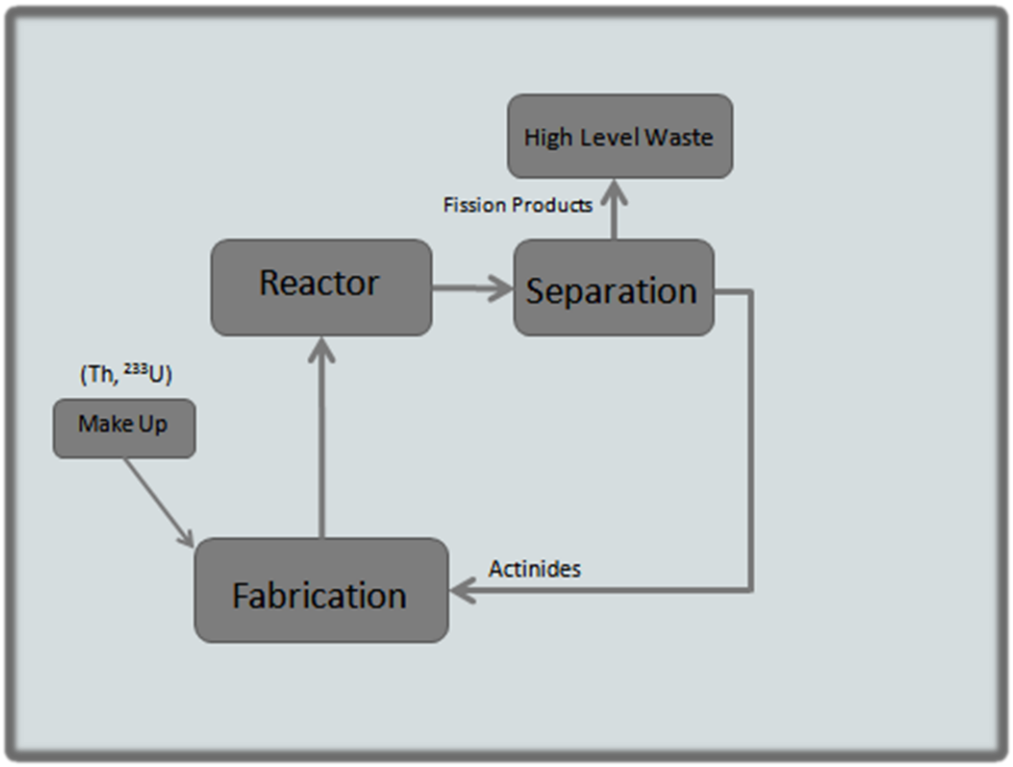

Figure 4. Material flow for a closed thorium fuel cycle with no losses material flow

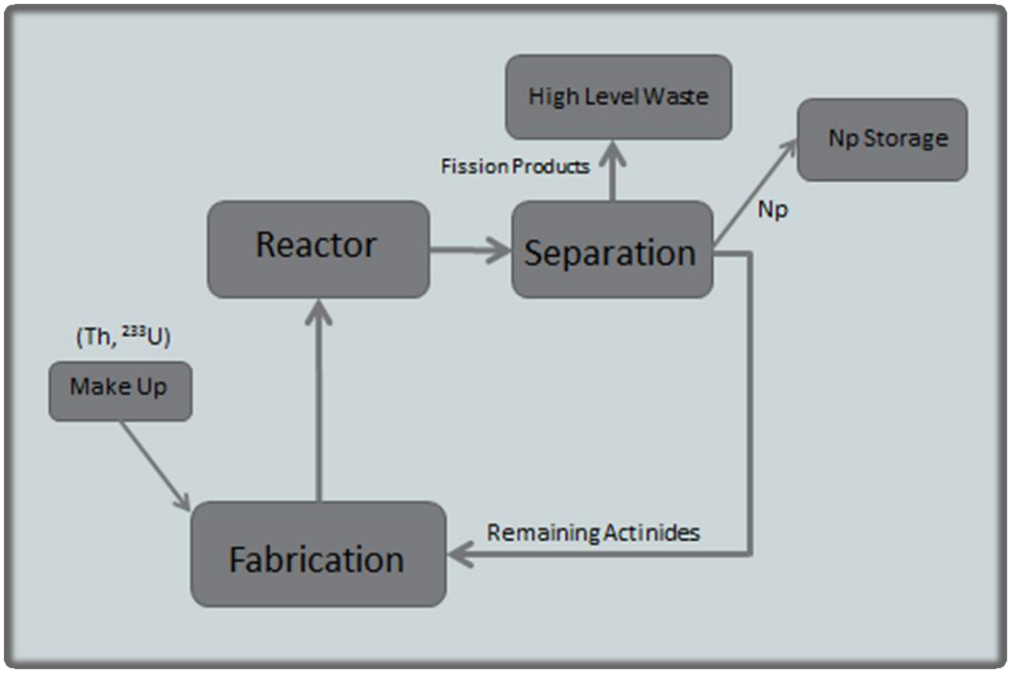

Figure 5. Material flow for a closed thorium fuel cycle with no losses with neptunium removed each cycle

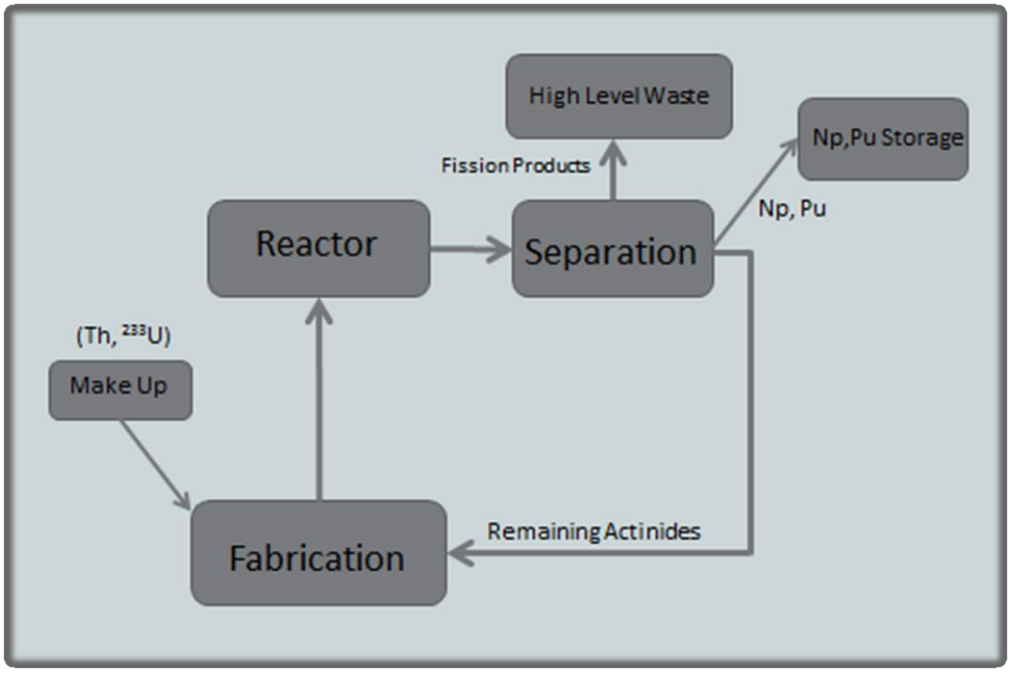

Figure 6. Material flow for a closed thorium fuel cycle with no losses and both neptunium and plutonium removed each cycle

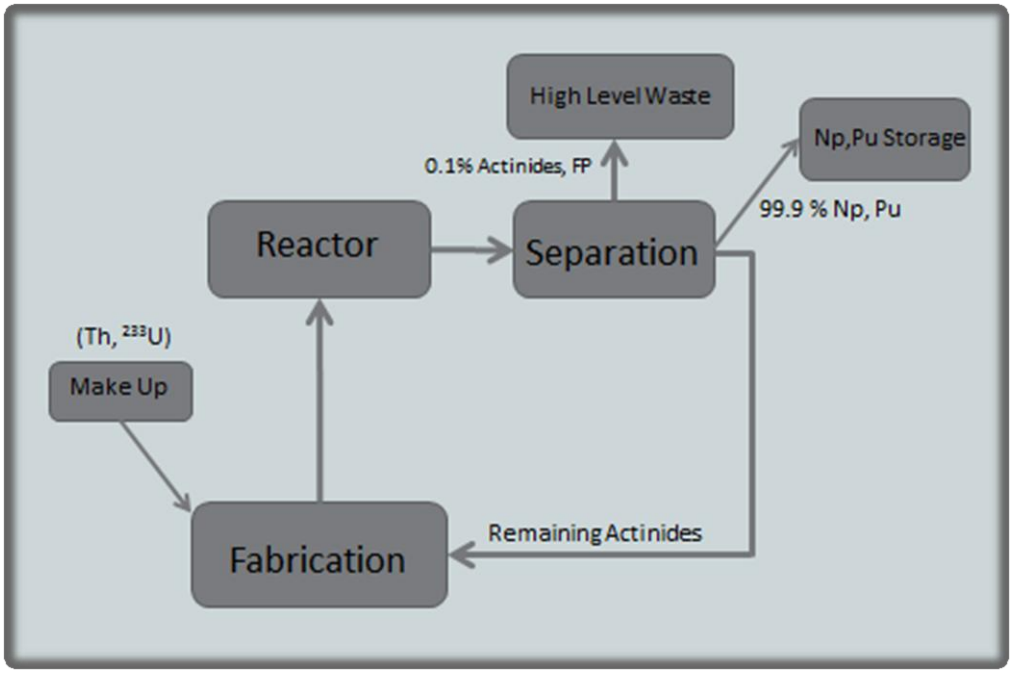

Figure 7. Material flow for a closed thorium fuel cycle with .1% losses and both neptunium and plutonium removed each cycle

To model the fuel cycle scenarios, a set of Python and Bourne shell scripts was developed. Python is used to generate input files for depletion in SCALE6.0. The Bourne shell script is used to call Python and SCALE6.0 in the correct sequence and organize input, output, and data files into the correct directories. The scripts are necessary in order to allow the simulation to run continuously and assist with repetitive long calculations in between depletion runs. The quarter fuel assembly is modeled in SCALE6.0 using TRITON 2D depletion sequence. The scripts take the isotopics output from SCALE6.0 and calculates what goes to storage, high level waste, and what goes to fabrication. The amount of make-up is calculated while iteratively solving for the correct fuel volume. The script then creates two new depletion input files with initial guesses of fissile material to solve for the correct cycle length. Equation 2.1 is used to find the concentration of fissile material that gives the correct cycle length. This is similar to the method used to solve for fissile material concentrations in the once-through

calculations except that it only requires one iteration since the uncertainty is much smaller giving a much smaller error using a linear method. The fuel density is iteratively calculated until it gives the correct fuel volume and fissile material concentration. A new input file is then created to model the depletion of the current cycle. This process is repeated until the isotopic concentrations have a very small change from cycle to cycle. Figure 8 is a flow diagram describing this process. ^{252}Cf is an isotope that gives a good metric for when a fuel cycle is close to equilibrium since it goes to equilibrium very slowly. The cycle length is solved to give a K-inf of 1.03 at the end of the second batch with an error no more than 100 pcm.

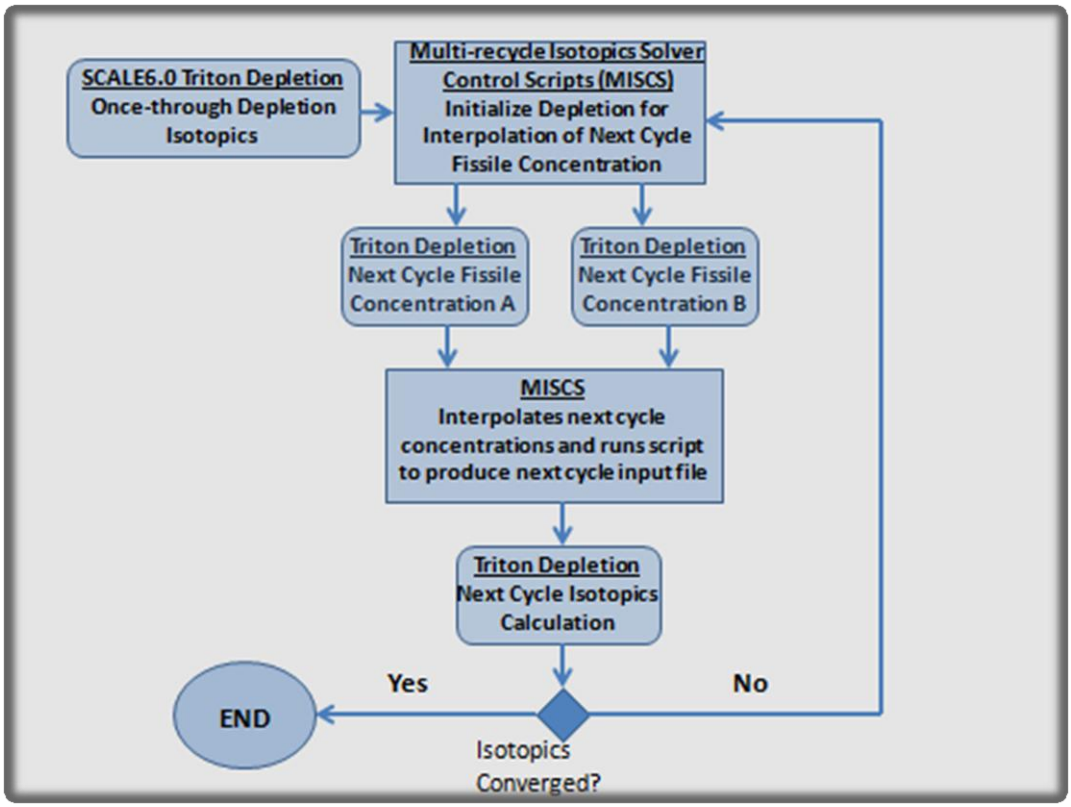

Figure 8. Flow diagram describes multi-recycle control sequence. Each iteration is one residence cycle

Correct mass flows from one cycle to the next require solving for the density that gives the required fuel volume before making a new depletion input. The concentration of the fissile

isotope is already given when solving for the correct density. First, a small amount of thorium make up is added. Then ^{233}U is added to give the correct ratio of fissile material. The partial densities are summed up. If the volume of the fuel is still less than the available fuel volume in the reactor then the process starts over and more thorium is added. This loop continues until the fuel fills the correct fuel volume and is found with the correct concentrations. Figure 9 illustrates this process.

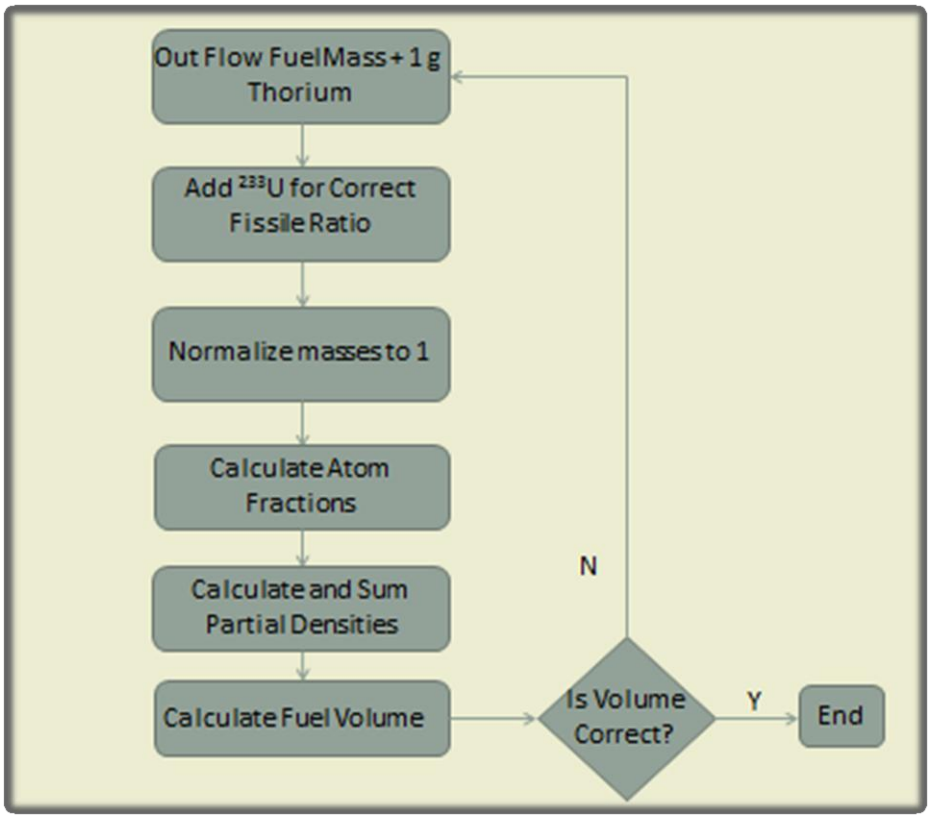

Figure 9. Diagram shows loop used to solve for composition giving correct fuel volume

Radio-toxicity Calculation

Radiotoxicity can be defined as either the volume of water or the volume of air required to dilute hazardous radioactive materials to an acceptable level determined by the Recommended Concentration Guides (RCG's). The recommended concentration gives a radio-toxicity equivalent to pitch blend[20]. ORIGEN-S, the standalone depletion and decay code apart of the

SCALE6.0 package is used to calculate decay for 2226 nuclides. Opus processes the output data and displays radio-toxicity according to the RCGs[18].

In order to calculate radiotoxicity for multi-recycle cases with no losses the ft71 restart files are called upon in the ORIGEN-S input. The ft71 restart files contain the input isotopic data for each depletion step from the multi-recycle depletion runs. The correct depletion step must be manually selected for the ORIGEN-S decay calculation to use the correct isotopics at the end of the 5 year cooldown. In the multi-recycle cases with no losses the .1% losses are not explicitly taken out by the script in between depletion runs so .1% the radio-toxicity calculated in ORIGEN-S is the actual load going to the repository. 99.9% of the fuel gets recycled back into the reactor and only the losses go to permanent HLW repository.

The multi-recycle case where .1% of actinide losses are taken directly by the script does not use an ft71 restart file to provide ORIGEN-S with input isotopics. Instead a script directly generates an ORIGEN-S input file with the isotopics copied in since these concentrations are known from when they were taken out in between cycles as losses.

Methodology developed for this research provided the ability to evaluate once-through cycle depletion isotopics, multi-recycle depletion isotopics, and back end radio-toxicity of different fuel cycle scenarios. An iterative process was created to solve for the fissile material concentration that gave the correct cycle length. In order calculate multi-recycle isotopics and radio-toxicity a methodology was implemented using Python and Bourne shell scripts to create and run SCALE6.0 depletions and to model the back end flow of the fuel.

ONCE-THROUGH CYCLE ISOTOPICS STUDY

In order to compare thorium fuel to uranium fuel several once-through cycle equivalent cycle length scenarios are evaluated using depletion in SCALE6.0. The selected fuels simulated in this study are standard UO_2, ThO_2 with $^{233}UO_2$, natural UO_2 with TRU, ThO_2 with TRU, WGP (weapons grade plutonium) with UO_2, WGP with ThO_2, RGP (reactor grade plutonium) with UO_2, and RGP with ThO_2. This chapter is split into five sections. The first section describes how the SCALE6.0 depletion model is set up. The second section compares isotopics of enriched UO_2 fuel against isotopics of ThO_2 and $^{233}UO_2$ fuel. The third section compares natural UO_2 with TRU fuel against ThO_2 with TRU fuel. The fourth section compares natural UO_2 with WGP fuel against ThO_2 with WGP fuel. The final section of this chapter compares natural UO_2 fuel with RGP against ThO_2 with RGP fuel.

Description and Parameters

The objective of this study is to calculate and analyze isotopics from several fuel compositions. The fuels were modeled in a quarter assembly of a Westinghouse PWR with 17 x 17 lattice. It was assumed the total thermal power in the reactor was 3000 MW. TRITON, a program in the SCALE6.0 package is used to model depletion. PMC/Centrum is used to prepare self-shielding cross-sections. NEWT is used to deterministically solve the 2D Transport equation. The cross-section library used is the 238 group ENDF/B-VII. All depletion calculations use the parameter Addnux=3. Addnux specifies how many isotopes are tracked in the depletion calculation. In SCALE6.0 Addnux=3 is the option with the most isotopes available. Addnux=3 adds 166 additional isotopes in trace quantities. Table 1 shows the assumptions about the geometry and operating power of the reactor model. Figure 9 shows the model geometry in NEWT for the quarter fuel assembly.

Table 1. Core Geometry and Temperatures for Westinghouse 17x17 PWR

Core Geometry and Temperatures	
Lattice	17 x 17
Reactor Power	3000 MW
Total Fuel Volume	9317167 cc
Fuel pellet radius	.4096 cm
Helium Gap OR	0.4178 cm
Fuel clad IR	.4178 cm
Fuel clad OR	.4750 cm
Guide tube IR	.5613 cm
Guide tube OR	0.6121 cm
Fuel pitch	1.2598 cm
Assembly Pitch	21.5036 cm
Number of Fuel Rods	264
Number of Guide tubes	25
Fuel Temperature	900 ^{o}C
Moderator Temperature	557 ^{o}C
Cladding Temperature	620 ^{o}C
Gap Temperature	700 ^{o}C

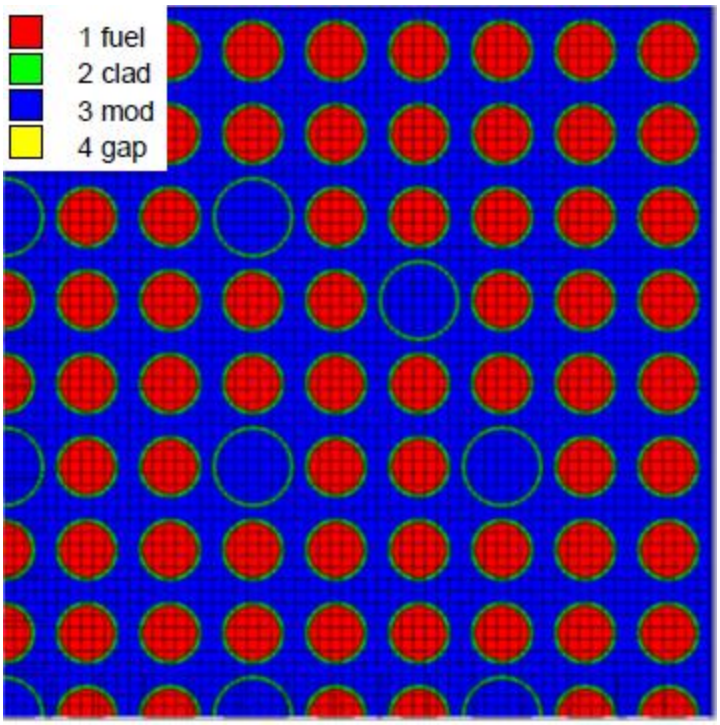

Figure 10. Westinghouse quarter fuel assembly. Red is fuel pin, green is cladding, blue is moderator, and yellow is helium gap (between fuel pin and cladding)

The parameters for the NEWT calculation include a B1 critical buckling search, which forces the spectrum to a critical spectrum. This is done to model reactor conditions since a

reactor running at full power is critical. This is only approximate since realistically burnable poisons or borated water absorb neutrons at the begging of cycle (BOC) to control the excess reactivity. The quarter fuel assembly is modeled with white boundary conditions since the fuel assembly is symmetric. The calculation uses S_6 level symmetric quadrature. The inner and outer eigenvalues are set to converge at 1 pcm for the once-through cases and 3 pcm for the multi-recycle calculations. P_1 scattering order is used. A P_1 scattering order is reasonably accurate in a thermal spectrum in areas away from material interfaces and strong absorbers. The error associated with using the P_1 scattering order is a few pcm, sufficient for a radio-toxicity study. Each fuel cell has 49 meshes for the once-through calculations.

UO_2 vs. ThO_2 with $^{233}UO_2$

The first two cases considered are UO_2 (UOX) fuel enriched to 4.32% and Th-$^{233}UO_2$ (Th-U233) with 3.955% ^{233}U by weight. In these cases no transuranics are included in the fresh fuel. In the UOX case the discharge burnup is 51242 MWd/tHM. In the Th-U233 case the discharge burnup is 55751 MWd/tHM Table 2 displays the values for K-inf for both fuel types. Figure 3.2 shows K-inf for the two cases as a function of FPD (full power days). Figure 10 shows the Th-^{233}U fuel has a larger reactivity swing than the UO_2 fuel. The Th-^{233}U fuel has about a 5% higher initial K-inf than the UO_2 fuel.

The Th-^{233}U fuel produces much less transuranics since the fresh fuel requires many more neutron captures to transmute into plutonium and higher transuranics. Table 3, 4, and 5 show the isotopic composition of the fresh fuel and spent fuel for the two cases in g/tHM, where tHM refers to the initial loading. The concentration of ^{233}U in the Th-U233 spent fuel is 42% of the concentration in the fresh fuel. The concentration of plutonium in the UOX fuel is more than four orders of magnitude larger than in the Th-U233 fuel after the 5 year cooldown. Overall, the

concentration of minor actinides in the UOX fuel is two orders of magnitude larger than in the Th-U233 fuel, but this is because ^{237}Np makes up more than 90% of the minor actinides weight. Most of the Minor actinides are more than five orders of magnitude greater in the UOX fuel than in the Th-U233 fuel.

Table 2. K-inf as a function of FPD

Full Power Days	UOX	Th-U233
0.00	1.39764	1.47394
13.50	1.34241	1.41977
40.50	1.32902	1.39930
67.50	1.31823	1.38439
101.25	1.30441	1.36782
141.75	1.28757	1.34934
243.00	1.24711	1.30530
405.00	1.19025	1.23736
607.25	1.12930	1.15804
849.75	1.06322	1.06936
971.50	1.02981	1.03002
1093.50	0.99972	0.99648
1336.50	0.94554	0.94036

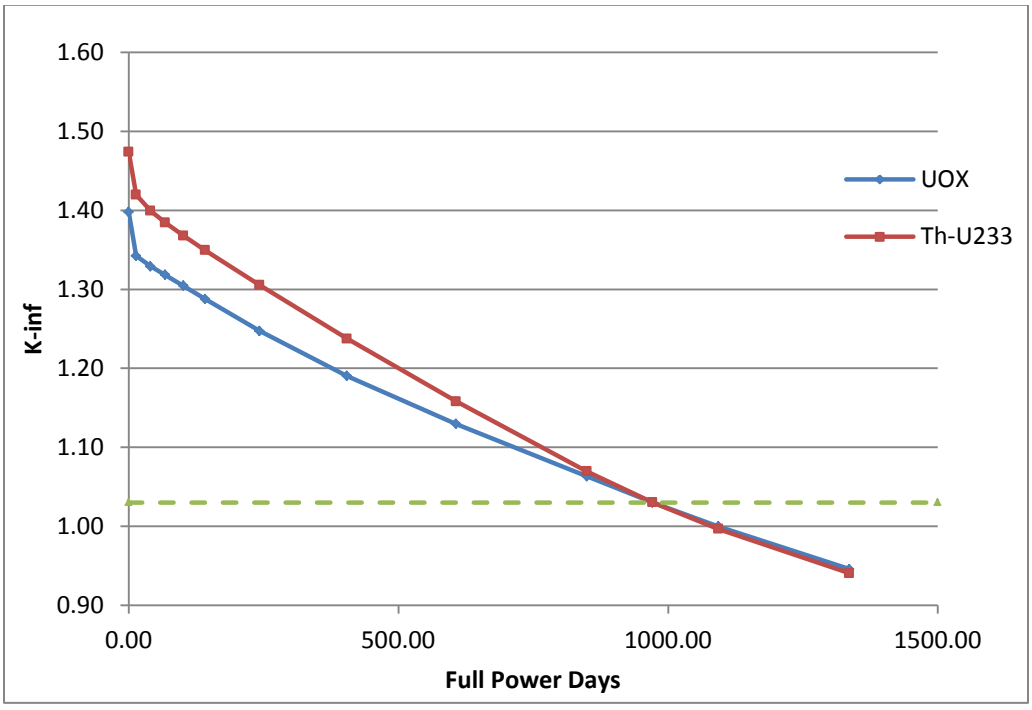

Figure 11. K-inf as a function of FPD

Table 3. Concentrations of suburanic actinides and uranium in fresh and spent fuel in grams per metric ton of heavy metal. Highlighted values were input as zero but treated as trace quantities by SCALE6.0

Concentration of Suburanic Actinides and Uranium in g/tHM								
Fresh Fuel			Discharged Fuel			After 5 Year Cooldown		
Isotope	UOX	Th-U233	Isotope	UOX	Th-U233	UOX	Th-U233	Th-U33/UOX
th228	1.12E-37	6.39E-43	th228	6.23E-06	6.77E-01	5.48E-05	2.02E+00	3.68E+04
th229	5.03E-40	4.63E-24	th229	1.91E-06	4.14E-01	1.98E-06	8.01E-01	4.06E+05
th230	4.16E-13	4.56E-13	th230	9.84E-04	9.88E-01	2.35E-03	1.06E+00	4.52E+02
th231	1.14E-27	1.14E-21	th231	1.16E-06	2.51E-01	3.00E-08	4.52E-09	1.51E-01
th232	4.19E-13	9.60E+05	th232	4.53E-04	9.16E+05	1.31E-03	9.16E+05	6.99E+08
th233	2.52E-37	2.04E-19	th233	9.62E-10	8.41E-01	0.00E+00	0.00E+00	0.00E+00
th234	3.99E-27	2.30E-42	th234	1.33E-05	1.47E-01	1.34E-05	3.93E-12	2.94E-07
pa231	4.18E-13	3.56E-42	pa231	3.78E-04	7.74E+01	4.15E-04	7.76E+01	1.87E+05
pa233	4.21E-13	4.56E-38	pa233	2.40E-05	1.42E+03	2.42E-05	5.41E-07	2.23E-02
pa234	1.05E-36	0.00E+00	pa234	3.83E-09	2.10E-01	2.01E-10	5.92E-17	2.94E-07
u232	4.19E-13	9.82E-24	u232	9.83E-04	8.70E+01	2.88E-03	8.30E+01	2.89E+04
u233	0.00E+00	3.95E+04	u233	0.00E+00	1.67E+04	0.00E+00	1.81E+04	0.00E+00
u234	1.89E+02	5.07E-20	u234	9.21E+01	5.38E+03	1.05E+02	5.38E+03	5.13E+01
u235	4.32E+04	0.00E+00	u235	7.38E+03	1.11E+03	7.38E+03	1.11E+03	1.51E-01
u236	4.27E-13	0.00E+00	u236	5.90E+03	2.23E+02	5.90E+03	2.23E+02	3.77E-02
u237	9.85E-22	0.00E+00	u237	1.20E+01	5.55E-01	4.27E-05	1.87E-09	4.37E-05
u238	9.56E+05	0.00E+00	u238	9.20E+05	2.71E-01	9.20E+05	2.71E-01	2.94E-07

Table 4. Concentrations of plutonium in fresh and spent fuel in grams per ton heavy metal. Highlighted values were input as zero but treated as trace quantities by SCALE

Concentration of Plutonium in g/tHM								
Fresh Fuel			Discharged Fuel			After 5 Year Cooldown		
Isotope	UOX	Th-U233	Isotope	UOX	Th-U233	UOX	Th-U233	Th-U33/UOX
pu236	0.00E+00	0.00E+00	pu236	2.91E-03	3.43E-05	8.84E-04	1.05E-05	1.18E-02
pu237	0.00E+00	0.00E+00	pu237	7.91E-04	6.72E-06	5.45E-16	4.63E-18	8.49E-03
pu238	0.00E+00	0.00E+00	pu238	3.14E+02	3.77E+00	3.28E+02	3.68E+00	1.12E-02
pu239	0.00E+00	0.00E+00	pu239	6.20E+03	5.20E-01	6.29E+03	5.21E-01	8.27E-05
pu240	0.00E+00	0.00E+00	pu240	2.94E+03	1.14E-01	2.95E+03	1.14E-01	3.86E-05
pu241	0.00E+00	0.00E+00	pu241	1.80E+03	7.84E-02	1.41E+03	6.16E-02	4.37E-05
pu242	0.00E+00	0.00E+00	pu242	8.74E+02	2.03E-02	8.74E+02	2.03E-02	2.32E-05
pu243	0.00E+00	0.00E+00	pu243	2.46E-01	6.95E-06	5.04E-13	6.98E-19	1.39E-06
pu244	0.00E+00	0.00E+00	pu244	3.53E-02	4.56E-07	3.53E-02	4.56E-07	1.29E-05
Total	0.00E+00	0.00E+00	Total	1.21E+04	4.50E+00	1.19E+04	4.39E+00	3.71E-04

Table 5. Concentrations of minor actinides in fresh and spent fuel in grams per ton of heavy metal. Highlighted values were input as zero but treated as trace quantities by SCALE

Concentration of Minor Actinides in g/tHM								
Fresh Fuel			Discharged Fuel			After 5 Year Cooldown		
Isotope	UOX	Th-U233	Isotope	UOX	Th-U233	UOX	Th-U233	Th-U233/UOX
np237	6.64E-43	0.00E+00	np237	6.99E+02	1.54E+01	7.13E+02	1.59E+01	2.24E-02
np238	0.00E+00	0.00E+00	np238	2.12E+00	5.52E-02	2.77E-07	3.73E-12	1.35E-05
np239	3.80E-38	0.00E+00	np239	9.23E+01	5.02E-04	2.03E-04	2.48E-09	1.22E-05
am241	0.00E+00	0.00E+00	am241	6.77E+01	1.10E-03	4.51E+02	1.78E-02	3.96E-05
am242	0.00E+00	0.00E+00	am242	1.63E-01	3.87E-06	1.96E-05	2.64E-10	1.35E-05
am242m	0.00E+00	0.00E+00	am242m	1.56E+00	2.10E-05	1.52E+00	2.05E-05	1.35E-05
am243	0.00E+00	0.00E+00	am243	2.36E+02	2.88E-03	2.36E+02	2.88E-03	1.22E-05
cm241	0.00E+00	0.00E+00	cm241	1.86E-06	1.68E-11	3.32E-23	2.99E-28	9.01E-06
cm242	0.00E+00	0.00E+00	cm242	2.54E+01	3.27E-04	1.48E-02	1.94E-07	1.31E-05
cm243	0.00E+00	0.00E+00	cm243	7.31E-01	4.86E-06	6.47E-01	4.31E-06	6.65E-06
cm244	0.00E+00	0.00E+00	cm244	1.01E+02	5.63E-04	8.38E+01	4.67E-04	5.57E-06
cm245	0.00E+00	0.00E+00	cm245	7.72E+00	2.45E-05	7.72E+00	2.45E-05	3.17E-06
cm246	0.00E+00	0.00E+00	cm246	9.60E-01	2.25E-06	9.59E-01	2.24E-06	2.34E-06
cm247	0.00E+00	0.00E+00	cm247	1.45E-02	2.01E-08	1.45E-02	2.01E-08	1.39E-06
cm248	0.00E+00	0.00E+00	cm248	1.17E-03	1.12E-09	1.17E-03	1.12E-09	9.56E-07
Total	3.80E-38	0.00E+00	Total	1.23E+03	1.54E+01	1.49E+03	1.60E+01	1.07E-02

Natural UO_2 with TRU vs. ThO_2 with TRU

The second set of cases considered UOX mixed with 12.277% TRUOX and ThOX mixed with 13.47% TRUOX. The U-TRU fuel has a discharge burnup of 50746 MWd/tHM. The Th-TRU fuel has a discharge burnup of 54872 MWd/tHM. Figure 11 shows the K-inf for the two quarter fuel assemblies. Table 6 shows the K-inf as a function of FPD for the two cases. Both cases start with a similar excess in reactivity. Initially, Reactivity drops quicker in the Th-TRU fuel since there is a larger percentage of MA's in the fuel.

The Th-TRU fuel starts out with a higher concentration of TRU's than the U-TRU fuel and has a lower concentration of TRU's at EOL. In both fuels the concentration of minor actinides increases during depletion and the concentration of plutonium decreases. The amount

of ^{233}U that is bred is approximately 18% of starting fissile material in the Th-TRU fuel. Table 7, 8, and 9 display the concentrations of isotopes in spent and fresh fuel for both fuel types.

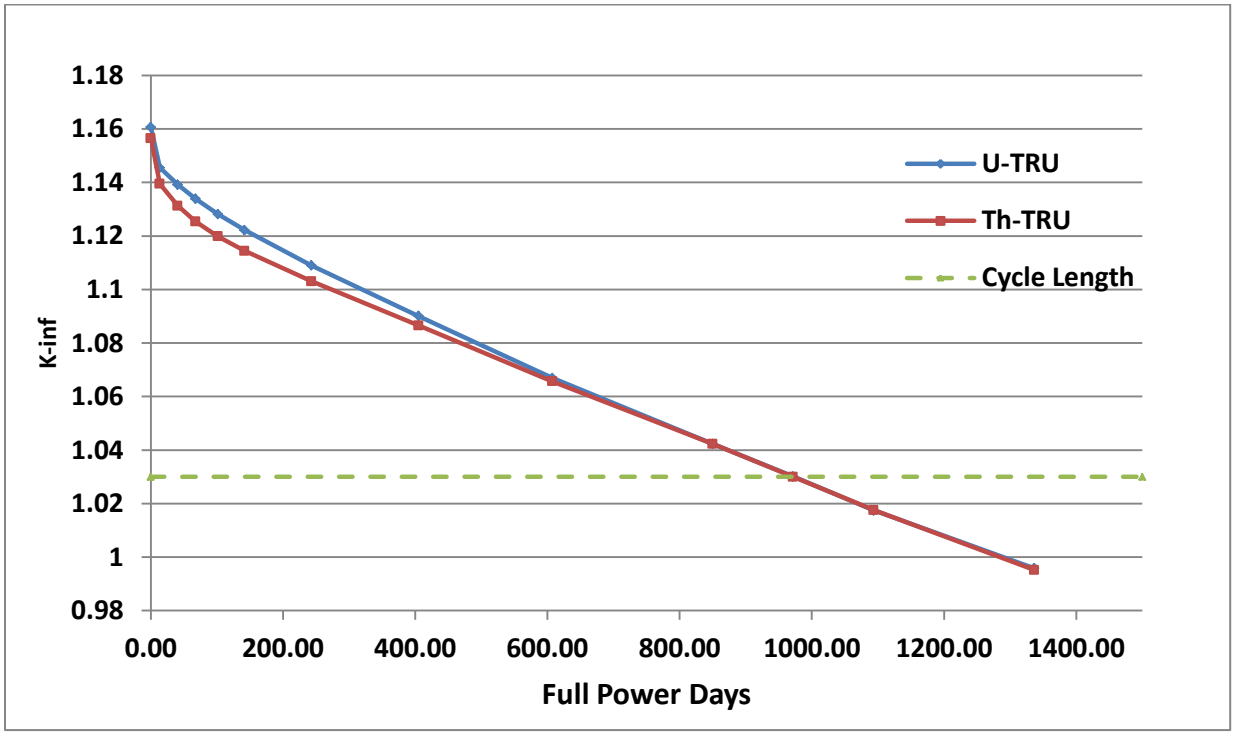

Figure 12. K-inf as a function of FPD

Table 6. K-inf as a function of FPD

FPD	U-TRU	Th-TRU
0.00	1.16060	1.15649
13.50	1.14549	1.13945
40.50	1.13915	1.13130
67.50	1.13388	1.12544
101.25	1.12814	1.11986
141.75	1.12219	1.11440
243.00	1.10899	1.10307
405.00	1.09009	1.08656
607.25	1.06693	1.06571
849.75	1.04233	1.04229
971.50	1.03014	1.03001
1093.50	1.01745	1.01754
1336.50	0.99586	0.99518

Table 7. Concentrations of suburanic actinides and uranium in fresh and spent fuel in grams per ton heavy metal. Highlighted values were input as zero but treated as trace quantities by SCALE

Concentration of Suburanics and Uranium in g/tHM								
Fresh Fuel			Discharged Fuel			After 5 Year Cooldown		
Isotopes	U-TRU	Th-TRU	Isotopes	U-TRU	Th-TRU	U-TRU	Th-TRU	Th-TRU/U-
th228	1.92E-42	2.24E-42	th228	2.11E-04	5.21E-01	1.00E-03	1.52E+00	1.52E+03
th229	7.24E-40	8.08E-40	th229	6.98E-05	2.55E-01	7.01E-05	5.86E-01	8.35E+03
th230	4.14E-13	4.48E-13	th230	1.69E-03	1.78E+00	6.15E-03	1.80E+00	2.93E+02
th231	1.64E-28	1.64E-21	th231	1.13E-06	2.79E-01	1.46E-08	9.79E-10	6.70E-02
th232	4.08E-27	8.65E+05	th232	5.93E-04	8.40E+05	1.30E-03	8.40E+05	6.49E+08
th233	0.00E+00	1.51E-19	th233	9.37E-10	4.03E-01	0.00E+00	0.00E+00	0.00E+00
th234	3.62E-27	6.56E-43	th234	1.21E-05	1.45E-02	1.22E-05	2.43E-12	2.00E-07
pa231	0.00E+00	5.50E-42	pa231	4.30E-04	1.69E+02	4.48E-04	1.69E+02	3.77E+05
pa233	5.10E-26	5.59E-26	pa233	1.35E-04	6.85E+02	1.36E-04	1.11E-04	8.17E-01
pa234	0.00E+00	0.00E+00	pa234	1.28E-08	6.42E-02	1.83E-10	3.66E-17	2.00E-07
u232	2.84E-29	0.00E+00	u232	2.32E-02	6.57E+01	4.97E-02	6.27E+01	1.26E+03
u233	0.00E+00	0.00E+00	u233	0.00E+00	1.48E+04	0.00E+00	1.55E+04	0.00E+00
u234	1.66E+02	6.92E-22	u234	2.14E+02	1.36E+03	4.28E+02	1.58E+03	3.70E+00
u235	6.18E+03	5.30E-23	u235	3.59E+03	2.38E+02	3.60E+03	2.41E+02	6.70E-02
u236	5.12E+03	9.15E-23	u236	4.82E+03	2.43E+01	4.84E+03	3.78E+01	7.81E-03
u237	8.36E-21	4.27E-25	u237	8.15E+00	4.61E-02	3.33E-04	3.36E-04	1.01E+00
u238	8.66E+05	4.66E-25	u238	8.37E+05	7.34E-02	8.37E+05	1.67E-01	2.00E-07

Table 8. Concentrations of Plutonium in fresh and spent fuel in grams per ton heavy metal. Highlighted values were input as zero but treated as trace quantities by SCALE

Concentration of Plutonium in g/tHM								
Fresh Fuel			Discharged Fuel			After 5 Year Cooldown		
Isotopes	U-TRU	Th-TRU	Isotopes	U-TRU	Th-TRU	U-TRU	Th-TRU	Th-TRU/U-TRU
pu236	3.31E-26	3.85E-26	pu236	4.14E-02	3.68E-02	1.26E-02	1.12E-02	8.89E-01
pu237	1.53E-24	1.74E-24	pu237	1.91E-02	1.98E-02	1.32E-14	1.37E-14	1.04E+00
pu238	2.96E+03	3.25E+03	pu238	5.40E+03	5.70E+03	5.44E+03	5.76E+03	1.06E+00
pu239	6.24E+04	6.85E+04	pu239	3.79E+04	2.07E+04	3.79E+04	2.07E+04	5.46E-01
pu240	2.93E+04	3.22E+04	pu240	2.68E+04	2.60E+04	2.69E+04	2.62E+04	9.73E-01
pu241	1.25E+04	1.37E+04	pu241	1.40E+04	1.41E+04	1.10E+04	1.11E+04	1.01E+00
pu242	8.50E+03	9.32E+03	pu242	9.11E+03	1.03E+04	9.11E+03	1.03E+04	1.13E+00
pu243	2.19E-20	2.64E-20	pu243	7.86E-01	9.36E-01	4.39E-12	6.93E-12	1.58E+00
pu244	0.00E+00	0.00E+00	pu244	1.58E-01	2.00E-01	1.58E-01	2.00E-01	1.26E+00
Total	1.16E+05	1.27E+05	Total	9.31E+04	7.68E+04	9.04E+04	7.41E+04	8.19E-01

Table 9. Concentrations of minor actinides in fresh and spent fuel in grams per ton heavy metal. Highlighted values were input as zero but treated as trace quantities by SCALE

Concentration of Minor Actinides in g/tHM								
Fresh Fuel			Discharged Fuel			After 5 Year Cooldown		
Isotopes	U-TRU	Th-TRU	Isotopes	U-TRU	Th-TRU	U-TRU	Th-TRU	Th-TRU/U-TRU
np237	5.85E+03	6.41E+03	np237	3.96E+03	3.24E+03	4.00E+03	3.27E+03	8.17E-01
np238	2.29E-20	2.72E-20	np238	5.63E+00	5.02E+00	1.41E-05	1.36E-05	9.61E-01
np239	3.39E-38	0.00E+00	np239	6.26E+01	6.48E-03	1.87E-03	2.16E-03	1.15E+00
am241	1.19E+03	1.30E+03	am241	2.04E+03	2.02E+03	5.02E+03	5.01E+03	1.00E+00
am242	6.91E-21	8.42E-21	am242	1.39E+00	1.62E+00	1.00E-03	9.63E-04	9.61E-01
am242m	1.34E-21	1.63E-21	am242m	7.96E+01	7.65E+01	7.77E+01	7.46E+01	9.61E-01
am243	3.68E-40	4.43E-40	am243	2.18E+03	2.51E+03	2.18E+03	2.51E+03	1.15E+00
cm241	0.00E+00	0.00E+00	cm241	2.47E-05	2.86E-05	4.41E-22	5.10E-22	1.16E+00
cm242	2.95E-41	3.63E-41	cm242	2.51E+02	2.94E+02	3.10E-01	3.20E-01	1.03E+00
cm243	0.00E+00	0.00E+00	cm243	1.12E+01	1.33E+01	9.92E+00	1.18E+01	1.19E+00
cm244	0.00E+00	0.00E+00	cm244	1.06E+03	1.26E+03	8.75E+02	1.04E+03	1.19E+00
cm245	0.00E+00	0.00E+00	cm245	1.36E+02	1.78E+02	1.35E+02	1.78E+02	1.31E+00
cm246	0.00E+00	0.00E+00	cm246	6.51E+00	1.00E+01	6.51E+00	1.00E+01	1.54E+00
cm247	0.00E+00	0.00E+00	cm247	1.26E-01	1.99E-01	1.26E-01	1.99E-01	1.58E+00
cm248	0.00E+00	0.00E+00	cm248	7.36E-03	1.24E-02	7.36E-03	1.25E-02	1.69E+00
Total	7.03E+03	7.71E+03	Total	9.80E+03	9.61E+03	1.23E+04	1.21E+04	9.85E-01

WGP with UO_2 vs. WGP with ThO_2

The third set of cases being compared are UOX mixed with 4.565% weapons grade plutonium dioxide(WGP) and ThOX mixed with 5.943% WGP. The WGP is made up of 96% ^{239}Pu and 4% ^{240}Pu. The U-WGP fuel has a discharge burnup of 50913 MWd/tHM. The Th-WGP fuel has a discharge burnup of 55471 MWd/tHM. Figure 13 shows K-inf as a function of FPD. Table 10 displays the values for K-inf as a function on FPD. The Th-WGP fuel starts with a higher concentration of plutonium than the U-WGP fuel and has a lower concentration of plutonium after depletion since the ^{238}U transmutes to plutonium. Also, the U-WGP fuel produces twice the concentration of minor actinides in the spent fuel. The Th-WGP fuel produces a concentration of ^{233}U that is approximately 26% of the starting fissile concentration.

Reactivity excess is similar in both fresh fuels. The Th-WGP fuel has a slightly higher excess reactivity. Tables 11, 12, and 13 show the isotopic compositions of the two fuels before and after depletion.

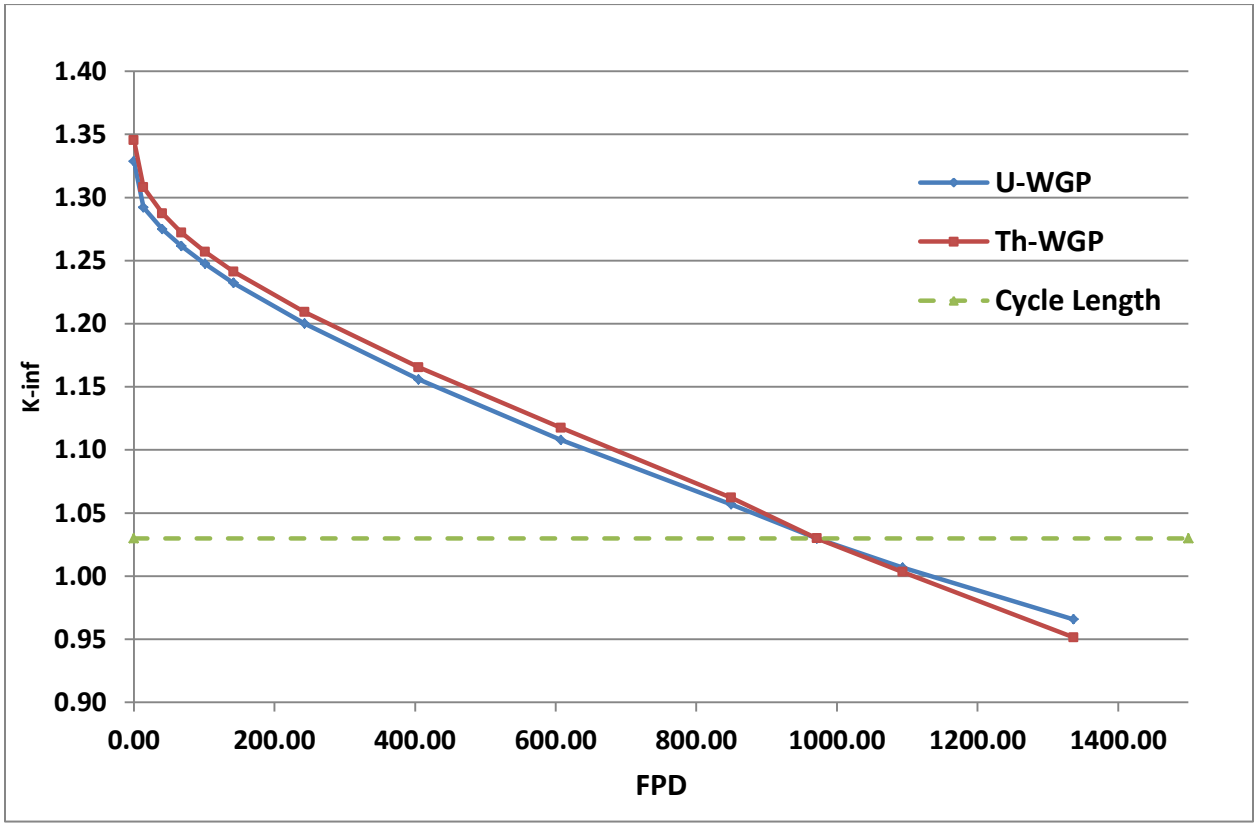

Figure 13. K-inf as a function of FPD

Table 10. K-inf as a function of FPD.

FPD	U-WGP	Th-WGP
0.00	1.32877	1.34543
13.50	1.29211	1.30805
40.50	1.27480	1.28739
67.50	1.26152	1.27221
101.25	1.24749	1.25701
141.75	1.23228	1.24131
243.00	1.20003	1.20919
405.00	1.15578	1.16541
607.25	1.10793	1.11749
849.75	1.05684	1.06213
971.50	1.02985	1.02999
1093.50	1.00678	1.00329
1336.50	0.96586	0.95154

Table 11. Concentration of suburanic actinides and uranium in fresh and spent fuel in grams per ton heavy metal. Highlighted values were input as zero but treated as trace quantities by SCALE

Concentration of Suburanic Actinides and Uranium in g/tHM								
Fresh Fuel			Discharged Fuel			After 5 Year Cooldown		
Isotope	U-WGP	Th-WGP	Isotope	U-WGP	Th-WGP	U-WGP	Th-WGP	Th-WGP/U-WGP
th228	1.60E-42	1.54E-21	th228	1.30E-05	3.06E-01	4.01E-04	2.20E+00	5.48E+03
th229	6.32E-40	9.40E+05	th229	3.90E-06	9.08E+05	3.17E-05	6.68E-01	2.11E+04
th230	4.15E-13	1.63E-19	th230	1.03E-03	6.33E-01	1.98E-10	1.57E+00	7.89E+09
th231	1.77E-28	9.84E-43	th231	1.06E-06	5.80E-02	1.02E-04	1.48E-09	1.46E-05
th232	4.44E-27	5.18E-42	th232	6.45E-04	1.30E+02	3.99E-06	9.08E+05	2.28E+11
th233	0.00E+00	3.66E-38	th233	1.26E-09	1.06E+03	2.58E-03	0.00E+00	0.00E+00
th234	3.93E-27	0.00E+00	th234	1.32E-05	1.46E-01	1.01E-08	5.94E-13	5.88E-05
pa231	0.00E+00	1.92E-42	pa231	3.88E-04	7.16E-01	1.41E-03	1.30E+02	9.24E+04
pa233	0.00E+00	7.08E-40	pa233	3.19E-05	3.32E-01	0.00E+00	2.94E-07	0.00E+00
pa234	0.00E+00	4.53E-13	pa234	4.49E-09	1.54E+00	1.32E-05	8.95E-18	6.79E-13
u232	2.58E-29	0.00E+00	u232	1.86E-03	9.49E+01	5.31E-03	9.06E+01	1.71E+04
u233	0.00E+00	0.00E+00	u233	1.01E+02	1.47E+04	0.00E+00	1.57E+04	0.00E+00
u234	1.80E+02	0.00E+00	u234	0.00E+00	1.96E+03	1.23E+02	1.97E+03	1.60E+01
u235	6.67E+03	4.42E-23	u235	2.48E+03	3.63E+02	2.49E+03	3.64E+02	1.46E-01
u236	5.57E+03	6.74E-24	u236	5.26E+03	3.41E+01	5.26E+03	3.72E+01	7.07E-03
u237	9.10E-21	0.00E+00	u237	1.06E+01	8.46E-02	1.21E-04	9.86E-05	8.15E-01
u238	9.42E+05	0.00E+00	u238	9.08E+05	2.25E-02	9.08E+05	4.09E-02	4.51E-08

Table 12. Concentration of plutonium in fresh and spent fuel in grams per ton heavy metal. Highlighted values were input as zero but treated as trace quantities by SCALE

Concentration of Plutonium in g/tHM								
Fresh Fuel			Discharged Fuel			After 5 Year Cooldown		
Isotope	U-WGP	Th-WGP	Isotope	U-WGP	Th-WGP	U-WGP	Th-WGP	Th-WGP/U-WGP
pu236	1.07E-30	1.60E-30	pu236	5.29E-03	5.08E-05	1.61E-03	1.54E-05	9.56E-03
pu237	3.17E-26	4.48E-26	pu237	1.72E-03	4.32E-04	1.18E-15	2.98E-16	2.52E-01
pu238	1.44E-23	1.92E-23	pu238	5.32E+02	1.57E+02	5.83E+02	2.36E+02	4.05E-01
pu239	4.38E+04	5.70E+04	pu239	1.44E+04	2.99E+03	1.45E+04	2.99E+03	2.06E-01
pu240	1.83E+03	2.37E+03	pu240	8.91E+03	5.99E+03	8.94E+03	6.03E+03	6.74E-01
pu241	3.79E-20	4.94E-20	pu241	5.08E+03	4.14E+03	3.99E+03	3.25E+03	8.15E-01
pu242	0.00E+00	0.00E+00	pu242	1.58E+03	2.03E+03	1.58E+03	2.03E+03	1.29E+00
pu243	0.00E+00	0.00E+00	pu243	3.71E-01	5.05E-01	6.86E-13	1.25E-12	1.82E+00
pu244	0.00E+00	0.00E+00	pu244	4.59E-02	6.69E-02	4.59E-02	6.69E-02	1.46E+00
Total	4.56E+04	5.94E+04	Total	3.05E+04	1.53E+04	2.96E+04	1.45E+04	4.91E-01

Table 13. Concentration of minor actinides in fresh and spent fuel. Highlighted values were input as zero but treated as trace quantities by SCALE

Concentration of Minor Actinides in g/tHM								
Fresh Fuel			Discharged Fuel			After 5 Year Cooldown		
Isotope	U-WGP	Th-WGP	Isotope	U-WGP	Th-WGP	U-WGP	Th-WGP	Th-WGP/U-WGP
np237	4.65E-42	0.00E+00	np237	9.15E+02	2.88E+00	9.33E+02	8.64E+00	9.26E-03
np238	0.00E+00	0.00E+00	np238	2.16E+00	7.92E-03	1.52E-06	1.26E-06	8.33E-01
np239	3.65E-38	0.00E+00	np239	8.21E+01	5.16E-04	3.63E-04	4.76E-04	1.31E+00
am241	0.00E+00	0.00E+00	am241	3.06E+02	2.59E+02	1.39E+03	1.14E+03	8.22E-01
am242	0.00E+00	0.00E+00	am242	4.56E-01	5.34E-01	1.08E-04	8.96E-05	8.33E-01
am242m	0.00E+00	0.00E+00	am242m	8.54E+00	7.12E+00	8.34E+00	6.95E+00	8.33E-01
am243	0.00E+00	0.00E+00	am243	4.21E+02	5.53E+02	4.21E+02	5.53E+02	1.31E+00
cm241	0.00E+00	0.00E+00	cm241	6.53E-06	7.59E-06	1.16E-22	1.35E-22	1.16E+00
cm242	0.00E+00	0.00E+00	cm242	7.27E+01	8.96E+01	5.28E-02	5.65E-02	1.07E+00
cm243	0.00E+00	0.00E+00	cm243	2.24E+00	2.83E+00	1.98E+00	2.51E+00	1.26E+00
cm244	0.00E+00	0.00E+00	cm244	1.75E+02	2.32E+02	1.44E+02	1.92E+02	1.33E+00
cm245	0.00E+00	0.00E+00	cm245	1.68E+01	2.27E+01	1.68E+01	2.27E+01	1.36E+00
cm246	0.00E+00	0.00E+00	cm246	1.24E+00	2.25E+00	1.23E+00	2.24E+00	1.82E+00
cm247	0.00E+00	0.00E+00	cm247	1.97E-02	3.58E-02	1.97E-02	3.58E-02	1.82E+00
cm248	0.00E+00	0.00E+00	cm248	1.34E-03	2.60E-03	1.34E-03	2.60E-03	1.95E+00
Total	3.65E-38	0.00E+00	Total	2.00E+03	1.17E+03	2.91E+03	1.93E+03	6.62E-01

RGP with UO_2 vs. RGP with ThO_2

The last set of fuels being compared are UOX mixed with 10% reactor grade plutonium dioxide (RGP) and ThOX mixed with 11.22% RGP. The RGP is comprised of 2.52% ^{238}Pu, 53.38% ^{239}Pu, 25.07% ^{240}Pu, 10.68% ^{241}Pu, 7.27% ^{242}Pu, and 1.07% ^{241}Am. The U-RGP fuel has a discharge burnup of 50788 MWd/tHM. The discharge burnup of the Th-RGP fuel is 55036 MWd/tHM. Figure 14 shows the K-inf for both fuels as a function of FPDs. Table 14 displays the values of K-inf as a function of FPDs. Reactivity excess is very similar in both cases with only a difference of about 168 pcm at BOL. Table 15, 16, and 17 display the isotopic compositions of the fresh and spent fuel. The spent Th-RGP fuel has a lower concentration of plutonium and MA's than the spent U-RGP fuel even though it starts with approximately 10% more plutonium. The concentration of ^{233}U produced in the Th-RGP fuel is approximately 21% of the starting concentration of fissile material.

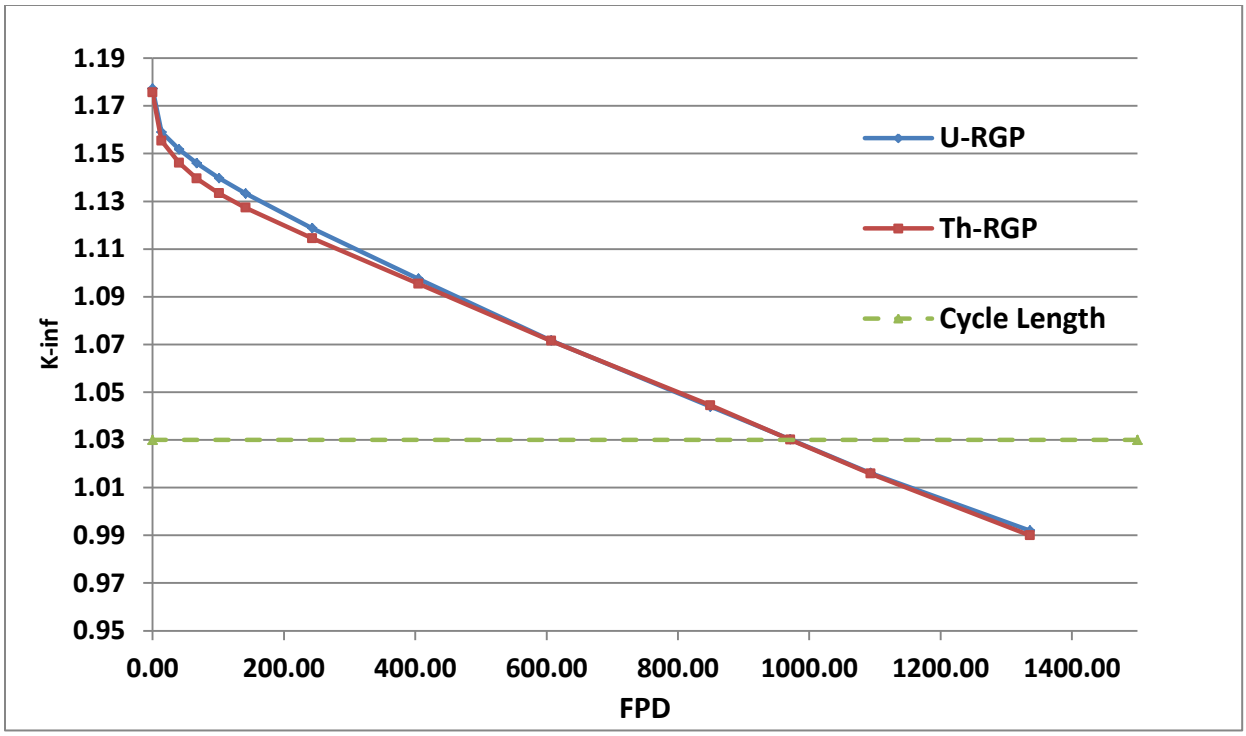

Figure 14. K-inf as a function of FPD

Table 14. K-inf as a function of FPD

FPD	U-RGP	Th-RGP
0.00	1.17724	1.17556
13.50	1.15898	1.15541
40.50	1.15173	1.14606
67.50	1.14591	1.13951
101.25	1.13969	1.13335
141.75	1.13323	1.12730
243.00	1.11868	1.11447
405.00	1.09748	1.09542
607.25	1.07159	1.07151
849.75	1.04394	1.04443
971.50	1.03020	1.03006
1093.50	1.01609	1.01580
1336.50	0.99196	0.98995

Table 15. Concentration of suburanic actinides and uranium in grams per ton heavy metal. Highlighted values were input as zero but treated as trace quantities by SCALE

Concentration of Suburanic Actinides and Uranium in g/tHM								
Fresh Fuel			Discharged Fuel			After 5 Year Cooldown		
Isotope	U-RGP	Th-RGP	Isotope	U-RGP	Th-RGP	U-RGP	Th-RGP	Th-RGP/U-RGP
th228	1.92E-42	2.24E-42	th228	2.20E-05	5.82E-01	1.48E-04	1.71E+00	1.15E+04
th229	7.14E-40	7.99E-40	th229	6.53E-06	2.78E-01	6.66E-06	6.14E-01	9.22E+04
th230	4.14E-13	4.50E-13	th230	1.45E-03	1.76E+00	4.56E-03	1.78E+00	3.90E+02
th231	1.67E-28	1.66E-21	th231	1.08E-06	2.87E-01	1.39E-08	1.07E-09	7.73E-02
th232	4.18E-27	8.88E+05	th232	6.07E-04	8.61E+05	1.33E-03	8.61E+05	6.49E+08
th233	0.00E+00	1.57E-19	th233	1.01E-09	4.39E-01	0.00E+00	0.00E+00	0.00E+00
th234	3.71E-27	6.56E-43	th234	1.24E-05	1.89E-02	1.25E-05	2.23E-12	1.79E-07
pa231	0.00E+00	5.50E-42	pa231	4.21E-04	1.62E+02	4.38E-04	1.62E+02	3.70E+05
pa233	0.00E+00	3.52E-38	pa233	3.12E-05	7.44E+02	3.18E-05	1.11E-06	3.49E-02
pa234	0.00E+00	0.00E+00	pa234	3.34E-09	7.56E-02	1.88E-10	3.36E-17	1.79E-07
u232	2.86E-29	0.00E+00	u232	2.88E-03	7.37E+01	7.66E-03	7.04E+01	9.19E+03
u233	0.00E+00	0.00E+00	u233	0.00E+00	1.50E+04	0.00E+00	1.57E+04	0.00E+00
u234	1.70E+02	6.04E-22	u234	1.67E+02	1.45E+03	2.82E+02	1.57E+03	5.55E+00
u235	6.29E+03	4.64E-23	u235	3.40E+03	2.62E+02	3.41E+03	2.63E+02	7.73E-02
u236	5.25E+03	8.00E-23	u236	4.94E+03	2.51E+01	4.95E+03	3.61E+01	7.29E-03
u237	8.79E-21	3.72E-25	u237	8.70E+00	5.08E-02	2.92E-04	2.89E-04	9.88E-01
u238	8.88E+05	4.07E-25	u238	8.58E+05	6.74E-02	8.58E+05	1.54E-01	1.79E-07

Table 16. Concentrations of plutonium in grams per ton heavy metal. Highlighted values were input as zero but treated as trace quantities by SCALE

Concentration of Plutonium in g/tHM								
Fresh Fuel			Discharged Fuel			After 5 Year Cooldown		
Isotope	U-RGP	Th-RGP	Isotope	U-RGP	Th-RGP	U-RGP	Th-RGP	Th-RGP/U-RGP
pu236	2.77E-26	3.31E-26	pu236	7.39E-03	2.00E-03	2.24E-03	6.07E-04	2.71E-01
pu237	1.29E-24	1.50E-24	pu237	9.88E-03	9.46E-03	6.81E-15	6.52E-15	9.58E-01
pu238	2.53E+03	2.84E+03	pu238	2.83E+03	2.81E+03	2.95E+03	2.97E+03	1.01E+00
pu239	5.34E+04	5.99E+04	pu239	3.01E+04	1.35E+04	3.01E+04	1.35E+04	4.50E-01
pu240	2.51E+04	2.81E+04	pu240	2.24E+04	2.11E+04	2.25E+04	2.13E+04	9.45E-01
pu241	1.07E+04	1.20E+04	pu241	1.23E+04	1.21E+04	9.64E+03	9.52E+03	9.88E-01
pu242	7.27E+03	8.16E+03	pu242	8.10E+03	9.47E+03	8.10E+03	9.47E+03	1.17E+00
pu243	2.12E-20	2.58E-20	pu243	7.91E-01	9.66E-01	5.82E-12	9.33E-12	1.60E+00
pu244	0.00E+00	0.00E+00	pu244	1.70E-01	2.18E-01	1.70E-01	2.18E-01	1.28E+00
Total	9.89E+04	1.11E+05	Total	7.56E+04	5.90E+04	7.34E+04	5.68E+04	7.74E-01

Table 17. Concentrations of minor actinides in grams per ton heavy metal. Highlighted values were input as zero but treated as trace quantities by SCALE

Concentration of Minor Actinides in g/tHM								
Fresh Fuel			Dicharged Fuel			After 5 Year Cooldown		
Isotope	U-RGP	Th-RGP	Isotope	U-RGP	Th-RGP	U-RGP	Th-RGP	Th-RGP/U-RGP
np237	4.62E-23	5.18E-23	np237	6.64E+01	9.45E+00	9.36E+02	3.27E+01	3.49E-02
np238	0.00E+00	0.00E+00	np238	1.45E+00	1.68E-02	1.09E-05	1.02E-05	9.34E-01
np239	3.53E-38	0.00E+00	np239	9.03E+02	2.14E-03	1.77E-03	2.07E-03	1.17E+00
am241	1.07E+03	1.20E+03	am241	1.64E+03	1.59E+03	4.25E+03	4.17E+03	9.81E-01
am242	7.12E-21	8.77E-21	am242	1.31E+00	1.56E+00	7.76E-04	7.25E-04	9.34E-01
am242m	1.38E-21	1.70E-21	am242m	6.16E+01	5.76E+01	6.01E+01	5.62E+01	9.34E-01
am243	3.56E-40	4.33E-40	am243	2.06E+03	2.41E+03	2.06E+03	2.41E+03	1.17E+00
cm241	0.00E+00	0.00E+00	cm241	2.34E-05	2.75E-05	4.17E-22	4.90E-22	1.17E+00
cm242	3.05E-41	3.76E-41	cm242	2.39E+02	2.86E+02	2.59E-01	2.69E-01	1.04E+00
cm243	0.00E+00	0.00E+00	cm243	1.09E+01	1.31E+01	9.63E+00	1.16E+01	1.20E+00
cm244	0.00E+00	0.00E+00	cm244	1.10E+03	1.32E+03	9.08E+02	1.09E+03	1.20E+00
cm245	0.00E+00	0.00E+00	cm245	1.45E+02	1.88E+02	1.45E+02	1.88E+02	1.30E+00
cm246	0.00E+00	0.00E+00	cm246	8.32E+00	1.31E+01	8.31E+00	1.31E+01	1.57E+00
cm247	0.00E+00	0.00E+00	cm247	1.67E-01	2.68E-01	1.67E-01	2.68E-01	1.60E+00
cm248	0.00E+00	0.00E+00	cm248	1.08E-02	1.85E-02	1.08E-02	1.85E-02	1.72E+00
Total	1.07E+03	1.20E+03	Total	6.23E+03	5.89E+03	8.37E+03	7.97E+03	9.52E-01

This study demonstrates that for a once-through fuel cycle in a PWR different thorium fuels in a homogeneous configuration generate less plutonium and minor actinides . In the first

part of this study UOX is compared to Th-^{233}UOX fuel. The thorium fuel generated two orders of magnitude less minor actinides than the UOX fuel. The next part of the study compared uranium oxide fuel mixed with TRUs versus thorium oxide fuel mixed with TRUs. Fuels mixed with RGP and WGP behave similarly to TRUs since they contain significant concentrations of plutonium. TRUOX fuel has the highest concentration of transuranics by a significant margin. Despite the thorium fuel starting with a higher concentration of TRUs and plutonium to get the same cycle length the concentration of transuranics was smaller than the U-TRU discharged fuel. The weapons grade plutonium comparison and reactor grade plutonium comparisons showed similar results to the TRUOX fuel.

MULTI-RECYCLE ISOTOPICS STUDY

The multi-recycle thorium fuel isotopics study was performed in order to gain an understanding of the benefits of recycling thorium in order to reduce the volume of transuranic waste. A combination of text editing scripts with UNIX shell scripts and SCALE6.0 allowed for modeling of multi-recycle depletion. The Python text editing scripts generate input files while the Unix shell script controls the overall process by calling SCALE and Python. This chapter includes a description of the 65 group library that was generated to speed up the multi-recycle calculations. The next section compares the isotopics of different separation scenarios. The final part of this isotopics study evaluates the effect of separation efficiency on buildup of transuranics. The radio-toxicity results in this chapter are normalized to the radio-toxicity of equivalent amount of mined un-irradiated natural uranium required to give an equivalent energy output and cycle length after enrichment in a once-through LWR fuel cycle. This allows the fuel cycle scenario to be compared to the amount of radio-toxicity unearthed just from mining operations in the current once-through fuel cycle[17]. Ideally, if irradiated fuel quickly decays to a level where it is comparable to mined natural uranium, then the concern for the waste being released into the environment after a very long time may be lessened.

Collapsing Cross-section Libraries and Computation Resource Management

Multi-recycle calculations require up to 100 depletion calculations in series with nearly a total of 150 depletion calculations. A depletion calculation with a 238 group cross-section library can take up to 17 hours. There are several parameters that can be adjusted to reduce the run time with only a small increase in error. The inner and outer eigenvalues can be adjusted to converge at several pcm instead of 1 pcm and is still good enough for a radiotoxicity calculation. Reducing the number of mesh grids has a significant speed up with a very small change in K-inf.

However, reducing the number of energy groups has the greatest effect. Collapsing the energy groups from 238 to 65 gives a speed up by a factor of nearly six resulting in a depletion calculation that only takes 3 hours both on a UNIX cluster or on a home computer with a core i7 960. In total a full multi-recycle calculation which has 3 depletion calculations, 2 in parallel, takes about roughly 300 hours. Approximately 13 GB of disk space is required to run the calculation since the temporary directory must be located within the working directory in order to access ft71 files and to link the cross-section library.

The 238 group ENDF/B-VII library was collapsed by analyzing absorption reaction rates in each energy group. The collapsed groups were formed by averaging the reaction rates. The initial collapse was to a 44 group structure that was collapsed to mimic a group structure from the ENDF/B-VI library. The difference in absorption reaction rate in each group from the original 238 group structure was analyzed and groups were added where the results were weak. This process was repeated until the error of actinide concentrations between the collapsed library and the original 238 group library was less than 1%, which the current 65 group library satisfies. The 1% mark is somewhat arbitrary but useful for a fuel cycle scenario study since the speedup is by nearly a factor of six and an error much smaller than the error of the cross-section data itself. Figure 15 shows a log plot that compares the collapsed group structure of the 65 group library compared to the 238 group library.

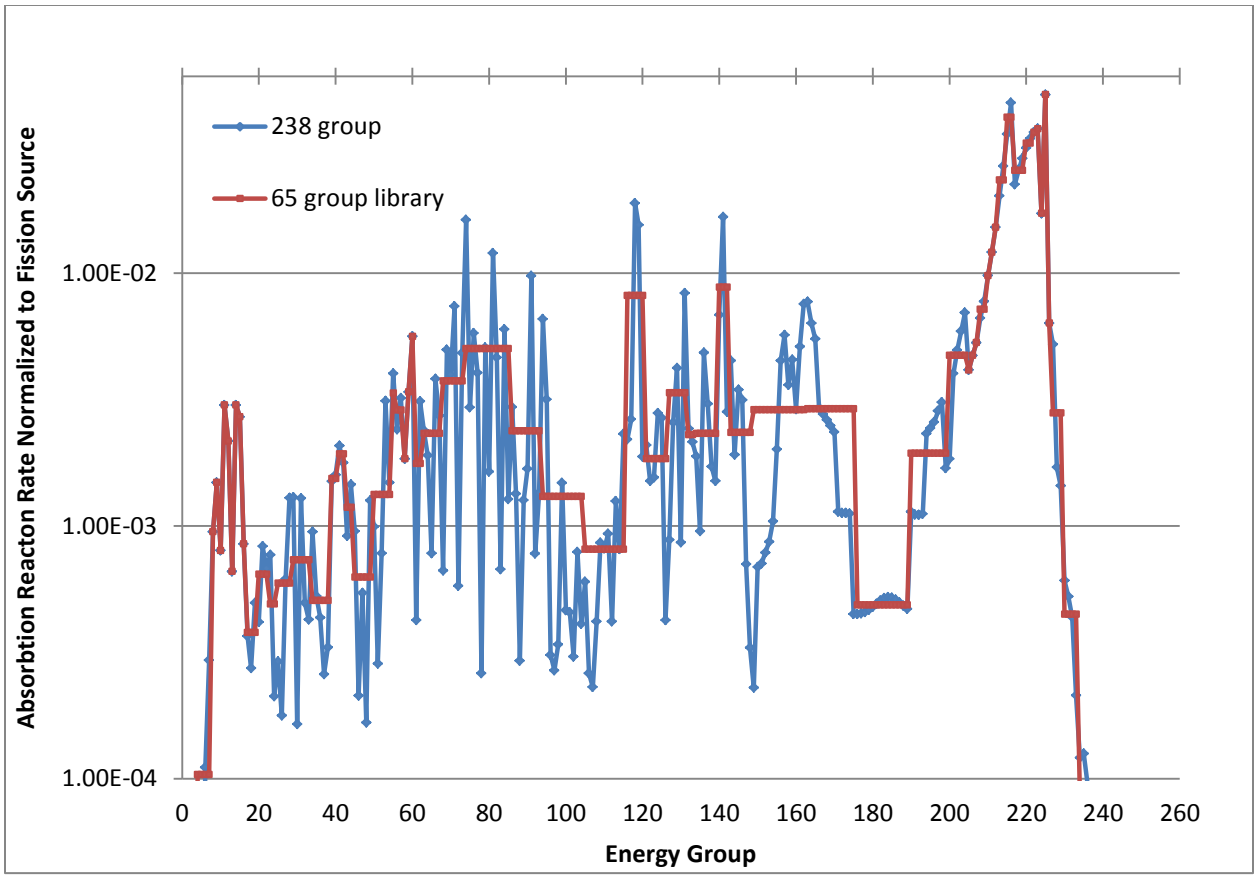

Figure 15. Fission source normalized absorption rate of 238 group and 65 group averaged over 238 group structure

The 65 group library follows the 238 group library best in the thermal spectrum and reasonably well in the fission spectrum, but does more poorly in the fast, epithermal, and resonance ranges. The 65 group library does not do well when used for calculating K-inf. It has a difference of 180 pcm at BOC even though it gives the correct cycle length. However, when used to calculate isotopics it has less than a 1% error for the concentration of each isotope after a burnup of about 55 GWd/tHM. It is more important to have a small error in isotopics than in reactivity since the isotopics is to calculate radio-toxicity.

Impact of Partitioning Scenarios on Generation of Transuranics with no Loses Assumed

Three scenarios were analyzed with the assumption that no losses are taken when reprocessing. Equilibrium concentrations were calculated for a case with no separation, a case

with neptunium separated, and a case with plutonium and neptunium separated. In each case the fission products are removed with 100% efficiency after every 3 batch residence cycles followed by a five year cool down. The cycle length (between refueling) is 18 months as in the once-through fuel cycle calculations. This means that every residence cycle is 4.5 years. Therefore, a total of 50 residence cycles is about 225 years. In the Np separation (partitioning) case and the Np and Pu separation case 100% of the Np and 100% the Np and Pu, respectively, are removed and placed in interim storage every residence cycle.

As each case moves toward equilibrium the reactivity curve shows a smaller swing after each residence cycle. The reactivity curve will move to the equilibrium cycle faster or slower depending on the recycling and separation scheme. By separating neptunium and plutonium fewer minor actinides are produced each residence cycle and equilibrium concentrations are generated quicker. This causes the K-inf curve to converge to the equilibrium cycle conditions faster. Figure 16, Figure 17, and Figure 18 show infinite criticality as a function of full power days (FPD) for cycle 1, 2, 10, and 50. When neptunium and plutonium are removed each residence cycle the change in reactivity swing between residence cycles is less than in the case without separation.

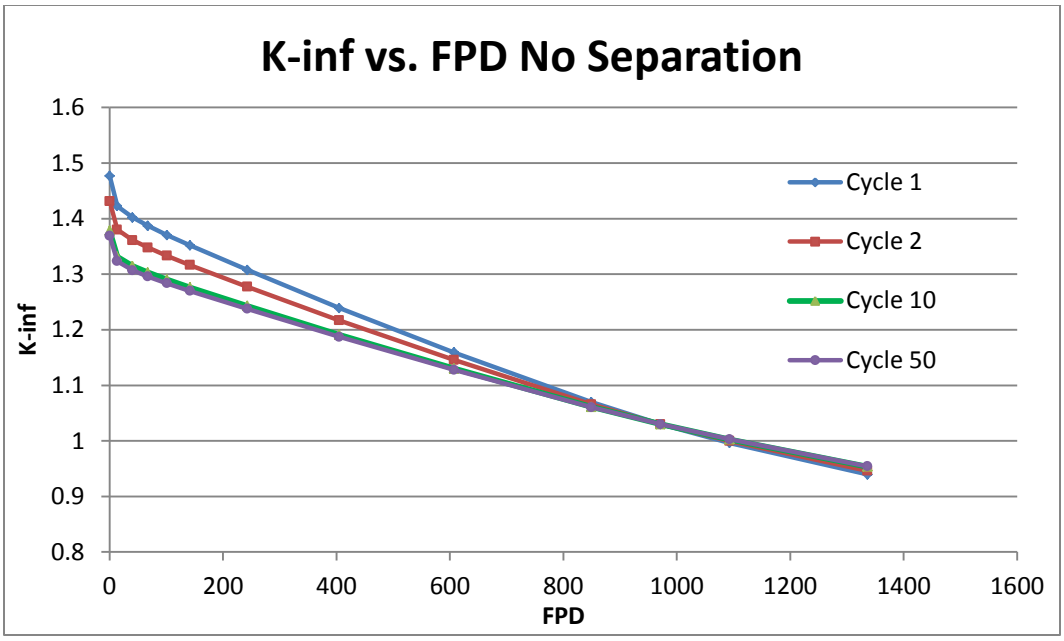

Figure 16. K-inf as a function of FPD for cycle 1, 2, 10 and 50 with no separation or losses

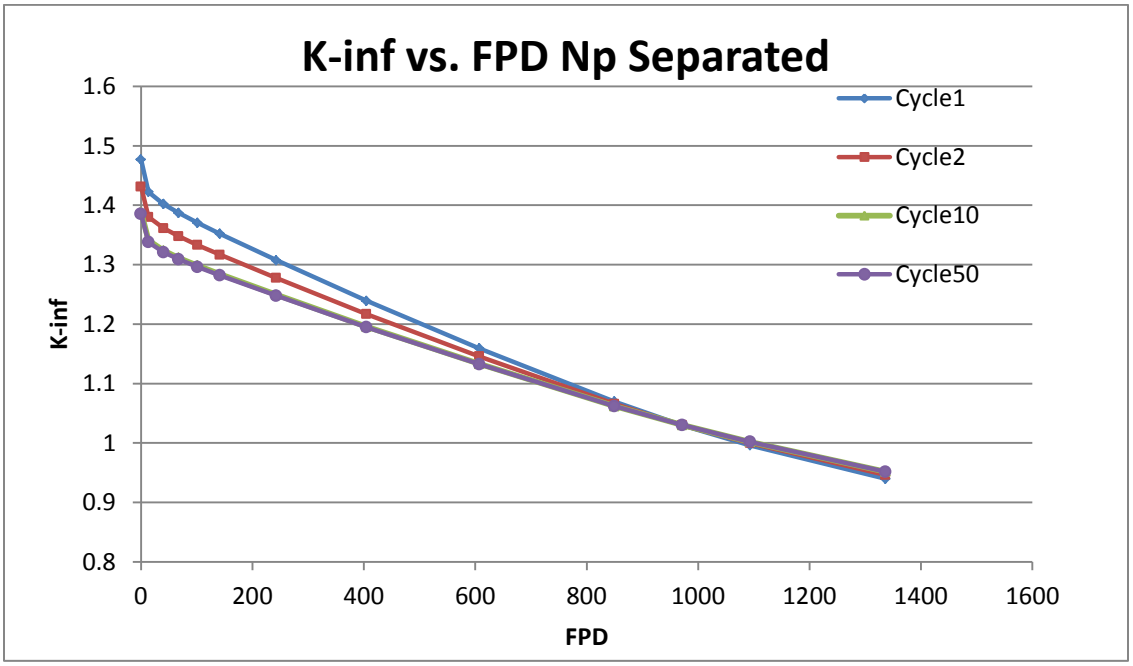

Figure 17. K-inf as a function of FPD for cycle 1, 2, 10 and 50 with Np separated and no losses

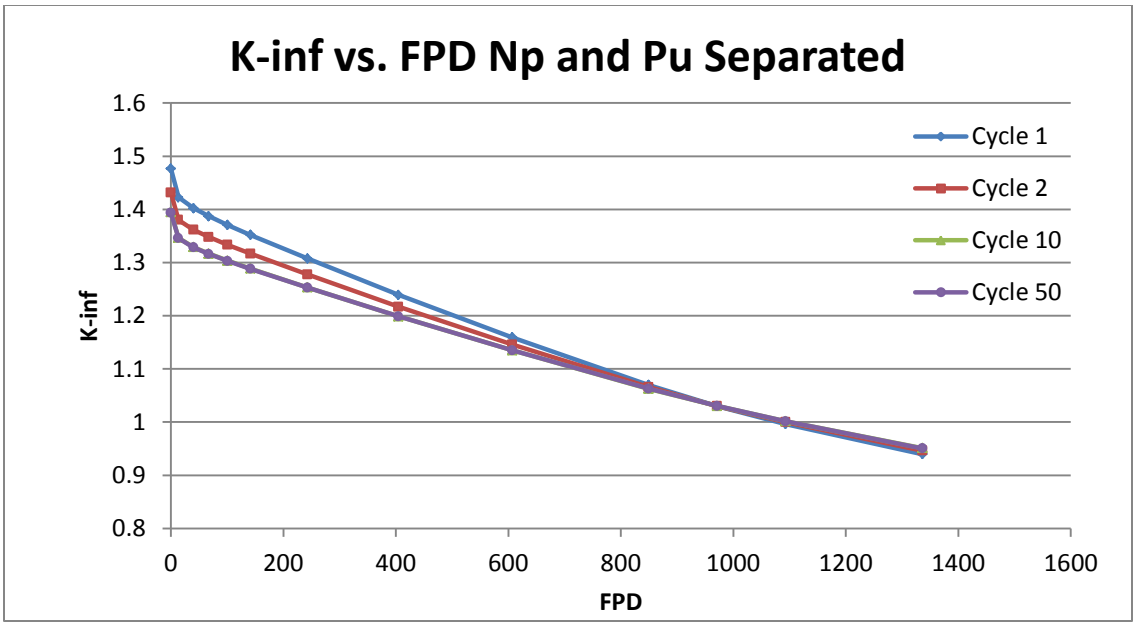

Figure 18. K-inf as a function of FPD for cycle 1, 2, 10 and 50 with Np and Pu separated and no losses

In addition to effecting reactivity, separation scenarios effect how much ^{233}U and thorium makeup is added each residence cycle. Figure 19 shows ^{233}U makeup every residence cycle for the three separation scenarios.

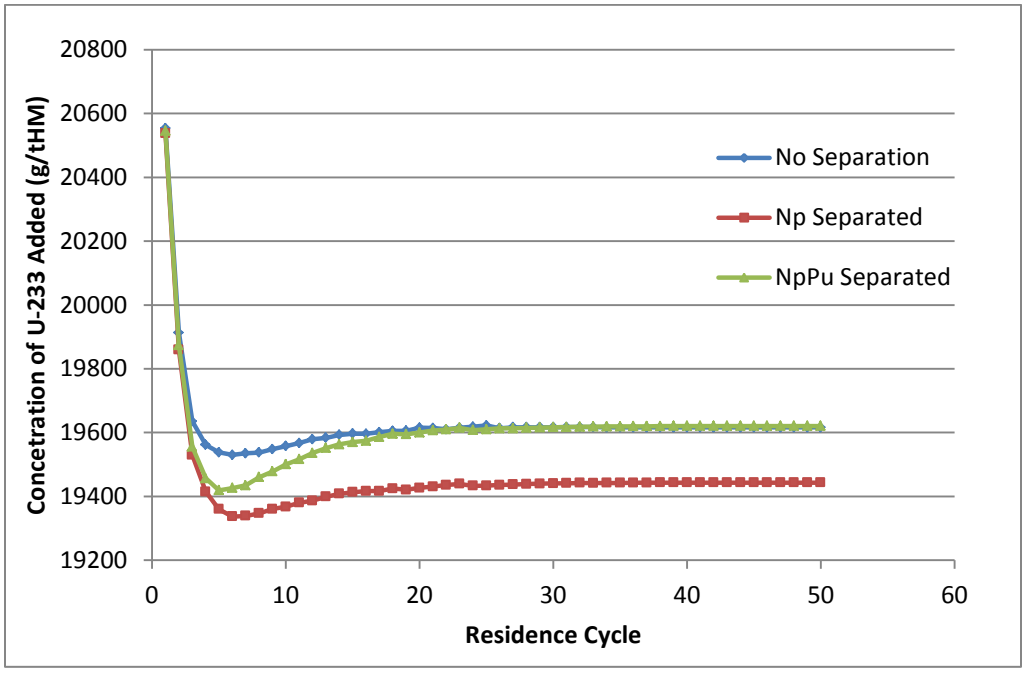

Figure 19. U-233 makeup each residence cycle for each separation scenario

Figure 19 shows that the scenario with no separation requires the most ^{233}U makeup to maintain the correct cycle length. Interestingly the Np partitioning scenario requires less ^{233}U makeup than the Np and Pu partitioning scenario. This is most likely because when only the neptunium is partitioned the remaining plutonium contains enough of the fissile isotope to contribute to criticality. Since neptunium makes up for most of the minor actinide concentration, its separation removes a large amount of neutron poisoning. Figure 20 shows thorium makeup for each residence cycle. The more material is partitioned in each cycle, the more thorium makeup is needed to fill the fuel volume.

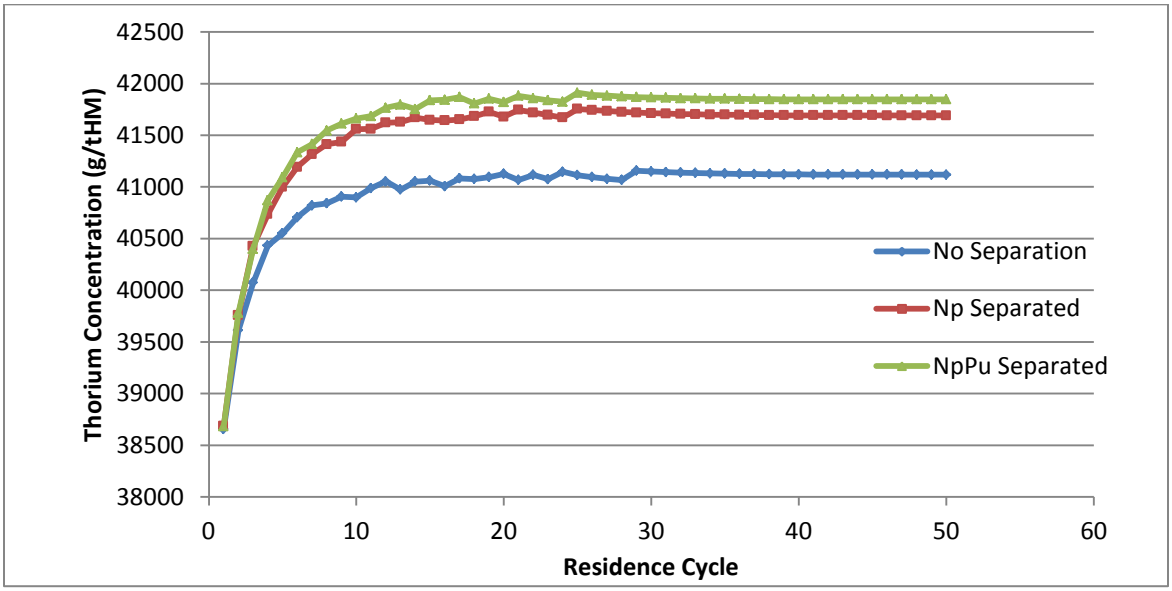

Figure 20. Thorium makeup added each residence cycle

^{232}U buildup can complicate reprocessing since it requires very expensive automated remote handling equipment due to high energy gamma rays. Figure 21 shows ^{232}U buildup in ppm in uranium each residence cycle. Initially the ^{232}U concentration is at 3,350 ppm the first residence cycle. After recycling the ^{232}U three times the concentration builds up to a maximum of 5,380 ppm. As minor actinides build up the equilibrium concentration of ^{232}U drops to 4,930

ppm. Even after the first residence cycle the concentration of ^{232}U is well beyond levels requiring additional shielding and remote handling facilities for reprocessing. Heavy water reactors produce orders of magnitude less 232U[10]. Perhaps by using an enhanced moderation lattice with smaller pins and a larger pitch ^{232}U buildup could be reduced by softening the spectrum, which decreases the rate of n,2n reactions in the fuel.

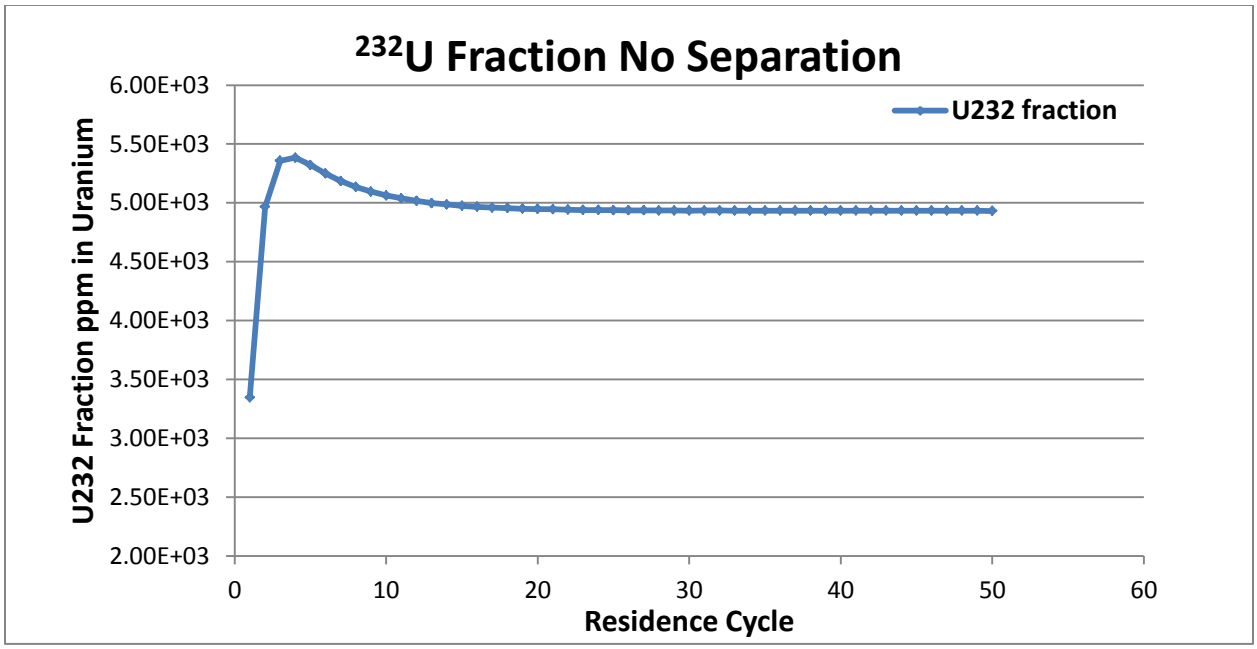

Figure 21. ^{232}U fraction in ppm of uranium in the no separation scenario. The ^{232}U fraction is after the 5 year cooldown.

Separating neptunium and plutonium each cycle mitigates the neutron absorption pathway to higher minor actinides reducing their production by more than an order of magnitude. Figure 22 shows the total concentration of minor actinides not including neptunium each cycle after the 5 year cooldown. Table 18 displays the total concentrations of minor actinides by element for the 1st, 2nd, 10th, and 50th residence cycle. The case with Np and Pu separated has the lowest minor actinide equilibrium cycle concentration and approaches equilibrium cycle concentrations more quickly. Both separation cases produce less plutonium and minor actinides

than the case with no separation. Figure 23 shows the total concentration of plutonium after the 5 year cooldown each cycle for the three no loss cases. Table 19 shows the concentration of plutonium after the 1st, 2nd, 10th, and 50th residence time. Removing neptunium each cycle has the greatest effect on reducing the amount of plutonium generated each residence cycle but removing plutonium has a greater effect on slowing the production of minor actinides.

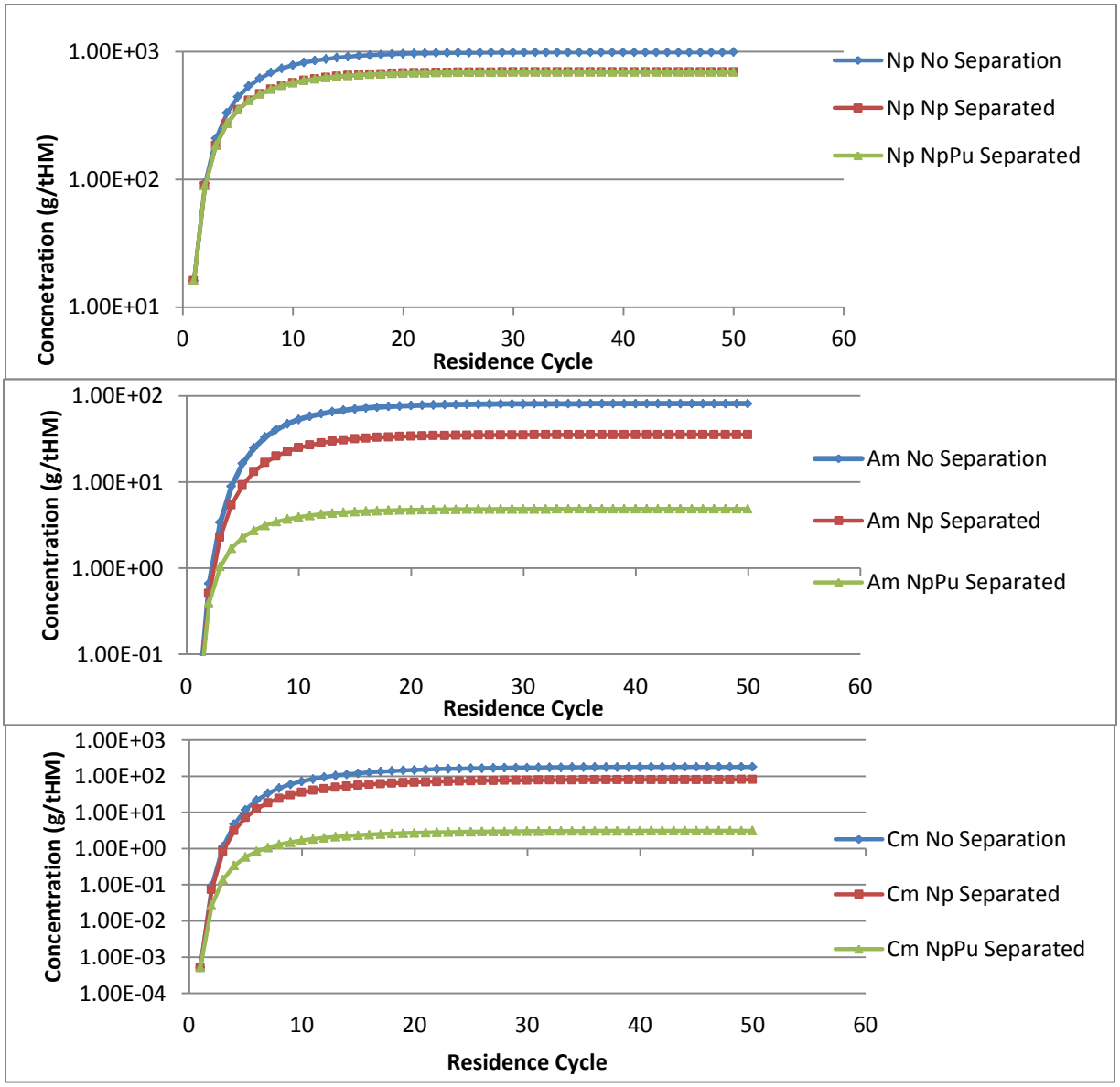

Figure 22. Total concentration in g/tHM of MA's over 50 recycles after the 5 year

Table 18. Total minor actinide concentrations by element (g/tHM)

Minor Actinide Concentrations in g/tHM After 5 year Cooldown			
No Separation No Losses			
Element	Np	Am	Cm
Cycle1	1.612E+01	2.134E-02	5.280E-04
Cycle2	9.339E+01	6.628E-01	9.439E-02
Cycle10	7.853E+02	5.315E+01	7.196E+01
Cycle50	9.926E+02	8.134E+01	1.813E+02
Np Separated No Losses			
Element	Np	Am	Cm
Cycle1	1.612E+01	2.134E-02	5.280E-04
Cycle2	8.921E+01	5.079E-01	7.357E-02
Cycle10	5.719E+02	2.500E+01	3.568E+01
Cycle50	6.949E+02	3.538E+01	8.076E+01
Np and Pu Separated No Losses			
Element	Np	Am	Cm
Cycle1	1.612E+01	2.134E-02	5.280E-04
Cycle2	8.921E+01	3.985E-01	2.700E-02
Cycle10	5.721E+02	3.921E+00	1.675E+00
Cycle50	6.947E+02	4.871E+00	3.122E+00

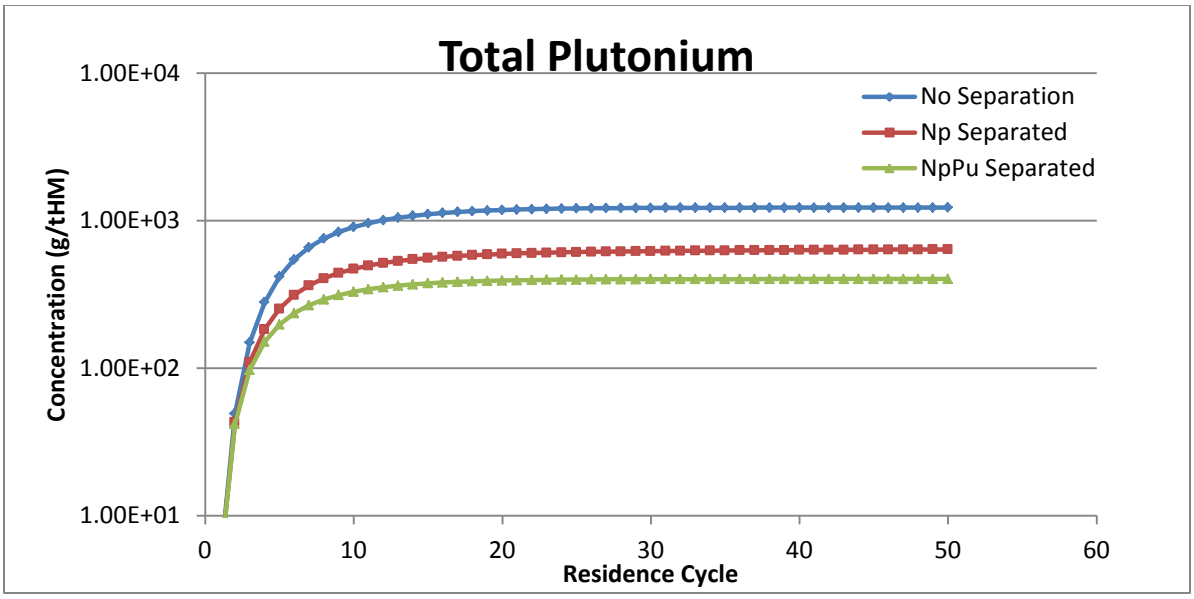

Figure 23. Total plutonium concentration in grams normalized to 10^6 grams heavy metal

Table 19. Total plutonium concentration for the three separation schemes after the 1st, 2nd, 10th, and 50th residence time (g/tHM)

Total Pu Concentration After 5 Year Cooldown in g/tHM			
Scenario	No Separation	Np Separated	NpPu Separated
Cycle1	4.4595E+00	4.4595E+00	4.46E+00
Cycle2	4.9401E+01	4.3048E+01	4.18E+01
Cycle10	9.0542E+02	4.7131E+02	3.29E+02
Cycle50	1.2270E+03	6.3861E+02	4.02E+02

Impact of Neptunium and Plutonium Separation Efficiency on Multi-recycle Scenarios

Multi-recycle isotopics were calculated for the Np and Pu separation scenario for 100%, 95%, and 70% separation efficiencies. Each case assumes a .1% loss during reprocessing each cycle before separation of Np and Pu. The .1% loss is assumed to be sent to a HLW permanent repository. Since the rest of the fuel is assumed to be recycled back indefinitely only the radio-toxicity of the losses in the HLW storage is considered when evaluating the multi-recycle scenario. Figure 24 shows the total concentration of neptunium, americium, and curium for each of the separation efficiencies after the 5 year cooldown before the fuel is reprocessed.

Figure 25 shows total concentration of plutonium for each of the separation efficiencies. Table 20 displays the total concentrations of neptunium, americium, and curium after 1, 2, 10 and 50 residence times, at different separation efficiencies after the 5 year cooldown. Table 21 displays the total concentration of plutonium.

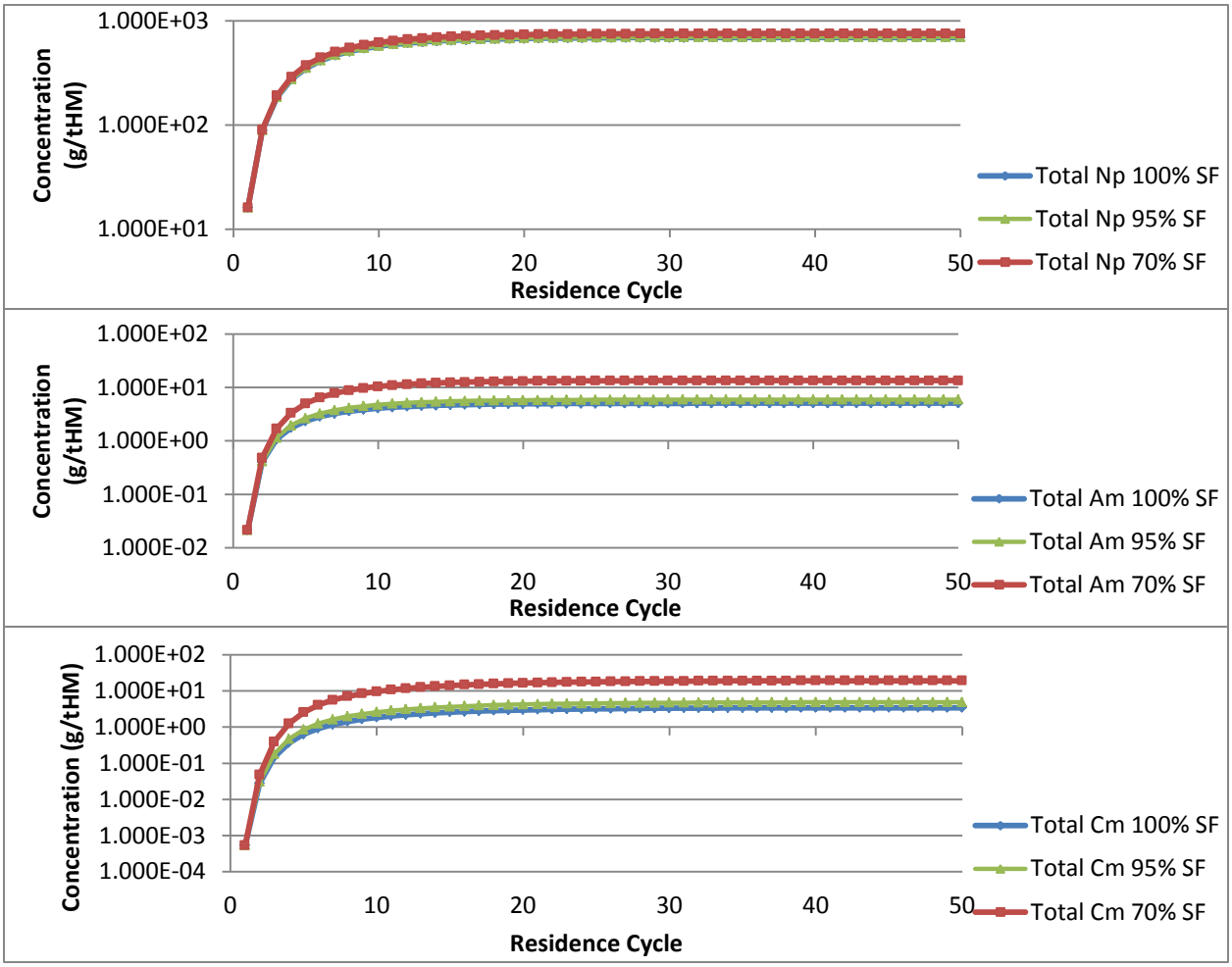

Figure 24. Total concentration of neptunium, americium, and curium for each of the separation efficiencies after the 5 year cooldown before the fuel is reprocessed

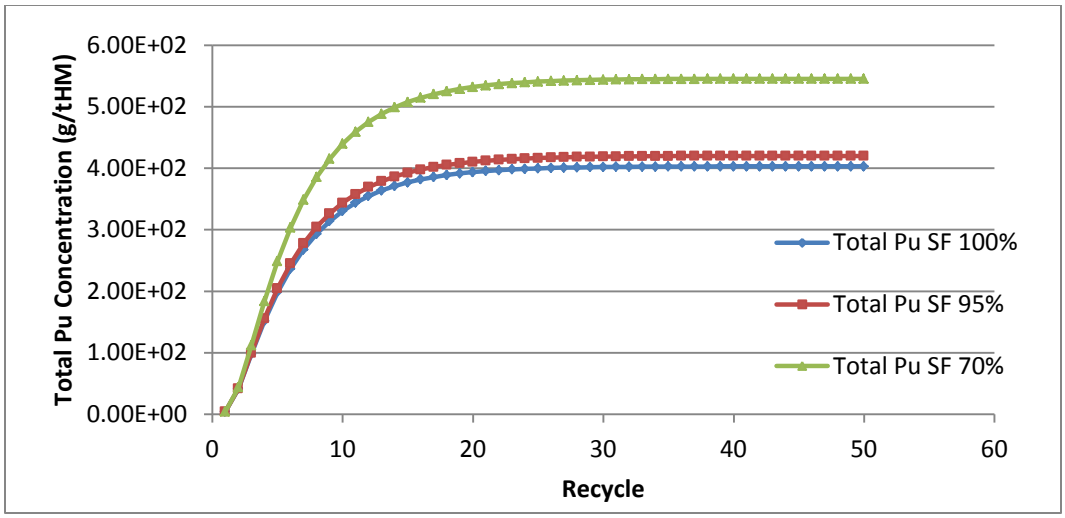

Figure 25. Total concentration of plutonium after 5 year cooldown for each of the separation efficiencies

Table 20. total concentrations of neptunium, americium, and curium after 1, 2, 10 and 50 residence times in the core, at the different separation efficiencies after the 5 year cooldown in g/tHM.

Scenario	Np+Pu Separated with 100% SF		
Element	Total Np (g/tHM)	Total Am (g/tHM)	Total Cm (g/tHM)
Cycle1	1.612E+01	2.134E-02	5.280E-04
Cycle2	8.918E+01	4.023E-01	2.779E-02
Cycle10	5.713E+02	4.075E+00	1.845E+00
Cycle50	6.925E+02	5.060E+00	3.433E+00
Scenario	Np+Pu Separated with 95% SF		
Element	Total Np (g/tHM)	Total Am (g/tHM)	Total Cm (g/tHM)
Cycle1	1.61E+01	2.13E-02	5.28E-04
Cycle2	8.94E+01	4.13E-01	3.05E-02
Cycle10	5.77E+02	4.74E+00	2.59E+00
Cycle50	7.00E+02	5.92E+00	4.87E+00
Scenario	Np+Pu Separated with 70% SF		
Element	Total Np (g/tHM)	Total Am (g/tHM)	Total Cm (g/tHM)
Cycle1	1.61E+01	2.13E-02	5.28E-04
Cycle2	9.04E+01	4.79E-01	4.73E-02
Cycle10	6.20E+02	1.04E+01	9.61E+00
Cycle50	7.55E+02	1.34E+01	1.92E+01

Table 21. Total plutonium concentration after each residence timer for different separation efficiencies in g/tHM

NpPu Separated Total Plutonium concentration in g/tHM			
Separation Efficiency	**100%**	**95%**	**70%**
Cycle1	**4.46E+00**	**4.46E+00**	**4.46E+00**
Cycle2	**4.17E+01**	**4.20E+01**	**4.40E+01**
Cycle10	**3.31E+02**	**3.44E+02**	**4.40E+02**
Cycle50	**4.03E+02**	**4.20E+02**	**5.45E+02**

It can be seen from the results that separation efficiency has little effect on the equilibrium concentration of neptunium. Neptunium is much lower in the transmutation chain and therefore is generated much quicker than heavier minor actinides. Changing separation efficiency has more of an effect on heavier actinides since they reach equilibrium slower. Decreasing the separation efficiency by 30% increases the concentration of americium by more than a factor of two and increases the concentration of curium by a factor of six. Plutonium is also significantly affected by the 30% decrease in separation efficiency, the plutonium concentration is increased by 26%.

This multi-recycle isotopics study evaluates multiple scenarios for recycling thorium fuel. In the first part of this study three idealized separation scenarios with no losses are compared. Separating neptunium and plutonium reduces production of americium and curium by almost two orders of magnitude. The second part of this study evaluates the effect of the separation efficiency for the neptunium and plutonium separation scenario with losses during reprocessing. The separation efficiency has a significant effect on the production of transuranics. For example, decreasing the separation efficiency from 100% to 70% increases the equilibrium cycle plutonium concentration by 26%, americium by nearly 100%, and curium by about 600%.

EVALUATION OF LONG-TERM RADIO-TOXICITY

Radio-toxicity is calculated for the previous fuel cycle scenarios using the isotopic data generated in SCALE6.0. In order to calculate radio-toxicity for the once-through cases and multi-recycle cases with no losses the ft71 restart file is used as an input for Origen-s. The multi-recycle cases with losses use a Python script that takes the output isotopics data and creates an Origen-S input file. Origen-S runs in only a few seconds. Both the ingested and inhaled radio-toxicity are calculated for all cases. The results are normalized to the radio-toxicity of the equivalent amount of natural uranium (without irradiation) which would be needed to produce the same energy if used to make LEU fuel for once-through LWR. In this chapter the first section covers the radio-toxicity of once-through fuel cycle scenarios. The second section of this chapter evaluates radio-toxicity of different transuranic partitioning scenarios. The last section of the chapter is a study of the impact of separation efficiency on long term radio-toxicity.

Once-Through Radio-toxicity

Radio-toxicity was calculated for each of the eight cases in order to compare their impact on a repository. Each case with uranium fuel case is paired with its respective thorium fuel case. It can be seen that the daughters of ^{233}U have a significant impact on long term storage. Figure 26 shows the inhaled radio-toxicity of thorium with ^{233}U fuel compared with UOX fuel. Figure 27 shows the inhaled and ingested radio-toxicity of thorium fuel compared to UOX.

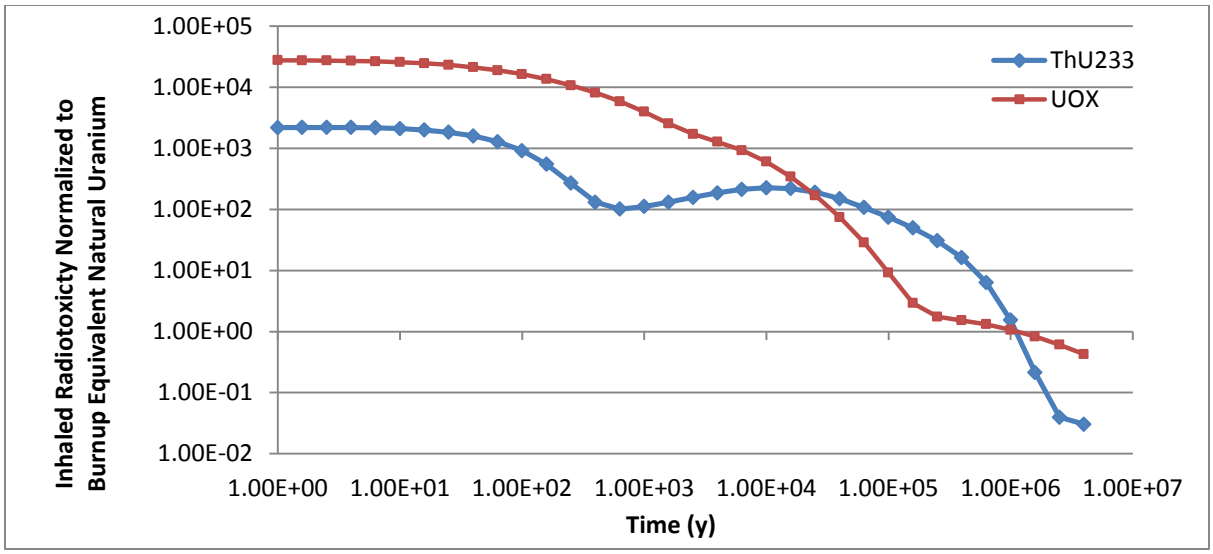

Figure 26. Inhaled radio-toxicity of Th-U233 fuel compared with UOX fuel normalized to burnup equivalent of natural uranium

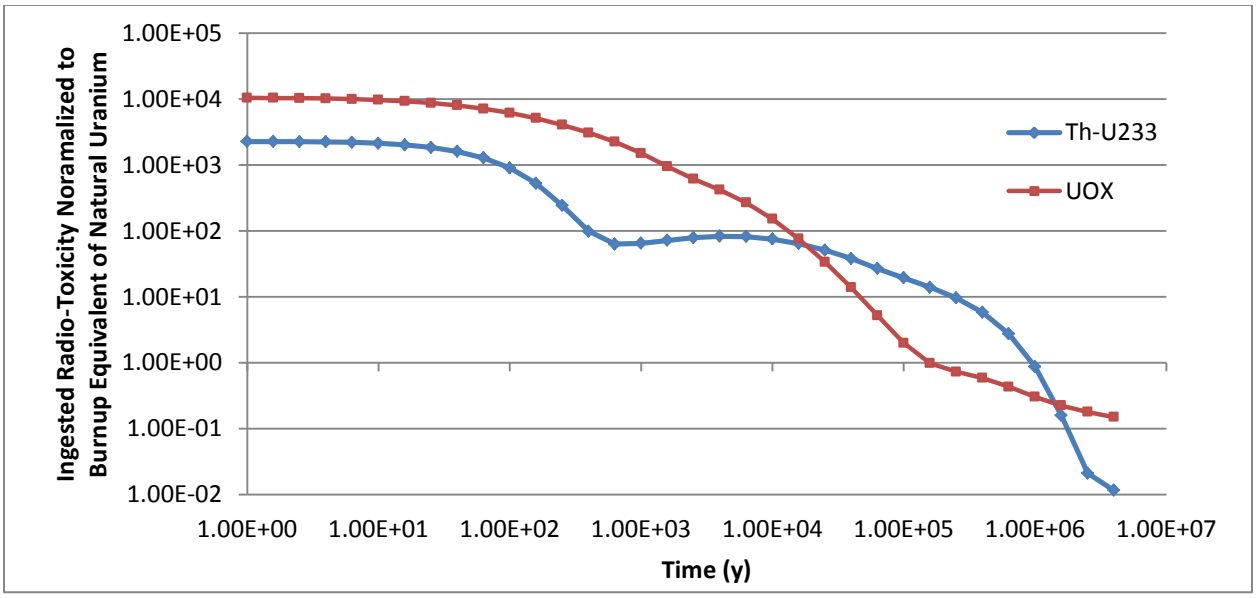

Figure 27. Ingested radio-toxicity of Th-U233 fuel compared with UOX fuel normalized to burnup equivalent of natural uranium

Radio-toxicity of thorium fuel drops after the first several hundred years until decay products of ^{233}U and ^{231}Pa dominate to a maximum around 10,000 years. Radio-toxicity of uranium is mostly dominated by isotopes of plutonium and americium until after 100,000 when ^{242}Pu and decay products of ^{241}Am take over. Interestingly, if the metric is which fuel's radio-toxicity

drops below natural uranium's then they are about the same. However, the risk for UOX is roughly two orders magnitude greater for the first 5,000 years and is greater than Th-U233 fuel for the first 10,000 years.

The three main isotopes that dominate radio-toxicity in thorium fuel are ^{228}Th, ^{232}U, and ^{229}Th. ^{228}Th is generated mostly from the alpha decay of ^{232}U. ^{232}U builds up in the reactor from the radiative capture of ^{231}Pa followed by a decay. Together ^{232}U and ^{228}Th account for nearly 90% of the radio-toxicity for the first 250 years. Afterwards ^{228}Th, which builds up from the decay of ^{233}U dominates radio-toxicity for over one-million years. The peak in radio-toxicity around 15,000 years of HLW from thorium fuel occurs when ^{228}Th is in secular equilibrium with ^{233}U. It may be possible to reduce the long term radio-toxicity of waste from thorium fuel by achieving higher burnup and further depleting ^{233}U before permanent storage. Figure 28 shows how the radio-toxicity of these three isotopes relates to spent thorium fuel radio-toxicity and uranium fuel radio-toxicity.

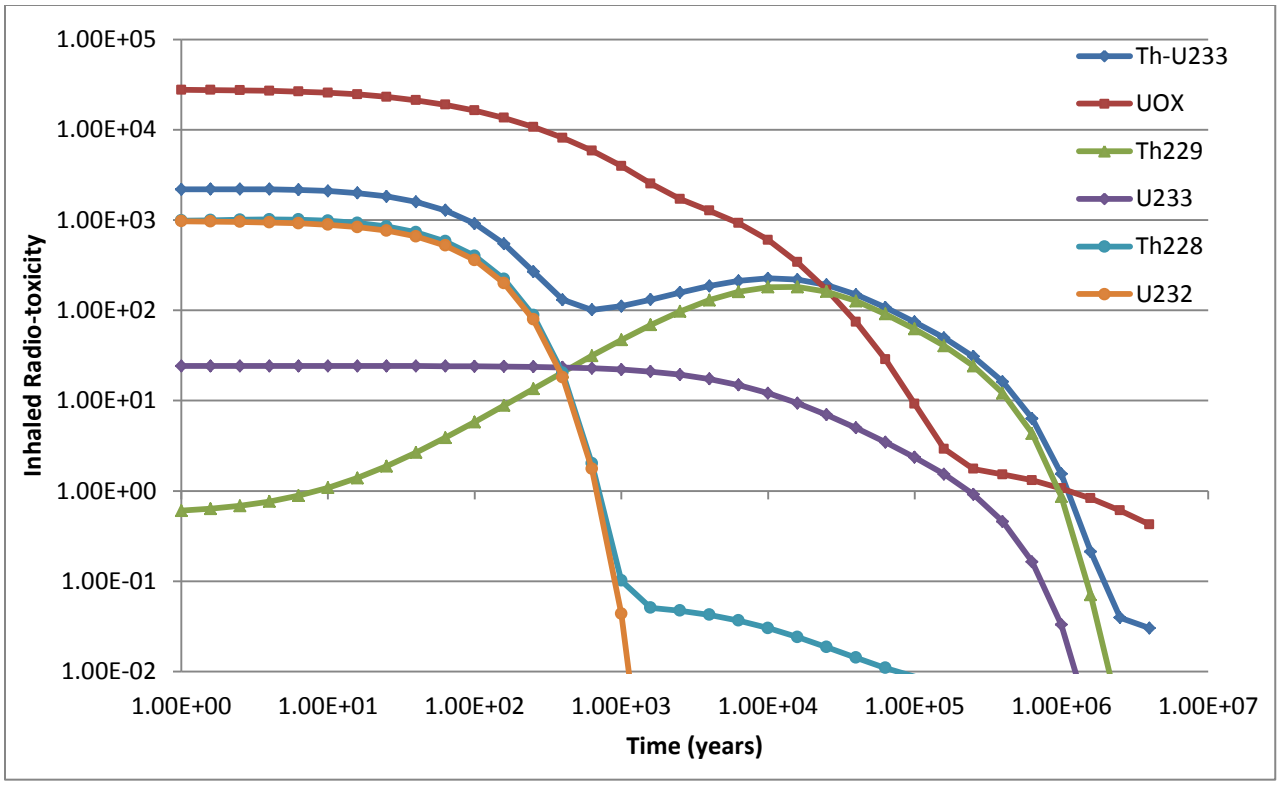

Figure 28. Contribution of primary isotopes to thorium fuel radio-toxicity compared to uranium fuel radio-toxicity

Plutonium, neptunium, and americium contribute the most to radio-toxicity in thorium and uranium fuels mixed with TRUOX. Regardless of the fertile isotope used the radio-toxicity of the transuranic fissile fuel dominates making the difference between thorium and uranium fuel less significant in a once-through cycle scenario. Even after a million years both TRUOX fuels are more toxic than the burnup equivalent of natural uranium. Figure 29 shows inhaled radio-toxicity of thorium and uranium fuel mixed with TRUOX. Figure 30 shows ingested radio-toxicity.

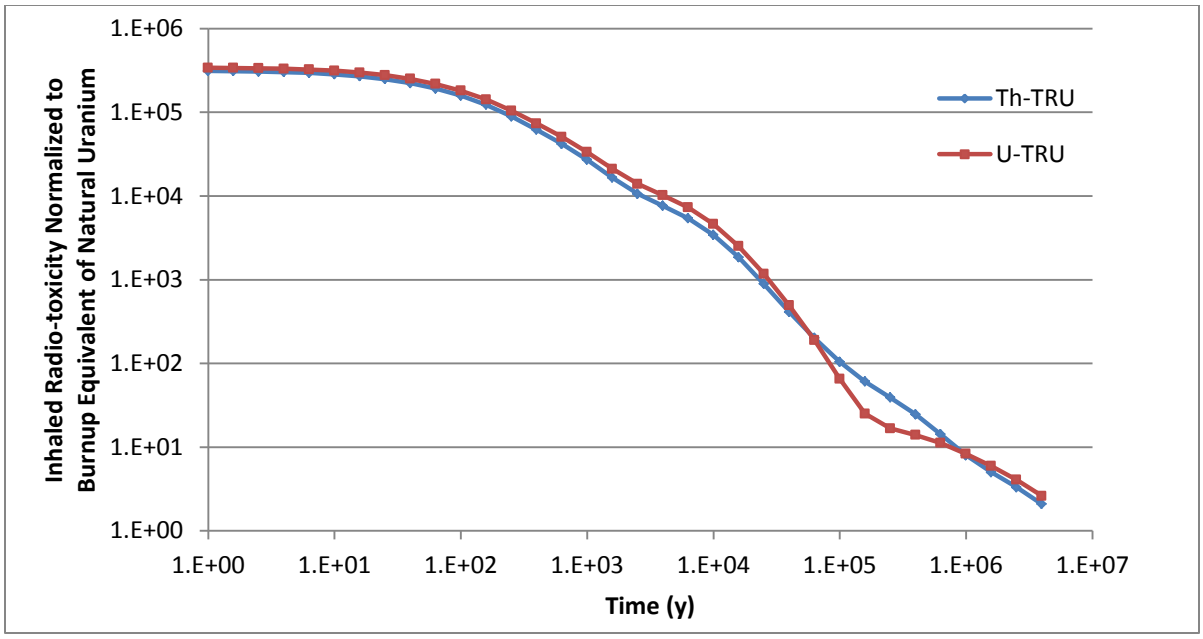

Figure 29. Inhaled radio-toxicity of thorium and uranium fuel mixed with TRUOX normalized to equivalent burnup of natural uranium

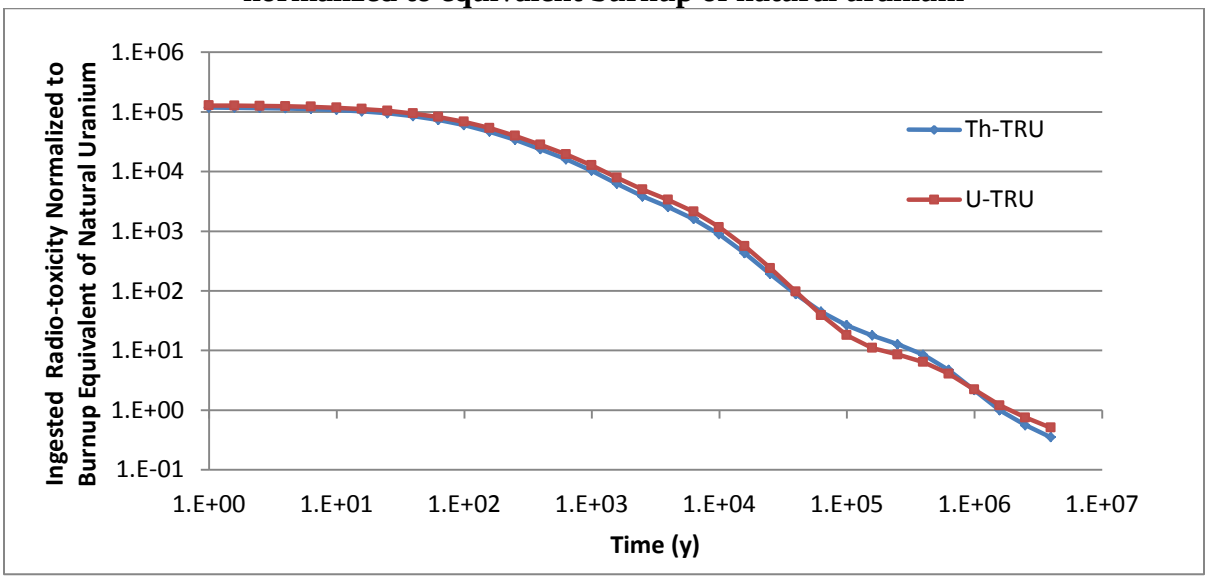

Figure 30. Ingested radio-toxicity of thorium and uranium fuel mixed with TRUOX normalized to equivalent burnup of natural uranium

Radio-toxicity of weapons grade plutonium mixed with thorium behaves similar to radio-toxicity of WGP mixed with uranium for the first 10,000 years. WGP mixed with natural uranium has a higher concentration of plutonium after discharge than when mixed with thorium

since plutonium is generated from ^{238}U so its radio-toxicity is nearly a factor two higher for the first 10,000 years. After 10,000 years most of the ^{240}Pu has decayed and radio-toxicity of uranium fuel drops more quickly than thorium fuel. Thorium fuel's activity decreases more steadily after 10,000 years since ^{233}U and its decay products are long lived. Figure 31 shows inhaled radio-toxicity of fuels mixed with weapons grade plutonium. Figure 32 shows ingested radio-toxicity.

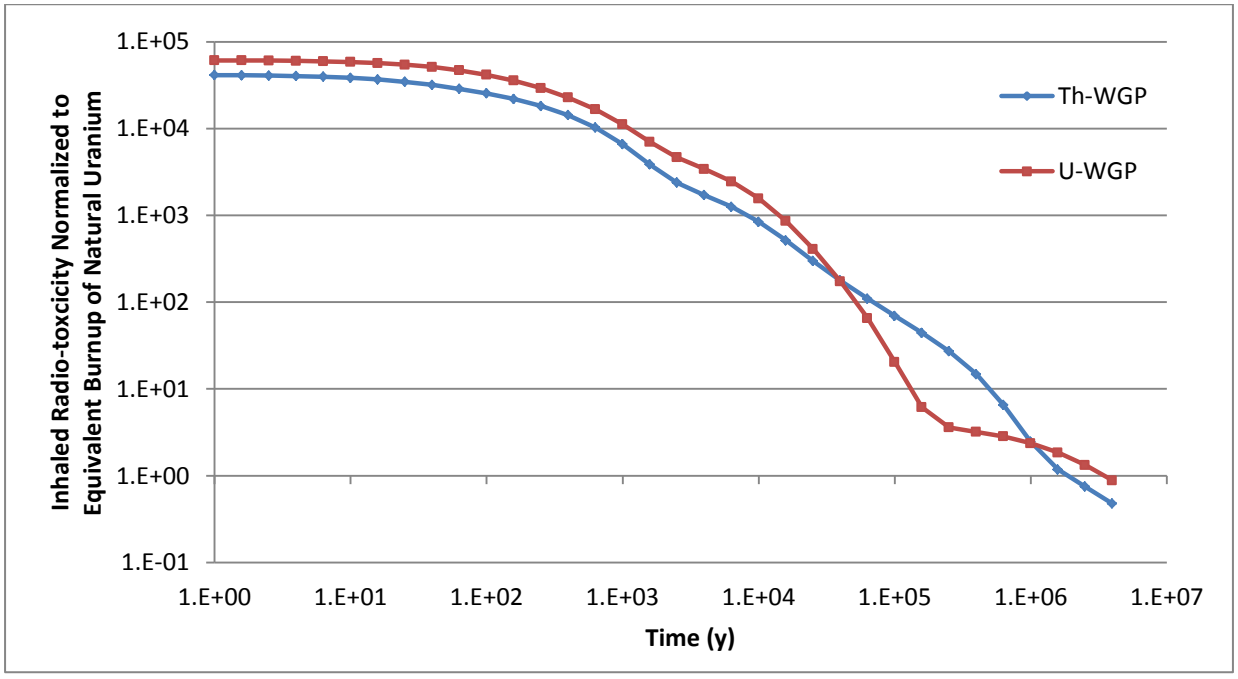

Figure 31. Inhaled radio-toxicity of WGP mixed with thorium and uranium normalized to equivalent burnup of natural uranium

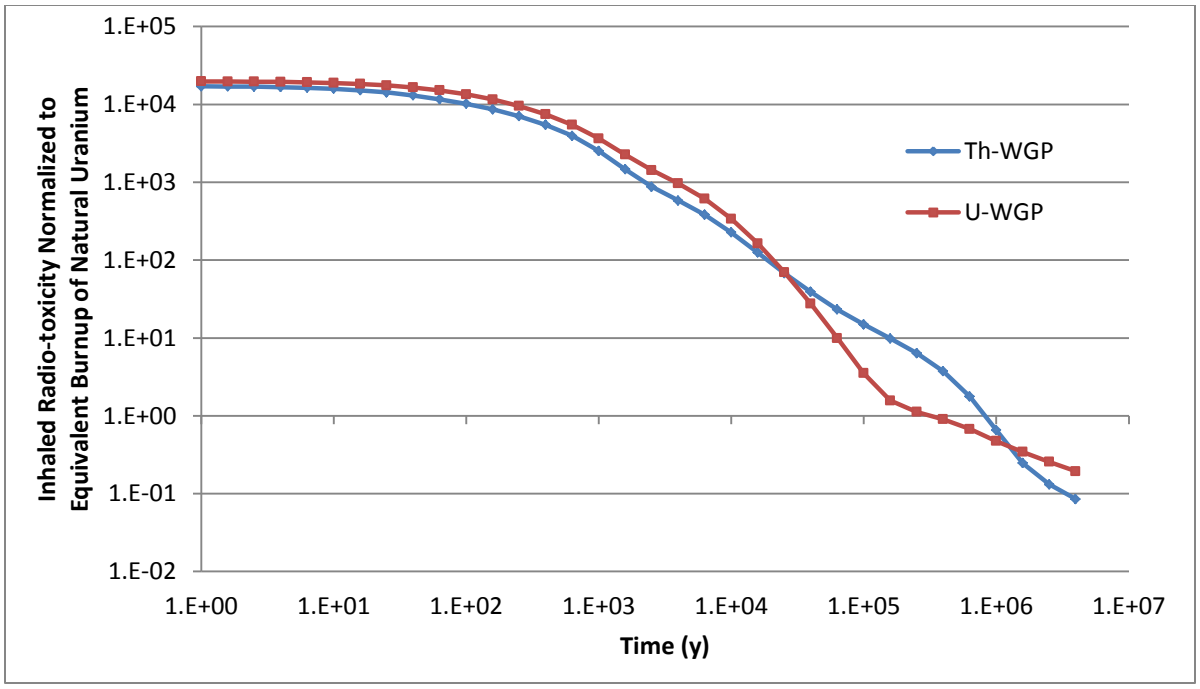

Figure 32. Ingested radio-toxicity of WGP mixed with thorium and uranium normalized to equivalent burnup of natural uranium

The case of thorium mixed with RGP compared to natural uranium is very similar to thorium or uranium mixed with TRUOX. Since reactor grade plutonium has a higher concentration of heavier plutonium isotopes minor actinides build up much quicker as the fuel is depleted. Figure 33 shows inhaled radio-toxicity of RGP mixed with thorium and RGP mixed with uranium. Figure 34 shows ingested radio-toxicity of RGP mixed with the two fuels. Overall the two fuels mixed with RGP have a lower radio-toxicity compared to fuels mixed with TRUOX. Similarly to other fuel comparisons the thorium mixed fuel starts with a lower radio-toxicity for the first 20,000 years then surpasses the uranium mixed fuel.

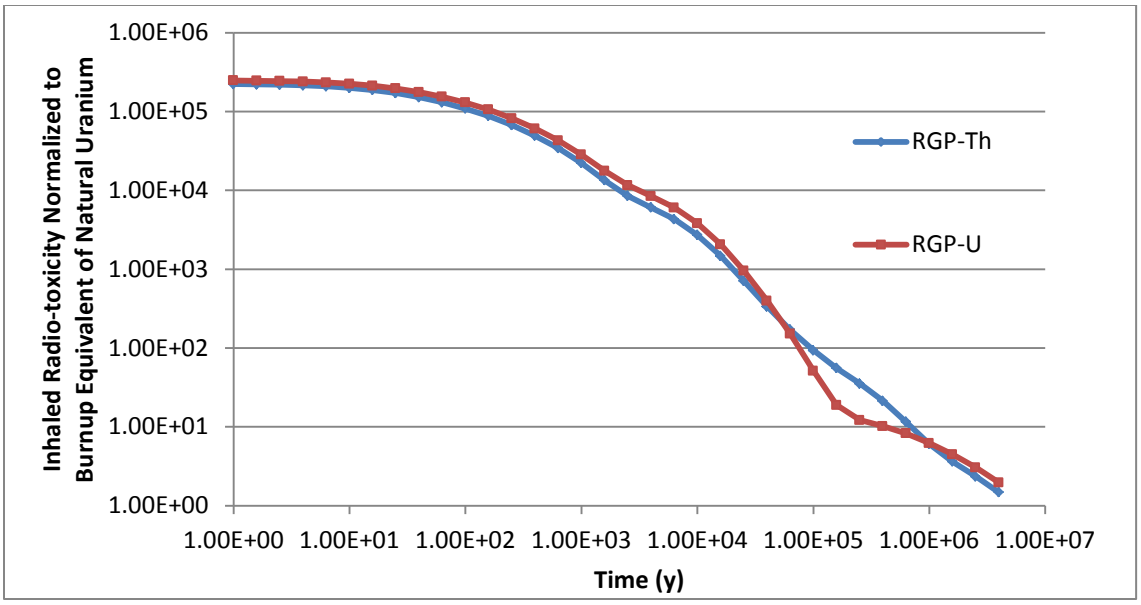

Figure 33. Inhaled radio-toxitity of thorium and uranium fuel mixed with RGP normalized to equivalent burnup of natural uranium

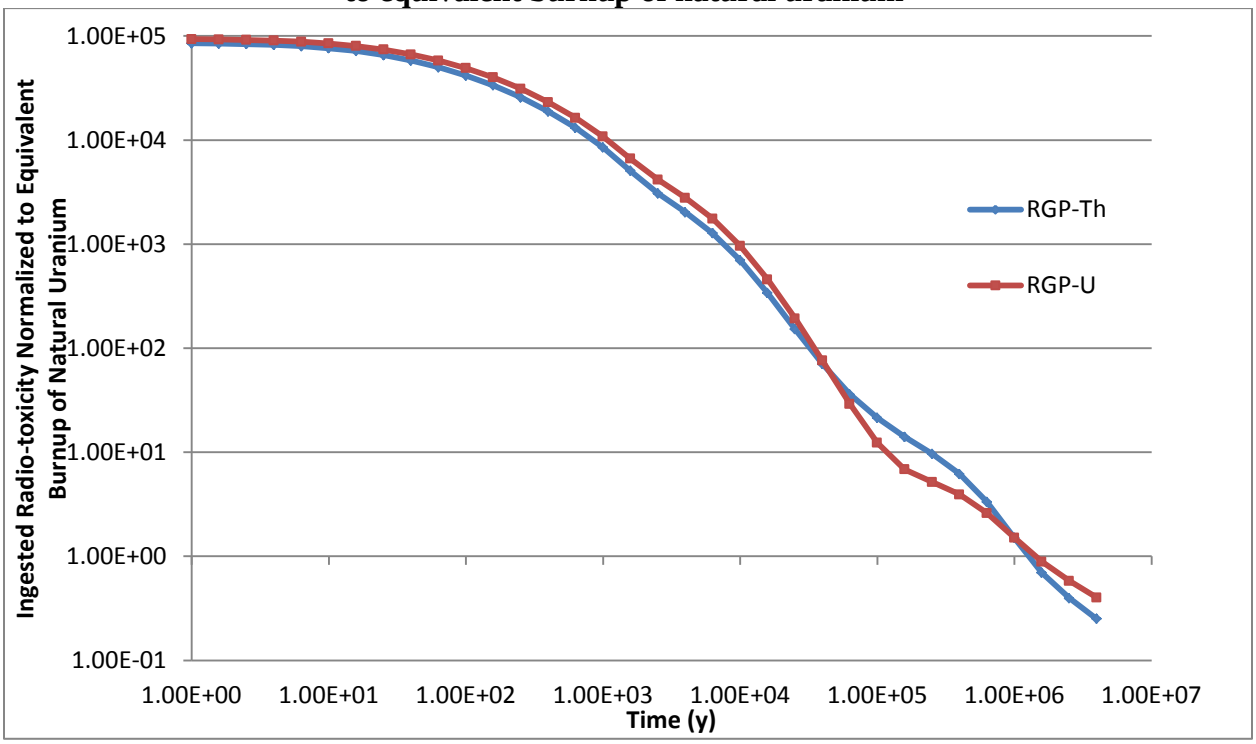

Figure 34. Ingested radio-toxicity of thorium and uranium fuel mixed with RGP normalized to equivalent burnup of natural uranium

Back End Radio-toxicity of Multi-recycle Partitioning Scenarios

Radio-toxicity was calculated for the three partitioning scenarios. These scenarios include no separation, separation of plutonium, and separation of neptunium and plutonium. The radio-toxicity calculation only includes the high level waste lost during reprocessing which accounts for 0.1% of the fuel mass. The remaining actinide portion of the fuel is assumed to be put back into the reactor. Fission products are not taken into account in this radio-toxicity calculation. Figure 35 shows inhaled radio-toxicity of the three scenarios for the 1^{st}, 2^{nd}, 10^{th}, and 50^{th} residence cycles. Figure 36 shows ingested radio-toxicity for the same. The scenario with neptunium and plutonium separated has the lowest radio-toxicity for the first 10,000 years by a large margin. After 10,000 years the difference between the separation scenarios and residence cycles is very small. Only separating neptunium has a small effect on reducing radio-toxicity for the first 10,000 years compared to separating plutonium and neptunium. All three separation scenarios are within 10% of each other after 10,000 years. Separating neptunium and plutonium after each residence cycle is very effective in reducing radio-toxicity after multiple residence cycles in the short term and after 1,000 years. It can be seen that there is a small difference in radio-toxicity between residence cycle 1 and residence cycle 50 at 1,000 years for the Np and Pu separated scenario. Also, it can be seen that for the Np and Pu separated scenario the radio-toxicity curves move towards equilibrium more quickly than without separation and when only neptunium is separated.

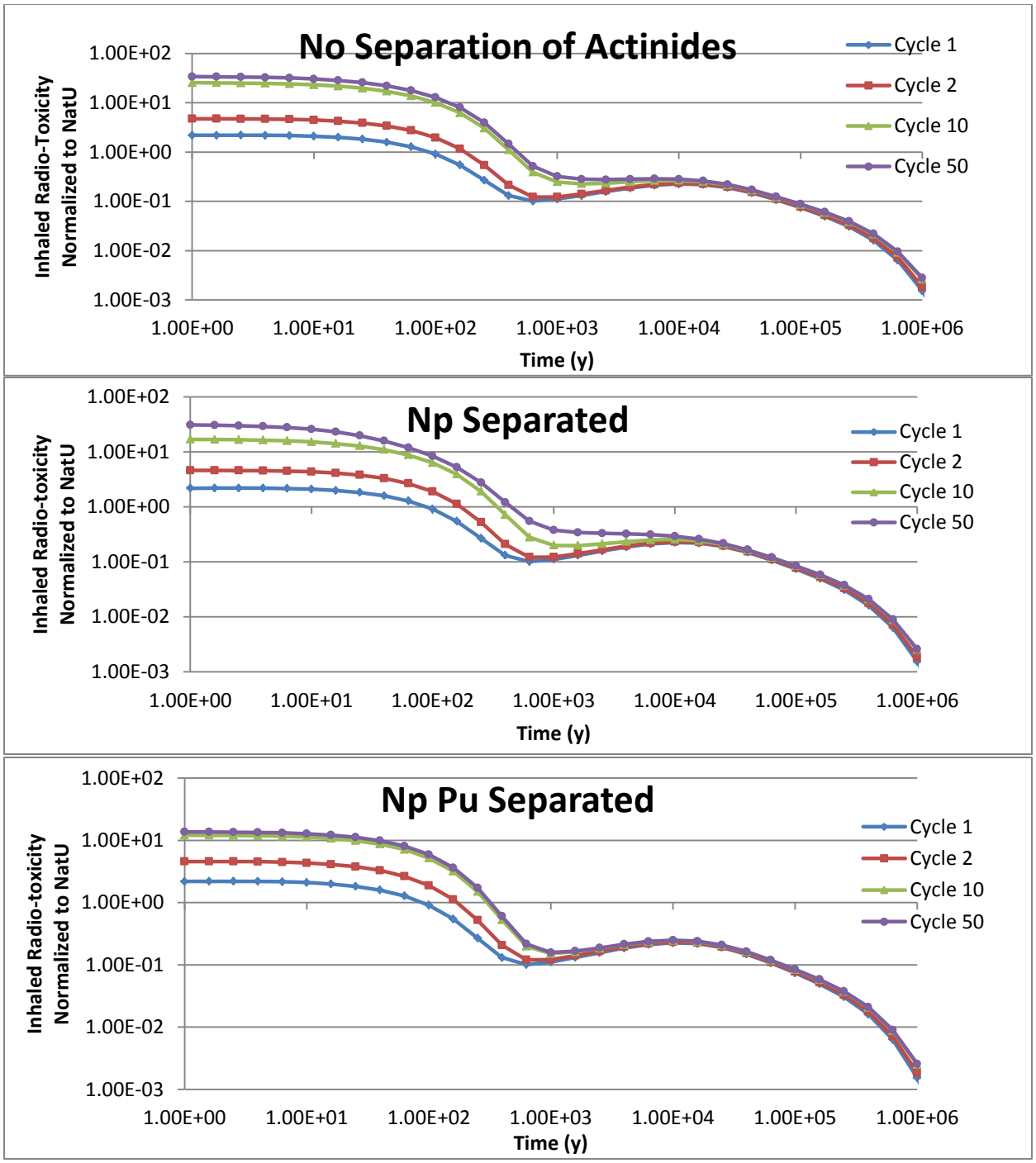

Figure 35. Inhaled radio-toxicity of partitioning scenarios normalized to equivalent burnup of natural uranium

Long term ingested radio-toxicity of the HLW has similar behavior to inhaled radio-toxicity. A major difference is there is not really a bump in ingested radio-toxicity after 1,000

years although the rate of decrease in radio-toxicity slows as decay products of ^{233}U dominate. The Np and Pu separated scenario shows quicker progress towards equilibrium than the other two scenarios with ingested radio-toxicity same as with inhaled radio-toxicity. Overall separating neptunium and plutonium does have a small effect on reducing ingested radio-toxicity. After residence cycle 50 the Np and Pu separated scenario has an ingested radio-toxicity half of the no separation scenario when the HLW first reaches the repository. However, after 10,000 years the difference between the two scenarios is only 10%.

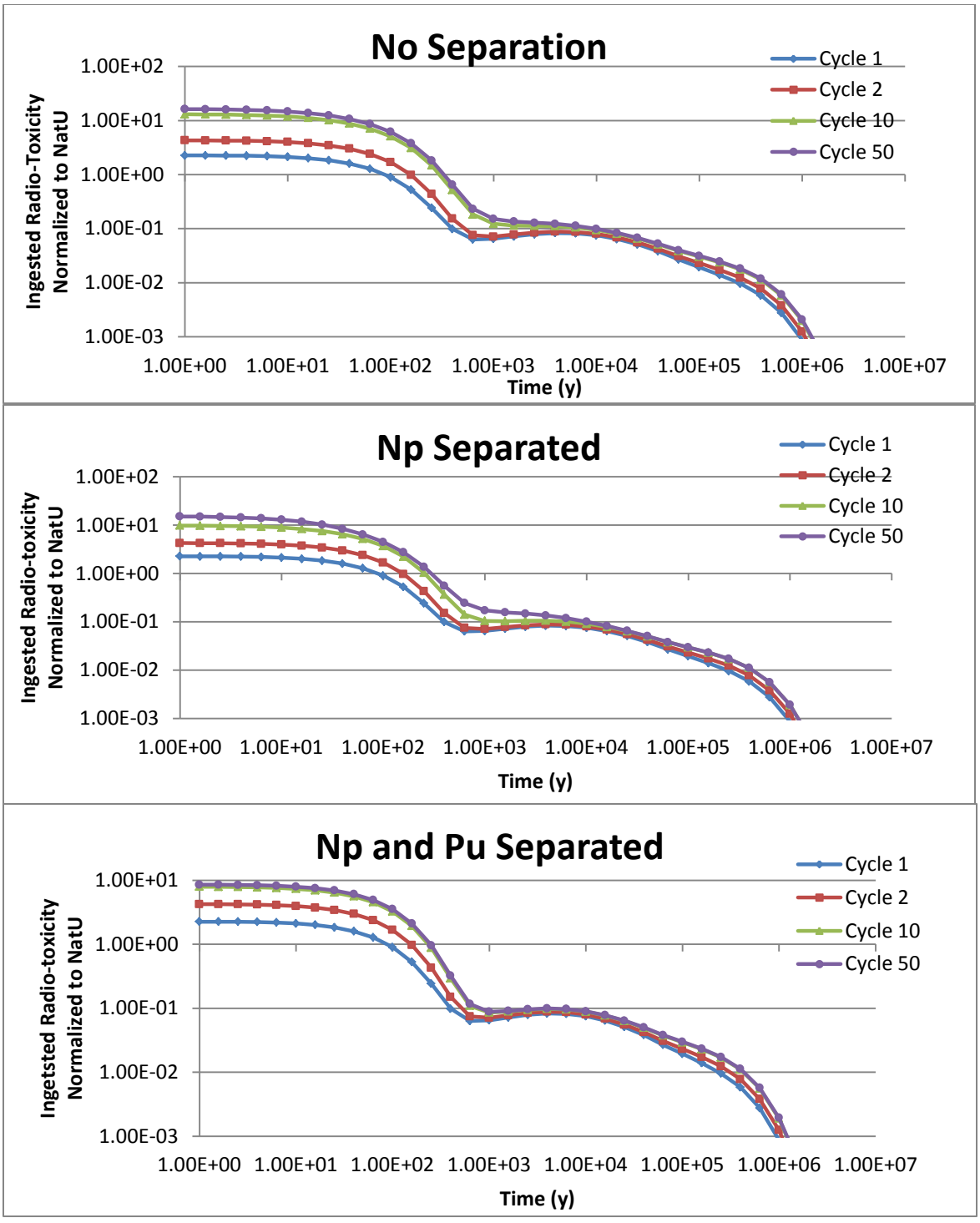

Figure 36. Ingested radio-toxicity of partitioning scenarios normalized to equivalent burnup of natural uranium

Impact of Separation Efficiency on Back End Radio-toxicity

Radio-toxicity is calculated for stored HLW from losses during reprocessing after 1, 2, 10 and 50 residence times. It is assumed that .1% of fuel reprocessed is lost to high level waste. Three separation efficiencies for the removal of plutonium and neptunium are compared to analyze the effect on radio-toxicity. Back end radio-toxicity is calculated for separation efficiencies of 100%, 95%, and 70% in order to have an understanding of how separation efficiency impacts radio-toxicity. Figure 37 shows the inhaled radio-toxicity of each separation efficiency case. Figure 38 shows ingested radio-toxicity. There is only a small effect from changing the separation efficiency from 100% to 70%. A separation efficiency of 70% only results in an inhaled radio-toxicity increase of 12% and an ingested radio-toxicity increase of 9% compared to the 100% separation efficiency after 1,000 years. However, not separating neptunium and plutonium results in nearly a two fold increase in inhaled radio-toxicity compared to the case with 70% separation efficiency. Separating neptunium and plutonium each cycle reduces the time it takes for radio-toxicity of losses from residence cycle 50 to drop below the radio-toxicity of burnup equivalent natural uranium by approximately 100 years.

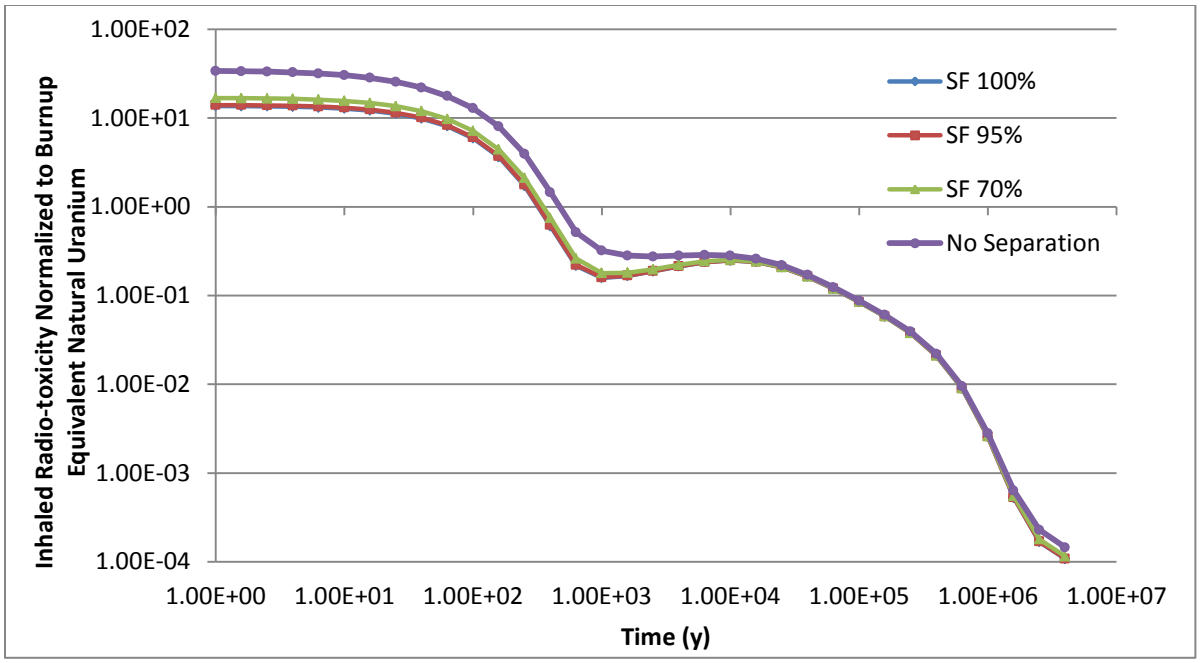

Figure 37. Inhaled radio-toxicity normalized to a burnup equivalent of natural uranium for different separation efficiencies of Np and Pu removal compared to scenario without separation after 50 residence times

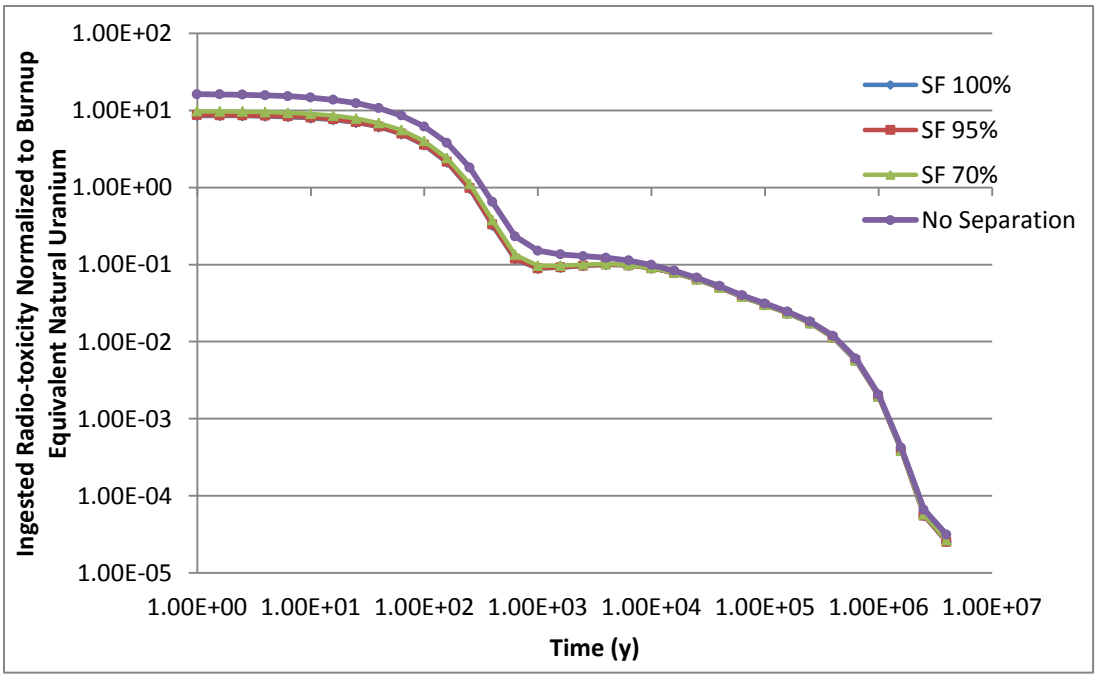

Figure 38. Ingested radio-toxicity normalized to a burnup equivalent of natural uranium for different separation efficiencies of Np and Pu removal compared to scenario without separation after 50 residence times

In this chapter multi-recycle thorium fuel radio-toxicity was evaluated for several transuranic partitioning scenarios and the impact of separation efficiency was analyzed. Typically reprocessing spent nuclear fuel is taken in context of increasing the utilization of the fuel. Reprocessing is also beneficial because it significantly reduces the load on the ultimate repository. By recycling thorium fuel the long term radio-toxicity load on the repository per residence cycle is reduced by two to three orders of magnitude except for the very last residence cycle if the makup fuel source is finite. Recycling the fuel reduces the time it takes for the waste to decay to the equivalent natural uranium ore level from several hundred thousand years to several hundred years. Separation of neptunium and plutonium after each residence cycle gives an additional benefit by halving the contribution to radio-toxicity load. Separating both neptunium and plutonium significantly reduces radio-toxicity compared to only separating neptunium since neptunium builds up quickly each cycle compared to ^{234}Pu. Depending on the difficulty required to separate neptunium and plutonium from other actinides, it could be worth the cost since it reduces the time it takes for the waste to decay to an acceptable level. The gain from a 95% separation efficiency vs. a 70% separation efficiency is small and may not be worth the cost. Most of the benefits are gained just by separating 70% of the neptunium and plutonium.

Long Term Radio-toxicity Impact of Thorium Multi-recycle Fuel Cycle Compared to a Once-through Fuel Cycle

In order to compare radio-toxicity of multi-recycle fuel cycles to once-through fuel cycles all of the HLW including the last full core of the multi-recycle fuel cycle must be considered. In the multi-recycle isotopics study the fuel is recycled 50 times in order to determine how long it takes for all isotopes to go to equilibrium. Therefore, the metric for this comparison is total actinide radio-toxicity of 50 residence cycles for the two fuel cycles being compared. The multi-recycle fuel cycle only sends one full core to the repository plus HLW from reprocessing loses due to 50 residence cycles. The corresponding once-through fuel cycle sends 50 full cores to the repository. The radio-toxicity due to reprocessing losses of the limiting case, residence cycle 50, is used to calculate the total long term radio-toxicity of the multi-recycle fuel cycle. This provides a conservative estimate of radio-toxicity. Figure 39 shows the total ingested radio-toxicity of 50 residence cycles for the different fuel cycles.

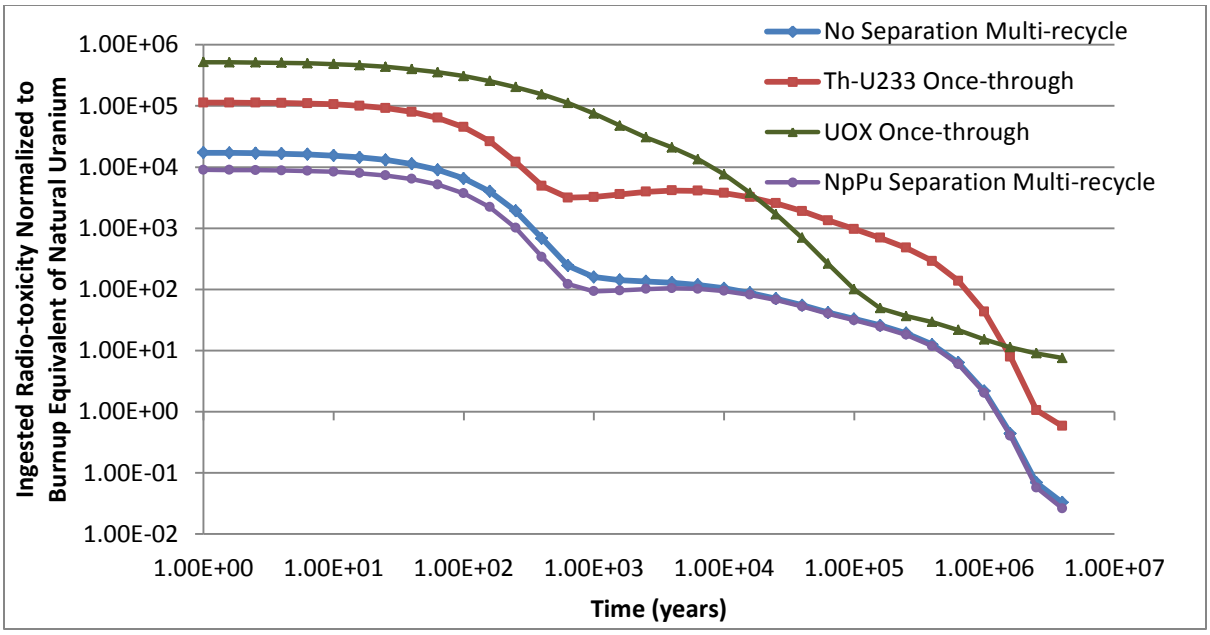

Figure 39. Total ingested radio-toxicity of no separation multi-recycle, Np and Pu separated multi-recycle, UOX once-through, and Th-^{233}UOX once through, normalized to burnup equivalent natural uranium

The results predict total ingested radio-toxicity of both multi-recycle scenarios to be roughly an order of magnitude lower than the once-through thorium fuel cycle. Most of the benefit of separating Np and Pu is in the first 1,000 years and is somewhat marginal compared to the overall benefit of recycling. Depending on the cost of separation it may or may not be worth the additional reduction in radio-toxicity by a factor of 2 for the first 1,000 years. A multi-recycle thorium fuel cycle provides a radio-toxicity reduction of nearly 2 orders of magnitude for the first 10,000 years compared to the current UOX once through fuel cycle. The multi-recycle thorium fuel cycle has lower ingested radio-toxicity than the UOX once through fuel cycle at any time of interest. Multi-recycle fuel cycles are better than once-through fuel cycles from a long term waste management perspective.

CONCLUSION

Summary

The first part of this thesis introduces background information about the nuclear fuel cycle and thorium fuel. The advantages of thorium fuel compared to uranium fuel are reviewed. Previous studies on thorium fuel cycles and recycling of thorium fuel are also discussed. While this research is similar in showing that multi-recycle of thorium fuel provides benefits by lowering the radio-toxicity impact to the ultimate repository, it also evaluates the benefits of selective partitioning of transuranics such as neptunium and plutonium.

The second chapter presents the developed methodology which is used to evaluate multi-recycle thorium fuel cycle scenarios and compare them with once-through fuel cycle scenarios. The methodology includes several automated scripts which control selective partitioning of transuranics, addition of top up fertile and fissile materials, and depletion parameters for the multi-recycle scenarios. The methodology also uses the Linear Reactivity Model to solve for the fissile isotope concentration to give the correct cycle length for once-through depletion and multi-recycle depletion.

In the third chapter once-through fuel isotopics are compared. Eight different fuel types are analyzed. Four of these fuels contain thorium and the other four contain natural uranium. The four mixed oxide fuel cases included thorium with ^{233}U and low enriched uranium, thorium with TRUOX and natural uranium with TRUOX, thorium with WGP and natural uranium with WGP, and thorium with RGP and natural uranium with RGP. The thorium fuels with TRUOX, RGP, and WGP started with more transuranics than natural uranium fuels to get the same cycle length but had a lower transuranic concentration at discharge. This shows that thorium fuels generate plutonium and minor actinides much more slowly than uranium fuels since it requires

many more neutron captures to build up. When comparing thorium mixed with ^{233}U versus low enriched uranium, the minor actinide concentration in the thorium fuel is predicted to be nearly five orders of magnitude less for all isotopes except for neptunium.

In the fourth chapter multi-recycle scenario isotopics are evaluated. The three partitioning scenarios of interest are: fission products separated but no transuranics separated, fission products and neptunium separated, and neptunium and plutonium separated in addition to fission products. Each of these three scenarios does not explicitly model losses during reprocessing although the radio-toxicity calculation comes from the assumption that there are .1% losses during reprocessing. Also, the impact of transuranic separation efficiency on minor actinide and plutonium buildup is evaluated. Separating only neptunium had a significant but small impact on reducing production of minor actinides. Separating neptunium reduces buildup of curium by a factor of two at most. By separating plutonium in addition to neptunium the buildup of americium and curium was reduced by more than an order of magnitude. Separation efficiency has a significant effect on reducing minor actinide production. By increasing the efficiency from 70% to 100% the predicted concentration of americium is decreased by roughly three times and curium is decreased roughly six times.

The fifth chapter presents radio-toxicity analysis for both once-through and multi-recycle fuel cycles. In the first part of the chapter radio-toxicity of thorium fuels are compared to uranium fuels in a once-through fuel cycle. In the second part of the chapter multi-recycle thorium fuel cycle scenarios are analyzed. The multi-recycle radio-toxicity includes results for the partitioning scenario study and the separation efficiency study. The last part of the fifth chapter compares multi-recycle fuel cycle radio-toxicity to once-through fuel cycle radio-toxicity.

Once-through cycle radio-toxicity results show that thorium fuel has one order of magnitude lower radio-toxicity than low enriched uranium fuel for the first 10,000 years until the decay daughters of ^{233}U dominate and thorium fuel becomes more radio-toxic until after roughly one million years where both fuels become less radio-toxic than natural uranium. In the other once-through scenarios plutonium and minor actinides dominate radio-toxicity to the point where thorium fuel and the uranium fuel counterpart are nearly identical for the first 10,0000-100,000 years until ^{233}U decay products dominate and the transuranics are mostly decayed away. It is important to note that thorium and ^{233}U fuel has two orders of magnitude lower radio-toxicity than reactor grade plutonium fuel mixed with either thorium or uranium. Since uranium fuel produces plutonium much quicker than thorium fuel it seems that multi-recycle thorium fuel cycles would be much less radio-toxic than a multi-recycle uranium fuel cycle.

The multi-recycle partitioning scenario study compared no partitioning to a neptunium partitioning case and to a neptunium and plutonium partitioned case. The results show significant reduction in discharged fuel radio-toxicity when separating both neptunium and plutonium. If only neptunium is separated then the decrease is only a few percent. Removal of both neptunium and plutonium reduces radio-toxicity by a factor of nearly two for the first 1,000 years and reduces the time to decay to natural uranium's radio-toxicity level from 354 years to 248 years, i.e., by about 100 years. Separating neptunium and plutonium has a much smaller effect on radio-toxicity after 10,000 years. All three separation scenarios are within 10% of each other after 10,000 years. The separation efficiency results predict that most of the benefits of separating neptunium and plutonium are gained at an efficiency of 70%. Increasing the separation efficiency from 70% to 100% only resulted in a predicted ingested radio-toxicity decrease of 9%.

The comparison of once-through radio-toxicity with multi-recycle radio-toxicity shows that recycling fuel is beneficial for long term waste management. After recycling fuel for 50 residence cycles the ingested radio-toxicity is reduced by roughly an order of magnitude compared to the once-through thorium fuel cycle. Also, 50 residence cycles of the multi-recycle thorium fuel cycle would produce two orders of magnitude less ingested radio-toxicity for the first 10,000 years than would 50 residence cycles of today's once-through uranium fuel cycles. Even after 10,000 years, HLW generated from a multi-recycle thorium fuel cycle would be significantly lower than HLW coming from the current once-through UOX fuel cycle.

Recommended Future Work

Additional studies could further enhance understanding of the benefits of a LWR thorium fuel cycle on back end radio-toxicity and potential issues. One such study could be the comparison of multi-recycle uranium fuel cycles which use a supply of ^{239}Pu in comparison with the multi-recycle thorium fuel cycle in this research. Also, further research could be done to better understand how to evaluate if highly radio-toxic fuel in the short term is more or less favorable than low radio-toxicity in the very long term. Another study would be to use more realistic isotopic vectors for the top up to see the effect additional thorium and uranium isotopes would have on long term radio-toxicity and generation of transuranics. These additional studies could help to further understand the effects of long term radio-toxicity generated from thorium vs. uranium fuel.

To further understand radio-toxicity of multi-recycle thorium fuel cycles uranium based multi-recycle fuel cycles should be evaluated. This would allow for better comparison and provide relative values for analysis of short term vs. long term radio-toxicity. Such a study

might provide additional insights into the advantages of further utilizing thorium fuel vs. uranium fuel in a multi-recycle scenario.

Further research to establish a metric to compare short term radio-toxicity vs. long term radio-toxicity is necessary for evaluating fuel cycle scenarios. In chapter 5 of this thesis an analysis of once-through radio-toxicity predicted that uranium fuel has a much higher radio-toxicity than thorium fuel for the first 15,000 years. Then ^{233}U decay products dominate radio-toxicity until after 1 million years making thorium fuel more radio-toxic than uranium fuel for a far longer time period even though the magnitude of radio-toxicity is much smaller for both fuels. Doing further research in public policy and environmental radiochemistry could help evaluate which among these scenarios is preferable.

More realistic top up vectors would improve the analysis of long term radio-toxicity of thorium fuels. Additional ^{234}U and ^{236}U could contribute to a faster buildup of minor actinides which would significantly increase radio-toxicity for more than 1,000 years. More accurate top up vectors could be generated from a depletion calculation for a thorium breeder reactor. Depending on whether the breeder is a thermal or fast reactor the heavier uranium isotope concentrations may or may not be negligible.

These additional studies could be carried out in order to better evaluate back end radio-toxicity of thorium fuel. Further research could provide additional understanding of how long term radio-toxicity would affect the environment. Future studies are important since they provide insight into a solution which could improve nuclear fuel utilization, back end radio-toxicity, and economics.

APPENDIX A

Bash Control Script

```
#!/bin/sh
a=1
z=50
if [ $a=1 ]
  then
     mkdir outputdata
     mkdir CycleAtmp
     mkdir CycleBtmp
     mkdir Cycletmp
     cp ./new65xnlib ./CycleAtmp
     cp ./new65xnlib ./CycleBtmp
     cp ./new65xnlib ./Cycletmp
     # Change Method of creating txt files for tables!!!!!
     echo "Cycle$a" > cycle.txt
     echo "Cycle$a" > kscript.txt
     grep "k-eff =" Cycle$a.output >> kscript.txt
     echo  "FPD     0.00  13.50  40.50  67.50  101.25  141.75  243.00  405.00  661.25  903.75
1025.50  1201.50  1444.50" > Kinftable.txt
     mv Kinftable.txt outputdata
     echo  "Uranium Mass Flow" > UMassFlow.txt
     mv UMassFlow.txt outputdata
     echo  "Uranium Out Vectors"   > UOutVectors.txt
     mv UOutVectors.txt outputdata
     echo  "Uranium In Vectors"   > UInVectors.txt
     mv UInVectors.txt outputdata
     echo  "U233 Makeup Equilibrim" >  UMakeupTable.txt
     mv UMakeupTable.txt outputdata
     echo  "Plutonium Vectors" > PuVector.txt
     mv PuVector.txt outputdata
     echo  "Plutonium Mass Flow" > PuMassFlow.txt
     mv PuMassFlow.txt outputdata
     echo  "MAMassFlow" > MAMassFlow.txt
     mv MAMassFlow.txt outputdata
     echo  "Pa Mass Flow" > PaMassFlow.txt
     mv PaMassFlow.txt outputdata
     echo  "Thorium makeup" > ThMakeupTable.txt
     mv ThMakeupTable.txt outputdata
     echo "0" > FissileConverge.txt
     echo "CycleA Solver" > FissileA.txt
     echo "CycleB Solver" > FissileB.txt
```

```
  else
     echo "" > /dev/null
fi
while [ $a != $z ]
do
   PrevFissileU=$(awk -v a="$a" 'NR==a' < FissileConverge.txt)
   u33=$(grep "u-233" Cycle$a.inp | awk 'NR==1 {print $4}')
   u35=$(grep "u-235" Cycle$a.inp | awk 'NR==1 {print $4}')
   oxy=$(grep "o  " Cycle$a.inp | awk 'NR==2 {print $4}')
   if [ $a = 1 ]
     then
        FissileU=$(echo "scale=7; ($u33)/(1.0-$oxy)" | bc)
     else
        FissileU=$(echo "scale=7; ($u33+$u35)/(1.0-$oxy)" | bc)
   fi
   echo $FissileU >> FissileConverge.txt
   DeltaFissU=$(echo "scale=7; $FissileU-$PrevFissileU" | bc)
   criteria=".0000003"
   #Unconverged=$(echo "$DeltaFissU > $criteria" | bc)
   Unconverged=1
   if [ $Unconverged = 1 ]
    then
       a=$(($a+1))
       FissileA=$(echo "scale=7; $FissileU+.0001" | bc)
       FissileB=$(echo "scale=7; $FissileU+.0003" | bc)
       echo $FissileA >> FissileA.txt
       echo $FissileB >> FissileB.txt
       ./CycleSolveA.py
       ./CycleSolveB.py
       export TMPDIR=./CycleAtmp
       scale6 Cycle${a}A.inp &
       export TMPDIR=./CycleBtmp
       scale6 Cycle${a}B.inp &
       wait
       KeffA=$(grep "Time=    972.00d" Cycle${a}A.output | awk '{print $3}')
       KeffB=$(grep "Time=    972.00d" Cycle${a}B.output | awk '{print $3}')
       m=$(echo "scale=7; ($KeffB-$KeffA)/($FissileB-$FissileA)" | bc)
       b=$(echo "scale=7; $KeffA-($FissileA*$m)" | bc)
       NewFissile=$(echo "scale=7; (1.03-$b)/$m" | bc)
       echo $NewFissile > NewFissile.txt
    else
       a=$(($a+1))
   fi
   echo "Cycle$a" >> kscript.txt
   ./openoutput.py
   echo "Cycle$a" >> cycle.txt
```

```
  export TMPDIR=./Cycletmp
  scale6 Cycle$a.inp &
  wait
  grep 'k-eff =' Cycle$a.output >> kscript.txt
done
./openoutput.py
./opusmulticycle.py
```

Python Reprocessing Script

```
#!/usr/bin/env python

#########################################################################
###############  I.  Opening and Reading Output   ###################
#########################################################################

import os, sys
CurrentDir=os.getcwd()

#  Opens a text file which has the 'Cycle#' txt for this cycle and previous cycles.
filecycle=open('cycle.txt','r')
CycleList=filecycle.readlines()
filecycle.close()

#  Gets rid of the next line character /n in CycleList.
for i in range(0,len(CycleList)):
  CycleList[i]=CycleList[i][0:-1]

#  Takes the last cycle in cyclelist for opening appropriate output.
CycleNumber= CycleList[len(CycleList)-1]

#Open Output File.
file= open(CycleNumber+'.output','r')
SCALEOUTPUT=file.read()


#Use string to cut up output file and assign to a new string.
a=SCALEOUTPUT.find('opus case')
b=SCALEOUTPUT.find('1                    sum of all depletion materials, opus case 1')
OpusDataRaw=SCALEOUTPUT[a:b]

#Save to new file opusdata.  Contains the raw opus data with junk in between.
file2=open('OpusdataRaw.txt','w')
file2.write(OpusDataRaw)
file.close()
```

```
file2.close()
file2=open('OpusdataRaw.txt','r')
OpusDataRaw=file2.read()
file2.close()

# Cuts out garbage from raw data to make clean data.
a=OpusDataRaw.find('th232')
b=OpusDataRaw.find('subtotal')
c=OpusDataRaw.find('th232',b)
d=OpusDataRaw.find('subtotal',c)
OpusData=OpusDataRaw[a:b] + OpusDataRaw[c:d]
file3=open('opusdataclean.txt','w')
file3.write(OpusData)
file3.close()
file3=open('opusdataclean.txt','r')
OpusList=file3.readlines()
file3.close()


################################################################################
########
##########  II.  String Manipulation and Data Organization Pre-calculation  ##########
################################################################################
########


# Splits list into smaller lists.
sectionstart=[]
for ind in range(0,len(OpusList)):
    OpusList[ind]=OpusList[ind].split()

# Finds where first isotope appears multiple times in list.
for num in range(0,len(OpusList)-1):
    if OpusList[num][0]==OpusList[0][0]:
        sectionstart.append(num)
a=sectionstart[1]

# Makes each isotope only one list with concentration as a function of time.
for line in range(0,a):
    for elem in range(1,len(OpusList[line+a])):
        OpusList[line].append(OpusList[line+a][elem])
UnsortedIsotopics=OpusList[0:85]

# Finds list index of a desired isotope.  Just type in 'Isotope' to find it.
def IsotopeFinder(IsotopeString,IsotopeList):
   for i in range(0,len(IsotopeList)):
```

```
    if IsotopeList[i][0]==IsotopeString:
        return i

# A list of isotopes in a desireable order.
IsotopeSortOrder=['ra226','th228','th229','th230','th231','th232','th233','th234','pa231','pa233','u23
2','u233','u234','u235','u236','u237','u238',

'pu236','pu237','pu238','pu239','pu240','pu241','pu242','pu243','pu244','np236','np237','np238','np
239','am241','am242','am242m',

'am243','am244','am244m','cm241','cm242','cm243','cm244','cm245','cm246','cm247','cm248','bk
249','cf249','cf250','cf251','cf252']

# Creates a sorted list of isotopes.
SortedIsotopics=[]
for n in range(0,len(IsotopeSortOrder)):

SortedIsotopics.append(UnsortedIsotopics[IsotopeFinder(IsotopeSortOrder[n],UnsortedIsotopics
)])



# Material going to high level waste after reprocessing.
WasteBin=[]
for iso in range(len(SortedIsotopics)):
  WasteBin.append([SortedIsotopics[iso][0],'%.7E' % (.001*float(SortedIsotopics[iso][-1]))])
  SortedIsotopics[iso][-1]='%.7E' % (.999*float(SortedIsotopics[iso][-1]))



# Separates Np and Pu with 99% efficiency.  .01% stays in rest of fuel.
NpPuStorage=[]
for iso in range(len(SortedIsotopics)):
  if 'np' in SortedIsotopics[iso][0]:
    NpPuStorage.append([SortedIsotopics[iso][0],'%.7E' % (.99*float(SortedIsotopics[iso][-
1]))])
    SortedIsotopics[iso][-1]='%.7E' % (.01*float(SortedIsotopics[iso][-1]))
  if 'pu' in SortedIsotopics[iso][0]:
    NpPuStorage.append([SortedIsotopics[iso][0],'%.7E' % (.99*float(SortedIsotopics[iso][-
1]))])
    SortedIsotopics[iso][-1]='%.7E' % (.01*float(SortedIsotopics[iso][-1]))
```

```
NpPuString=''
if CycleNumber=='Cycle1':
  file=open(CurrentDir+'/NpPuStorage.txt','w')
  file.write('Neptunium and Plutonium Waste Stream')
  file.close()
  NpPuString='Isotope'+' '
  for col in NpPuStorage:
    NpPuString=NpPuString+ col[0]+'   '

NpPuString=NpPuString+'\n'+CycleNumber+' '

for col in NpPuStorage:
  NpPuString=NpPuString+ col[1]+' '

file=open(CurrentDir+'/NpPuStorage.txt','a')
file.write(NpPuString)
file.close()


WasteString=''
if CycleNumber=='Cycle1':
  file=open(CurrentDir+'/HLWaste.txt','w')
  file.write('Neptunium and Plutonium Waste Stream')
  file.close()
  WasteString='Isotope'+' '
  for col in WasteBin:
    WasteString=WasteString+ col[0]+'   '

WasteString=WasteString+'\n'+CycleNumber+' '

for col in WasteBin:
  WasteString=WasteString+col[1]+' '

file=open(CurrentDir+'/HLWaste.txt','a')
file.write(WasteString)
file.close()

# Changes all numerical strings to floats for calculation.
for lin in range(0,len(SortedIsotopics)):
   for l in range(1, len(SortedIsotopics[lin])):
      SortedIsotopics[lin][l]=float(SortedIsotopics[lin][l])



# Atomic mass list for each isotope in order.
```

```
AtomicMasses=[226.0254, 228.0287, 229.0318, 230.0331, 231.0363, 232.0381, 233.0416,
234.0436, 231.0359, 233.0402, 232.0371, 233.0396, 234.0409, 235.0439, 236.0456, 237.0487,
238.0508,
          236.0461, 237.0484, 238.0496, 239.0522, 240.0538, 241.0568, 242.0587, 243.062,
244.0642, 236.0466, 237.0482, 238.0509, 239.0529, 241.0568, 241.0568, 241.0568, 243.0614,
          244.0643, 244.0643, 241.0576, 242.0588, 243.0614, 244.0627, 245.0655, 246.0672,
247.0703, 248.0723, 249.075, 249.0748, 250.0764, 251.0796, 252.0816]

# Fuel volume in quarter fuel assembly.
FuelVolume=104863.2409

# Creates list for makeup flow
MakeupFlow=[]
for l in range(0,len(SortedIsotopics)):
   MakeupFlow.append(0)


#########################################################
#---------- U233+U235 concnentration --------------#
#########################################################
                                ######
file=open('NewFissile.txt','r')
NewFissile=file.read()
FissileU=float(NewFissile)
                                ######
#########################################################
#-----------------------------------------------#
#########################################################


# Calculates total inflow mass
TotalInflow=0
for isot in range(0,len(SortedIsotopics)):
   TotalInflow=TotalInflow+SortedIsotopics[isot][len(SortedIsotopics[isot])-1]

InitialVolumeGuess=TotalInflow/9.5519
ThoriumTD=10
PackingFraction=.95

ElementSpef=['ra',    'th',    'th',    'th',    'th',    'th',    'th',    'th',    'pa',    'pa',    'u',    'u',    'u',
          'pu',    'pu',    'pu',    'pu',    'pu',    'pu',    'pu',    'np',    'np',    'np',    'np',    'am',    'am',    'am',
          'cm',    'cm',    'cm',    'cm',    'cm',    'cm',    'bk',    'cf',    'cf',    'cf',    'cf']

DensityOfOxide=[['u',10.96],  ['np',11.11],    ['pu',11.46],    ['am',11.68],    ['th',10],
          ['cm',11.7],    ['pa',10.47],    ['ra',7.5], ['cf',0], ['bk',0]]
for r in range(0,len(DensityOfOxide)):
```

```
    for m in range(0,len(ElementSpef)):
                if DensityOfOxide[r][0]==ElementSpef[m]:
                    ElementSpef[m]=[ElementSpef[m], DensityOfOxide[r][1]]

################################################################################
#############
################## III.  Reprocessing Parameter Definitions Pre-Loop
####################
################################################################################
#############

# Thorium Makeup
ThoriumMakeup=(FuelVolume-InitialVolumeGuess)*ThoriumTD*PackingFraction-
SortedIsotopics[IsotopeFinder('u233',SortedIsotopics)][len(SortedIsotopics[0])-1]

# U233 Makup
U233Makeup=(FissileU*(ThoriumMakeup+TotalInflow)-
SortedIsotopics[IsotopeFinder('u233',SortedIsotopics)][len(SortedIsotopics[0])-1] -
SortedIsotopics[IsotopeFinder('u235',SortedIsotopics)][len(SortedIsotopics[0])-1])/(1-FissileU)

# Adding Makeup Isotopes to Makup List
MakeupFlow[IsotopeFinder('u233',SortedIsotopics)]=MakeupFlow[IsotopeFinder('u233',SortedI
sotopics)]+U233Makeup
MakeupFlow[IsotopeFinder('th232',SortedIsotopics)]=MakeupFlow[IsotopeFinder('th232',Sorted
Isotopics)]+ThoriumMakeup

#Calculates mass after makeup is added.
OutFlowMass=[]
for i in range(0,len(SortedIsotopics)):
    OutFlowMass.append(SortedIsotopics[i][len(SortedIsotopics[i])-1] + MakeupFlow[i])

# Total out flow mass.
TotalOutflow=0
for isot in range(0,len(OutFlowMass)):
    TotalOutflow=TotalOutflow+OutFlowMass[isot]

# Renormalized compositions.
NormalizedComp=[]
for l in range(0,len(OutFlowMass)):
    NormalizedComp.append(OutFlowMass[l]/TotalOutflow)

# Normalized composition times atomic mass.
PartialMass=[]
for i in range(0,len(NormalizedComp)):
    PartialMass.append(NormalizedComp[i]*AtomicMasses[i])
```

```
# Average atomic mass of heavy metal.
Total_HM_Mass=0
for j in range(0,len(PartialMass)):
   Total_HM_Mass=Total_HM_Mass+PartialMass[j]

# Weight percent divided by atomic mass.
WtPctOverA=[]
for k in range(0,len(NormalizedComp)):
   WtPctOverA.append(NormalizedComp[k]/AtomicMasses[k])

# Total of weight percent divided by atomic mass.
TotalWtOverA=0
for n in range(0,len(WtPctOverA)):
   TotalWtOverA=TotalWtOverA+WtPctOverA[n]

# Atomic fraction.
AtomFraction=[]
for i in range(0,len(WtPctOverA)):
   AtomFraction.append(WtPctOverA[i]/TotalWtOverA)

PartialTD=[]
for j in range(0,len(AtomFraction)):
   PartialTD.append(AtomFraction[j]*ElementSpef[j][1])

TheoreticalDensity=0
for k in range(0,len(PartialTD)):
   TheoreticalDensity=TheoreticalDensity+PartialTD[k]

Density=TheoreticalDensity*PackingFraction

ActualVolume=TotalOutflow/Density

DeltaV=abs(FuelVolume-ActualVolume)

##########################################################################
########
##########                                              ###############
##########  IV.  Giant loop to iteratively solve for correct volume.    ##################
##########                                              ######################
##########################################################################
####################

while abs(DeltaV) > .1:
   a=a-1
   if ActualVolume < FuelVolume:
      ThoriumMakeup=ThoriumMakeup + 1
```

```
    else:
        ThoriumMakeup=ThoriumMakeup - 1
    # U233 Makup
    U233Makeup=(FissileU*(ThoriumMakeup+TotalInflow)-
SortedIsotopics[IsotopeFinder('u233',SortedIsotopics)][len(SortedIsotopics[0])-1] -
SortedIsotopics[IsotopeFinder('u235',SortedIsotopics)][len(SortedIsotopics[0])-1])/(1-FissileU)

    # Adding Makeup Isotopes to Makup List
    MakeupFlow[IsotopeFinder('u233',SortedIsotopics)]=U233Makeup
    MakeupFlow[IsotopeFinder('th232',SortedIsotopics)]=ThoriumMakeup

    #Calculates mass after makeup is added.
    OutFlowMass=[]
    for i in range(0,len(SortedIsotopics)):
        OutFlowMass.append(SortedIsotopics[i][len(SortedIsotopics[i])-1] + MakeupFlow[i])

    # Total out flow mass.
    TotalOutflow=0
    for isot in range(0,len(OutFlowMass)):
        TotalOutflow=TotalOutflow+OutFlowMass[isot]

    # Renormalized compositions.
    NormalizedComp=[]
    for l in range(0,len(OutFlowMass)):
        NormalizedComp.append(OutFlowMass[l]/TotalOutflow)

    # Normalized composition times atomic mass.
    PartialMass=[]
    for i in range(0,len(NormalizedComp)):
        PartialMass.append(NormalizedComp[i]*AtomicMasses[i])

    # Average atomic mass of heavy metal.
    Total_HM_Mass=0
    for j in range(0,len(PartialMass)):
        Total_HM_Mass=Total_HM_Mass+PartialMass[j]

    # Weight percent divided by atomic mass.
    WtPctOverA=[]
    for k in range(0,len(NormalizedComp)):
        WtPctOverA.append(NormalizedComp[k]/AtomicMasses[k])

    # Total of weight percent divided by atomic mass.
    TotalWtOverA=0
    for n in range(0,len(WtPctOverA)):
        TotalWtOverA=TotalWtOverA+WtPctOverA[n]
```

```
    # Atomic fraction.
    AtomFraction=[]
    for i in range(0,len(WtPctOverA)):
        AtomFraction.append(WtPctOverA[i]/TotalWtOverA)

    # Atomic fraction multiplied by oxide densities.
    PartialTD=[]
    for j in range(0,len(AtomFraction)):
        PartialTD.append(AtomFraction[j]*ElementSpef[j][1])

    #  Summing up to get Theoretical Density
    TheoreticalDensity=0
    for k in range(0,len(PartialTD)):
        TheoreticalDensity=TheoreticalDensity+PartialTD[k]

    Density=TheoreticalDensity*PackingFraction

    ActualVolume=TotalOutflow/Density

    DeltaV=FuelVolume-ActualVolume

#####################################   End of Giant Loop
###################################

#####################----------------------------------------------
########################

#  Reads Cycle# and increases the cycle # by 1.
DigitIndex=[]
DigitNet=[]
for i in range(0,len(CycleNumber)):
  if CycleNumber[i].isdigit():
     DigitIndex.append(i)
     DigitNet.append(CycleNumber[i])
Digit=''
for k in range(0,len(DigitNet)):
  Digit=Digit+DigitNet[k]
FinalDigitValue=float(Digit)+1
FinalDigit=str(FinalDigitValue)
CycleStr=CycleNumber[0:DigitIndex[0]]

# puts 'Cycle' and cycle number for next cycle together.
OutCycle=CycleStr+FinalDigit[0:-2]

#############################################################################
################
```

```
######################  V.  Creation of Tables for Data Analysis
##########################
#############################################################################
################

#  Call from SortedIsotopics, TotalInflow, U233Makeup, ThoriumMakeup, TotalOutflow,
Density, Specific Power
#  Open kscript to make a clean table of K-eff vs FPD/Burnup.

#  Creates a list with FPD for each K-inf step...
FullPowerDayList=[0.00,13.50,40.50,67.50,101.25,141.75,243.00,405.00,661.25,903.75,1025.5
0,1201.50,1444.50]
FullPowerDayStr=[]
for m in range(0,len(FullPowerDayList)):
  FullPowerDayStr.append(str(FullPowerDayList[m]))

#################### A.  K-inf Data
###########################################################
#  Opens the K-inf data text file.  Also makes it into a list.
file=open(CurrentDir+'/kscript.txt','r')
kscriptraw=file.read()
file.close()
a=kscriptraw.find(CycleNumber)
KList= kscriptraw[a:]
KList=KList.splitlines()
KList=KList[1:]
for i in range(0,len(KList)):
  KList[i]=KList[i].split()

#  Seperates the numbers in KinfList from the junk and turns it into floats.
KinfList=[]
for j in range(0,len(KList)):
  for m in range(0,len(KList[j])):
    try:
      KinfList.append(float(KList[j][m]))
    except ValueError:
       pass

#  Adds a label each cycle saying what cycle the data corresponds to.
KinfTable="
KinfTable=KinfTable+CycleNumber

#  Adds k values to string.
for k in range(0,len(KinfList)):
  KinfTable=KinfTable+'  '+str(KinfList[k])
KinfTable=KinfTable+'\n'
```

```
#  Writes to the table text file.
Kfile=open(CurrentDir+'/outputdata/Kinftable.txt','a')
Kfile.write(KinfTable)
Kfile.close()

##########################################################################################
##################

#  Makes a list with the isotope concentrations after the 5 year cooldown.
IsotopesAfterCD=[]
for i in range(0,len(SortedIsotopics)):
  IsotopesAfterCD.append(SortedIsotopics[i][len(SortedIsotopics[i])-1])

################## B.  Uranium Mass Flow
##########################################################
#  Makes a list with uranium isotopes.


UraniumList=[]
PlutoniumList=[]
PaList=[]
MAList=[]
for i in range(0,len(IsotopesAfterCD)):
  I=IsotopeSortOrder[i]
  if 'u'==I[0]:
    UraniumList.append([IsotopeSortOrder[i],IsotopesAfterCD[i]])
  elif 'pu' == I[:2]:
    PlutoniumList.append([IsotopeSortOrder[i],IsotopesAfterCD[i]])
  elif 'pa'== I[:2]:
    PaList.append([IsotopeSortOrder[i],IsotopesAfterCD[i]])
  elif 'th'== I[:2] or 'ra'==I[:2]:
    pass
  else:
    MAList.append([IsotopeSortOrder[i],IsotopesAfterCD[i]])


#  A string that contains the isotope names.
UraniumStr=''
for k in range(0,len(UraniumList)):
  UraniumStr=UraniumStr+UraniumList[k][0]+'  '

#  If the UMassFlow text file doesnt have isotope string names yet, then it adds it.
file=open(CurrentDir+'/outputdata/UMassFlow.txt','r')
UMassFlow=file.readlines()
file.close()
```

```
file=open(CurrentDir+'/outputdata/UMassFlow.txt','a')
try:
   UMassFlow[1]==UraniumStr
except IndexError:
   file.write('Isotope'+'  '+UraniumStr)
else:
    pass

#  Makes a string with uranium isotope concentrations.
UraniumMassStr=''
for j in range(0,len(UraniumList)):
  UraniumMassStr=UraniumMassStr+str(UraniumList[j][1])+'  '

#  Saves the data to the UMassflow txt file.
file.write('\n'+CycleNumber+'  '+UraniumMassStr)
file.close()

#################### C.  Uranium Out Vectors
############################################################

#  Creates a list containing a normalized uranium vector.
UraniumSum=0
for l in range(0,len(UraniumList)):
  UraniumSum=UraniumSum+UraniumList[l][1]
UraniumOutVector=[]
for s in range(0,len(UraniumList)):
  UraniumOutVector.append(UraniumList[s][1]/UraniumSum)

file=open(CurrentDir+'/outputdata/UOutVectors.txt','r')
UOutVectors=file.readlines()
file.close()
file=open(CurrentDir+'/outputdata/UOutVectors.txt','a')
try:
   UOutVectors[1]==UraniumStr
except IndexError:
   file.write('Isotope'+'  '+UraniumStr)
else:
    pass

UraniumOutVectorStr=''
for k in range(0,len(UraniumOutVector)):
  UraniumOutVectorStr=UraniumOutVectorStr+str(UraniumOutVector[k])+'  '

file.write('\n'+CycleNumber+'  '+UraniumOutVectorStr)
file.close()
```

```
################### D.  Uranium In Vectors
#########################################################


UraniumInList=[]
for i in range(0,len(OutFlowMass)):
  if IsotopeSortOrder[i][0]=='u':
     UraniumInList.append([IsotopeSortOrder[i],OutFlowMass[i]])

#  Creates a list containing a normalized uranium vector.
UraniumSum=0
for l in range(0,len(UraniumInList)):
  UraniumSum=UraniumSum+UraniumInList[l][1]
UraniumInVector=[]
for s in range(0,len(UraniumInList)):
  UraniumInVector.append(UraniumInList[s][1]/UraniumSum)

file=open(CurrentDir+'/outputdata/UInVectors.txt','r')
UInVectors=file.readlines()
file.close()
file=open(CurrentDir+'/outputdata/UInVectors.txt','a')
try:
   UInVectors[1]==UraniumStr
except IndexError:
   file.write('Isotope'+'  '+UraniumStr)
else:
    pass

UraniumInVectorStr=''
for k in range(0,len(UraniumInVector)):
  UraniumInVectorStr=UraniumInVectorStr+str(UraniumInVector[k])+'  '

file.write('\n'+CycleNumber+'  '+UraniumInVectorStr)
file.close()

##################  E.  Plutonium Mass Flow
#########################################################

PuStr=''
for i in range(0,len(PlutoniumList)):
  PuStr=PuStr+PlutoniumList[i][0]+'  '

file=open(CurrentDir+'/outputdata/PuMassFlow.txt','r')
PuMassFlow=file.readlines()
file.close()
file=open(CurrentDir+'/outputdata/PuMassFlow.txt','a')
```

```
try:
   PuMassFlow[1]==PuStr
except IndexError:
   file.write('Isotope'+'  '+PuStr)
else:
   pass

PuMassStr=''
for j in range(0,len(PlutoniumList)):
  PuMassStr=PuMassStr+str(PlutoniumList[j][1])+'  '

file.write('\n'+CycleNumber+'  '+PuMassStr)
file.close()

##################  F.  Plutonium Out Vectors
#####################################################

#PuTotal=0
#for l in range(0,len(PlutoniumList)):
#   PuTotal=PuTotal+PlutoniumList[l][1]
#
#PuVectorList=[]
#for k in range(0,len(PlutoniumList)):
#   PuVectorList.append(PlutoniumList[k][1]/PuTotal)
#
#file=open(CurrentDir+'/outputdata/PuVector.txt','r')
#PuVector=file.readlines()
#file.close()
#file=open(CurrentDir+'/outputdata/PuVector.txt','a')
#try:
#    PuVector[1]==PuStr
#except IndexError:
#    file.write('Isotope'+'  '+PuStr)
#else:
#    pass
#
#PuVectorStr=''
#for j in range(0,len(PuVectorList)):
#   PuVectorStr=PuVectorStr+str(PuVectorList[j])+'  '
#
#file.write('\n'+CycleNumber+'  '+PuVectorStr)
#file.close()
##################  G.  Protactinium Mass Flow
#####################################################

PaStr=''
```

```
for i in range(0,len(PaList)):
  PaStr=PaStr+PaList[i][0]+' '

file=open(CurrentDir+'/outputdata/PaMassFlow.txt','r')
PaMassFlow=file.readlines()
file.close()
file=open(CurrentDir+'/outputdata/PaMassFlow.txt','a')
try:
   PaMassFlow[1]==PaStr
except IndexError:
   file.write('Isotope'+' '+PaStr)
else:
   pass

PaMassStr=''
for k in range(0,len(PaList)):
  PaMassStr=PaMassStr+str(PaList[k][1])+' '

file.write('\n'+CycleNumber+' '+PaMassStr)
file.close()
################  H.  Minor Actinide Mass Flow
################################################

MAStr=''
for j in range(0,len(MAList)):
  MAStr=MAStr+MAList[j][0]+' '

file=open(CurrentDir+'/outputdata/MAMassFlow.txt','r')
MAMassFlow=file.readlines()
file.close()
file=open(CurrentDir+'/outputdata/MAMassFlow.txt','a')
try:
   MAMassFlow[1]==MAStr
except IndexError:
   file.write('Isotope'+' '+MAStr)
else:
   pass

MAMassStr=''
for l in range(0,len(MAList)):
  MAMassStr=MAMassStr+str(MAList[l][1])+' '

file.write('\n'+CycleNumber+' '+MAMassStr)
file.close()
```

```
################  I.  Makeup Data
#############################################################

file=open(CurrentDir+'/outputdata/UMakeupTable.txt','a')
file.write('\n'+CycleNumber+'  '+str(U233Makeup))
file.close()

file=open(CurrentDir+'/outputdata/ThMakeupTable.txt','a')
file.write('\n'+CycleNumber+'  '+str(ThoriumMakeup))
file.close()




#############################################################################
#################
######################  VI.  Formatting Isotopics for input insertion
#######################
#############################################################################
#################

#  Calculating specific power.
FullCoreVolume=9323718.206  #cc
FullCoreMass=FullCoreVolume*Density
ReactorThPower=3400 #MWth
SpecificPower=ReactorThPower*1e6/FullCoreMass

#  Fraction of oxygen in fuel.
OxygenFraction=32/(32+Total_HM_Mass)
NextCycleComp=[OxygenFraction]
for n in range(0,len(NormalizedComp)):
   NextCycleComp.append(NormalizedComp[n]*(1-OxygenFraction))

# Creates a list for future input string manipulation that includes oxygen.
InputIsotopeList=['o']
for i in range(0,len(IsotopeSortOrder)):
   InputIsotopeList.append(IsotopeSortOrder[i])

# Makes sure the input mass fractions add up to 1.  If this part is wrong, code is really messed up.
TotalInput=0
for j in range(0,len(NextCycleComp)):
   TotalInput=TotalInput+NextCycleComp[j]
if abs(1-TotalInput)>.0001:
   print 'Input Compositions are not Properly Normalized!'

#  Adds the mass fractions to the input composition list
```

```
for k in range(0,len(InputIsotopeList)):
   InputIsotopeList[k]=[InputIsotopeList[k],NextCycleComp[k]]

#  Selects isotopes for removal that won't be usable in SCALE
remover=[]
remover.append(IsotopeFinder('th231',InputIsotopeList))
for l in range(0,len(InputIsotopeList)):
   if InputIsotopeList[l][1] ==0:
     remover.append(l)

#  Removes selected isotopes from list
for n in range(0,len(remover)):
   InputIsotopeList.pop(remover[n]-n)

#  Converts floats back into strings for input production.
for i in range(0,len(InputIsotopeList)):
   InputIsotopeList[i][1]=str(InputIsotopeList[i][1])

#  Adds hyphen in the isotope strings to make compatable with SCALE th232 ----> th-232
for k in range(1,len(InputIsotopeList)):
   if InputIsotopeList[k][0][0]=='u':
      InputIsotopeList[k][0]=InputIsotopeList[k][0][:1]+'-'+InputIsotopeList[k][0][1:]
   else:
      InputIsotopeList[k][0]=InputIsotopeList[k][0][:2]+'-'+InputIsotopeList[k][0][2:]


##########################################################################################
####################
######################### VII.  String manipulation to create input files
########################
##########################################################################################
####################

#  Top part of input file
TopInputSlice= '=t-depl parm=(centrm,addnux=3) \nthoriumtest \nnew65xnlib \nread alias \n
$fuel 1 end \n  $clad 2 end \n  $mod 3 end \n  $gap 4 end \nend alias \nread composition \n
helium' \
'     $gap 1 700   end \n h2o         $mod den=0.7 1 557   end \n zirc4       $clad 1 620   end \n'

#  Part of input file after compositions.
MiddleInputSlice='read celldata \n' \
'  latticecell squarepitch fuelr=0.4095 $fuel gapr=0.418 $gap cladr=0.475 $clad hpitch=0.6299
$mod end \n' \
'end celldata \n' \
'read depletion \n' \
'  $fuel \n' \
```

```
'end depletion \n'

#  read in previous input file for splicing.
file= open(CycleNumber+'.inp','r')
SCALEINPUT=file.read()

#  Splices input file and makes bottom part of input.
a=SCALEINPUT.find('read opus')
BottomInputSlice=SCALEINPUT[a:]
file.close()

fuel= '   $fuel'
den='   den='
temp='   900'
end='   end'
EndOFBlock='end'

#  Creating a compositions block from InputIsotopeList.
CompositionsBlock=[]
for j in range(0,len(InputIsotopeList)):
   CompositionsBlock.append(InputIsotopeList[j][0]+fuel+den+str(Density)+'   ' +
InputIsotopeList[j][1]+temp+end + '\n')
CompositionsBlock.append('end composition \n')
CompSlice="".join(CompositionsBlock)

#  Creates a burndata block from strings and the specific power data.
BurnSlice='read burndata \n'\
'power='+'   ' + str(SpecificPower)+'   burn=81   nlib=3   end \n'\
'power='+'   ' + str(SpecificPower)+'   burn=81   nlib=2   end \n'\
'power='+'   ' + str(SpecificPower)+'   burn=324   nlib=2  down=54   end \n'\
'power='+'   ' + str(SpecificPower)+'   burn=485   nlib=2   end \n'\
'power='+'   ' + str(SpecificPower)+'   burn=1   nlib=1   down=54   end \n'\
'power='+'   ' + str(SpecificPower)+'   burn=486   nlib=2   down=1825  end \n'\
'end burndata \n'

#  Adds together parts of input to make input.
SCALEinput=TopInputSlice+CompSlice+MiddleInputSlice+BurnSlice+BottomInputSlice



#  Saves input File
file=open(OutCycle+'.inp','w')
file.write(SCALEinput)
file.close()
```

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