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Characterization of High Level Waste from a Hybrid LIFE Engine for Enhanced Repository Performance

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Characterization of High Level Waste from a Hybrid LIFE Engine for Enhanced Repository Performance

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ABSTRACT:

In the interest of providing unlimited greenhouse gas-free energy at low cost, the Laser Inertial Fusion Energy (LIFE) project provides a testbed for inertial confinement fusion technology. Proposed designs are a pure fusion reactor or a hybrid fusion-fission reactor, which includes a subcritical blanket of fissionable material to be irradiated by neutrons from the fusion reaction. Two possible fuels are considered: (1) used fuel from current reactors; (2) thorium. Amounts of high level waste (HLW) generated per kilowatt-hour (kW*h) produced are lower relative to current Light Water Reactors (LWR), but potential hazard associated with 1 ton of HLW from LIFE is superior. The scope of this study is to combine quantities and qualities of HLW from LIFE and determine the repository space required relative to HLW from LWR for a once through fuel cycle. Repository space was determined in terms of number of canisters required disposal of waste in the production of 1 kW*h. HLW properties were determined using the Oak Ridge Isotope GENeration code (ORIGEN-S) and waste was conditioned and stored in borosilicate glass. For a LWR, the fuel was burnt to 50 gigawatt-days per tonne heavy metal (GWd/tHM) then reprocessed through Plutonium Uranium Extraction (PUREX). For LIFE, fuel burnup varied from 478.6 to 971.8 GWd/tHM and both PUREX reprocessing and conditioning with no separation were analyzed. HLW load per canister was determined for each fuel by combining mass, decay heat, and composition constraints, but the decay heat constraint was eliminated, allowing the spent fuel to cool before solidification. If PUREX reprocessing is applied, LIFE requires 1.47E-10 and 1.39E-10 canisters per kW*h for used fuel and thorium fuel, respectively. A LWR requires 1.56E-10 canisters per kW*h. Limiting constraints for LIFE spent fuel were mass of the canister, mass fraction of the glass frit, or molybdenum trioxide mass fraction. If uranium and plutonium are not separated from LIFE spent fuel, then 2.10E-10 and 1.96E-10 canisters are required per kW*h, for the used fuel and thorium fuel, respectively. Required number of canisters decreases with increased fuel burnup. HLW waste disposal of LIFE is not only feasible, but more efficient than LWR with separation per kW*h. High burnups of LIFE offer the greatest waste performance benefit. Limitations of the study include assumption of generic processing or PUREX extraction for LIFE fuel. Future work will include environmental impact after canister failure.

INTRODUCTION:

The purpose of this analysis is to find the volume of high level waste (HLW) generated in a fuel cycle that include LIFE (Laser Inertial Fusion-based Energy) engines as compared to a LWR (Light Water Reactor) once-through fuel cycle. For the LIFE system, two options are considered: (1) LIFE is used to burn used fuel from LWR recovered through the AIROX process; (2) LIFE is fueled with thorium only. The volume of waste requiring deep geological disposal is determined in number of canisters. Additionally, a parametric analysis was performed in order to characterize the HLW waste being stored in the canisters. The report will first detail models used in the analysis, which include details for the repository and fuel cycles analyzed. Calculation methods will be detailed, including specific calculations performed and scripting tools used. Next, results of the parametric analysis and the cask loading results will be given and discussed. Finally, overall conclusions for both facets of the study will be given.

MODELS

Fuel cycles

LIFE fueled with recovered used LWR Fuel

Figure 1 shows the fuel cycle for a LIFE engine fed with used fuel form LWR. LWR fuel was burned through three cycles to 50 GWd/tHM. Enrichment was 5.0 wt % U-235. After a cooling time of twenty years, the fuel is recovered via the AIROX process and refabricated. Only volatile and partially semi-volatile fission products are extracted from the used fuel (Table 1). Elements removed are primary noble gasses, but also include cesium, tellurium, ruthenium, cadmium, and iridium. Next, this refabricated fuel was burned in LIFE. Simultaneously, the fission products removed via AIROX were depleted via the Origen-S code for 40 years. These same fission products were added back into the end-of-cycle waste from LIFE. The simplification made was that LIFE would run for 40 years, regardless of burnup, and the AIROX-removed fission products would decay simultaneously. The spent fuel from LIFE was let decay before vitrification and disposal. Two different options were assumed for the conditioning phase. The first option assumed that there was no reprocessing, and the fuel was simply mechanically separated from the carbon. In the second, it was assumed that the LIFE spent fuel underwent PUREX reprocessing.

LIFE fueled with thorium

Figure II details the thorium fuel cycle, which is simpler than the extended LWR-LIFE fuel cycle previously described in Figure 1. The thorium fuel cycle simply assumes that a LIFE engine converts thorium to ^{233}U and burns this directly, in a single pass mode. The spent fuel after cooling is either disposed in its original composition or reprocessed through THOREX.

LWR fuel cycle

For LWR reactor a once-through fuel cycle was assumed. The initial fuel is enriched 5.0 wt% in ^{235}U and is burned through for three cycles to 50 GWd/tHM. After cooling and before disposal the spent fuel is reprocessed through PUREX.

For all fuel cycles the cooling time before disposal was assumed to be a parameter, varying from 5 to 40 years. For the PUREX process, uranium and plutonium are separated out with 0.604% and 0.2966 % remaining in the waste stream, and all noble gasses are separated out completely. THOREX is still an experimental process, but for the purposes of this study, uranium, plutonium, and thorium are extracted similarly to PUREX with 0.604%, 0.2966 % respectively, and 0.700% remaining in the waste stream, respectively. The value for thorium efficiency was chosen by the author to insure conservatism.

The high level waste arising from each of these fuel cycles is assumed to be disposed in the form of borosilicate glass. This process is currently used to vitrify defense HLW from the weapons complex. Borosilicate glass consists of boron oxide and silica. The boron serves as a neutron absorber. (Saling & Fentiman, 2001)

Repository model

This study assumes the repository has the characteristics of the proposed Yucca Mountain repository. Assumptions and constraints are based off of the federal regulations relevant to this repository. Each canister is modeled as a cylinder with outer cladding, with vitrified HLW distributed homogeneously. Principal decay heat emitters are also homogeneously distributed with the canister. All released decay heat is absorbed in the borosilicate glass. In interim storage, the canisters are stacked on top of each other. Canisters are cooled naturally by air. The maximum temperature is on the centerline of the canisters, and heat conduction in the axial direction is neglected, in order to insure conservatism. Steady state heat transfer at time of emplacement with constant heat emission rate is assumed and radiation effects are ignored. LIFE with used LWR fuel and PWR undergo the same conditioning and vitrification: either PUREX or reprocessing without actinide extraction. LIFE with thorium fuel is assumed to undergo either THOREX reprocessing, or reprocessing without actinide (including thorium) extraction. For simplicity, it is assumed that process and corrosion chemicals are proportional to the amount of waste processed, and are the same for both PUREX and THOREX.

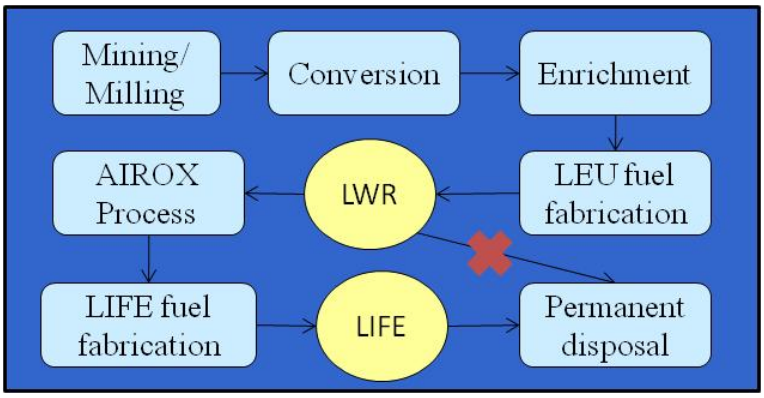

Figure 1: Fuel cycle for LIFE with LWR recovered fuel

Table 1: AIROX fission product separation efficiencies

Element	Separation efficiency (%)
H	100
Kr	100
Ru	100
Cd	75
Te	75
Ir	75
I	100
Xe	100
Cs	100
Other	0

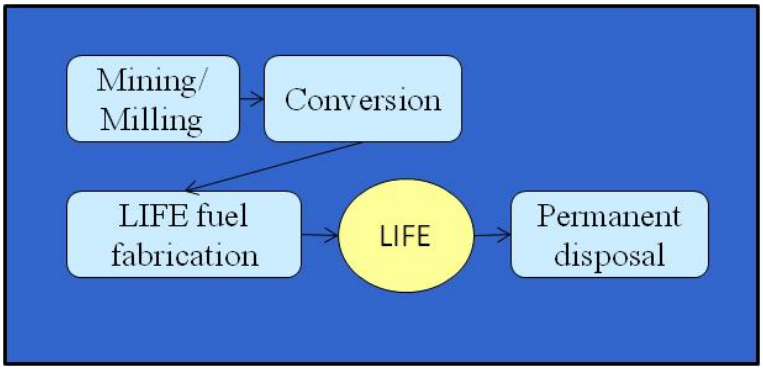

Figure 2: Fuel cycle for LIFE with thorium fuel

METHODOLOGY

In order to determine the volume of HLW waste generated in each of the fuel cycle multiple steps are necessary: (1) fuel depletion in the reactor; (2) spent fuel cooling; (3) reprocessing; (4) condition and vitrification.

For this study, the composition of the spent fuel discharged from a LIFE engine was provided (Fratoni, 2010) (Powers, 2010), whereas composition from the PWR was determined using the Origen-S code. (Gauld, 2009) Spent fuel cooling was also modeled with Origen-S for both systems.

Reprocessing, vitrification, and canister loading were computed with a newly designed MATLAB script. After the optional PUREX or THOREX reprocessing, the borosilicate glass composition, that includes processing and corrosion chemicals besides the spent fuel, was determined. For the case where the fuel is simply recovered without any actinide separation, it was assumed that amounts of chemicals were identical to those used in the vitrification during PUREX for PWR fuel. These are linearly proportional to the amount of waste being vitrified. Finally, the amount of high level waste that can be loaded in a canister was determined according to mass, volume, material, and waste composition constraints. Seven constraints were modeled. Variable descriptions are given in Table 2 and the linearized form is given in Table 3.

These constraints are based upon federal regulation. The first three constraints are independent of the HLW composition. The first constraint limits the canister mass to 2500 kg. The second constraint requires that the volume of vitrified HLW must be between 80% and 100% of the volume of the canister. The third constraint limits the mass fraction of glass frit to be between 70% and 85% of the vitrified waste. The fourth constraint imposes that the temperature of the canister cannot exceed 400ºC in the vitrified waste. The derived linear relationship between temperature and heat emission can be interpolated from Figure 3, and constants K_1 and K_2 can be used to graph the resulting constraint. The coefficients K_1 and K_2 are equally valid for both LIFE and PWR fuel, as they are approximation from the thermal hydraulics of the canister and the total heat emission of the canister, and not dependent of the composition of the nuclides in the waste producing heat emission. The fifth constraint prescribes that the concentration of plutonium must be less than 2.5 kg/m^3. The sixth constraint is that the amount of molybdenum trioxide cannot exceed 2 wt % of the vitrified HLW. The seventh and final constraint is that the amount of sodium dioxide content cannot exceed 10 wt % of vitrified HLW. All constraints will apply equally to LIFE or LWR fuel, since the assumption is made that the conditioning chemicals used are the same.

The combination of all the constraints determines the number of canister necessary for each fuel cycle. These constraints are combined using linear programming techniques, meaning they were linearized (if needed) and graphed to form a feasible solution space. These provide a space of feasible solutions given by combinations of HLW mass and glass mass. Assuming that the scope is to minimize the repository space, the preferred solution among the feasible combinations is the one that minimize the number of canisters, i.e. maximize the HLW waste load per canister. Analysis was normalized pet tHM and per GWd to facilitate comparison.

A MATLAB script was used to input composition data and calculate these variables and constraints, as well as to apply processing to the input composition. Additionally, it performed necessary normalizations for relevant data. A copy of the MATLAB script is given in the appendix.

Table 2: Variables used in analysis

Variable	Description
M_G	Mass of glass frit
M_W	Mass of HLW waste
K_1, K_2	Constants used to calculate heat flux linearization
ζ	Heat emission rate per unit mass of HLW waste
V_c	Volume of canister (.823 m^3)
$x_{W,PU}$	Weight fraction of plutonium
x_{MoO3}	Weight fraction of molybdenum trioxide
x_{W,NaO_2}	Weight fraction of sodium dioxide
x_{G,NaO_2}	Weight fraction of sodium dioxide in glass frit (assumed to be 0)

Table 3: Constraints for cask loading

Constraints for Cask Loading		
1	Total mass of the waste container must be less than 2500 kg	$2033 - M_G \leq M_W$
2	The volume of the vitrified HLW must be between 80 and 100% of the canister volume	$2393.7 - 1.505 * M_G \leq M_W \leq 2932.3 - 1.505 * M_G$
3	The mass fraction of the glass frit must be between 70 and 85%	$0.1765 * M_G \leq M_W \leq 0.4286 * M_G$
4	The highest temperature in vitrified HLW must be 400°C.	$M_G * K_1 + K_2 \leq M_W$
5	The concentration of plutonium in vitrified HLW must be less than 2.5 kg/m^3	$2.5 * \frac{V_c}{x_{WPU}} * M_G \leq M_W$
6	The mass fraction of molybdenum trioxide in vitrified HLW must be less than 2 wt%	$\left(\frac{0.02}{x_{MoO_3} - .02}\right) * M_G \leq M_W$
7	The upper bound for the mass fraction of sodium dioxide in vitrified HLW is 10%	$\frac{.1 - x_{GNa_2O}}{x_{WNa2O} - .1} * M_G \leq M_W$

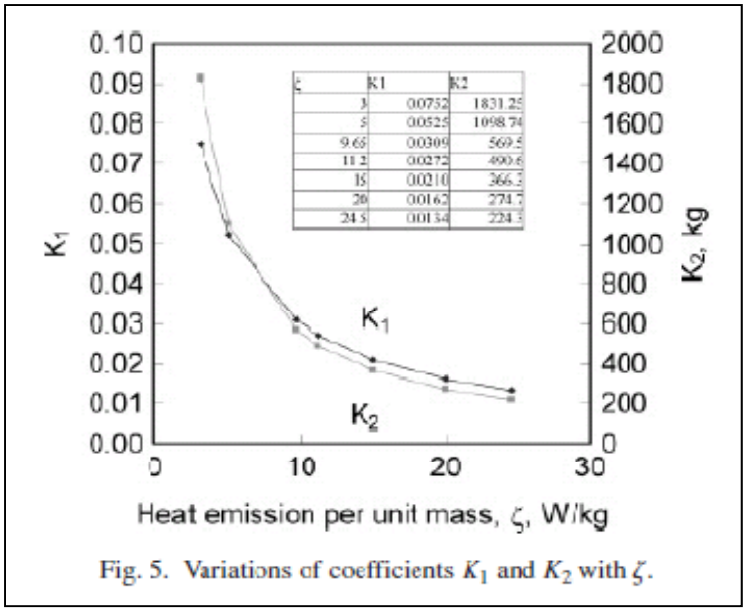

Figure 3: Variation of K_1 and K_2 with ζ

MATLAB Script

Inputs to the script from Origen-S were formatted in a Microsoft Excel file. The MATLAB script asked the user for the burnup to be analyzed, input the data, and offered PUREX and THOREX options with extraction. The script then found the parameters needed to graph the constraint equations. Outputs from the script were a graph of the feasibility solution as well as total HLW and number of canisters needed. These values were normalized per GWd and per tHM. A flow chart is given below in Figure 4. The input code for the thorium fuel is given in the appendix.

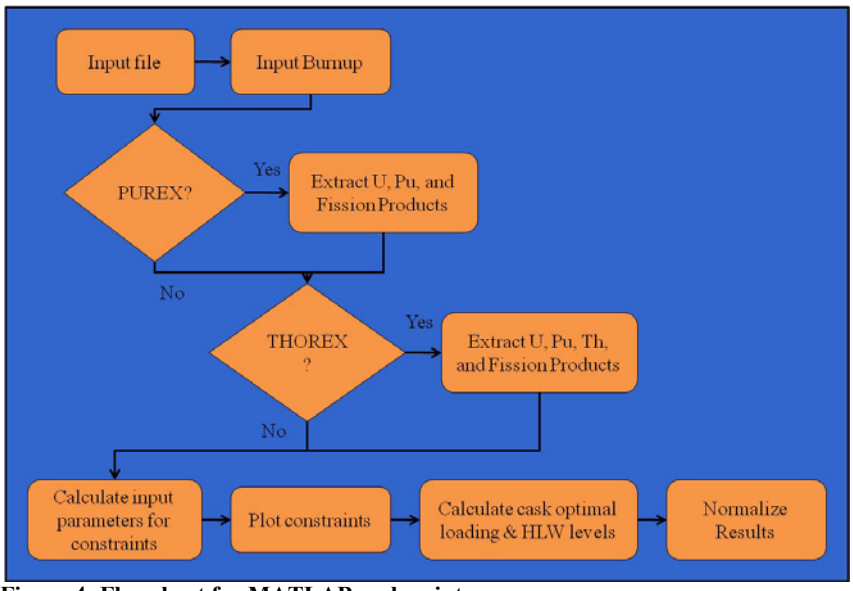

Figure 4: Flowchart for MATLAB and script

RESULTS AND DISCUSSION

Spent fuel properties comparison

The properties of the spent fuel as discharged from the reactor, either LIFE or LWR, were analyzed in order to identify the fuel cycle specific characteristics. Activity levels, decay heat, radiotoxicity (both inhalation and ingestion hazards), Neptunium-237 and precursor levels, total neutron source levels, product mass, transuranic (TRU) mass, fissile mass, fissile fraction, and fissile plutonium fraction were determined for selected burnup levels (Table 4) as a function of time after discharge. All quantities are provided per initial mass of heavy metal (tHM) and per unit of energy produced (GWd).

The PWR fuel activity is lowest per tHM (Figure 5) but highest per GWd (Figure 6). LIFE fuels behave similarly per GWd, and thorium fuel performs better in terms of initial tHM. Higher burnups minimizes activity, regardless of normalization.

Decay heat is lower for thorium fuel than the PWR fuel, for either normalization and for used PWR LIFE fuel per GWd (
Figure 7 and Figure 8). Higher burnups minimize decay heat most effectively. Inhalation hazard behaves similarly to decay heat, as in Figure 9 and Figure 10. Relative performances are the same, and higher burnups most effectively minimizes inhalation hazard.

Ingestion hazard most effectively minimizes the PWR per initial tHM (Figure 11) and thorium per GWd (Figure 12). Higher burnups minimize ingestion hazard, however, the relative decrease in ingestion hazard as burnup increased is smaller than for inhalation hazard.

Neptunium-237 and precursor levels are graphed in Figure 13 and Figure 14. Thorium has the lowest levels for either normalization, as a result of the lower atomic mass of the fertile thorium fuel. In general, LIFE used PWR fuel performs the worst. The exception was the fuel at burnup of 99.441 % FIMA. This has the lowest level per GWd and the second lowest level per tHM; thorium at burnup of 94.117 % also effectively minimizes levels.

Total neutron source was graphed per initial tHM and GWd in Figure 15 and Figure 16. PWR fuel minimizes the levels most effectively. However, high neutron source levels could provide a benefit in terms of proliferation resistance, as materials are more difficult to handle with the large levels of emitted neutrons, so high total neutron source is a positive attribute. Total neutron source increases with increasing burnup. Fission product mass behaves similarly, with PWR most effectively minimizing the quantity both per initial tHM (Figure 17) and per GWd (Figure 18). Fission product mass level increases with increasing burnup, as there were more fissions, and by extension, more fission products.

TRU mass is graphed per initial tHM and GWd in Figure 19 and Figure 20. TRU mass is most effectively minimized by the PWR in terms of initial tHM and by LIFE per GWd. TRU mass decreases with burnup for LIFE used PWR fuel and increase for LIFE thorium fuel. LIFE fueled with used PWR at burnup of 99.441% FIMA minimizes TRU most effectively for both normalizations. Fissile mass behaves similarly, with the exception that thorium fuel minimized the levels per tHM most effectively on average, as can be seen in Figure 21 and Figure 22. Similarly, LIFE fueled with used PWR at burnup of 99.441% FIMA minimizes fissile mass most effectively for both normalizations.

Finally, fissile fraction and fissile plutonium fraction were analyzed in Figure 23 and Figure 24, respectively. The PWR fuel minimizes the fissile fraction most effectively, followed by thorium fuel. Fissile fraction decreased with increase burnup. LIFE fueled with used PWR at burnup of 99.441% FIMA with minimized fissile mass most effectively. There are no conclusive

findings for fissile plutonium fraction. As can be seen in Figure 24, the fraction of fissile plutonium is highly dependent on time for both LIFE fuels.

In order to facilitate the analysis, each fuel was ranked for each characteristic on a relative scale (for both normalizations). Fuels were ranked from 1 (best at minimization of quantity) to 3 (worst). These were determined qualitatively from the graphs. If a clear hierarchy was not visible, the parameter was not analyzed. The results, including overall total rank, are given in Table 5. The best performing fuel is the one with the lowest "score." From this analysis, thorium fuel minimized hazards most effectively per GWd and used PWR fuel minimized hazards most effectively per initial tHM. However, per GWd, both LIFE fuels performed the most effectively.

However, a major exception to the general rules is the behavior of the used PWR fuel for LIFE at very high burnup. This, along with the thorium fuel at high burnup, minimized almost every category most effectively, for both normalizations. The only exceptions were fission product mass, which is reasonable because of the greater number of fissions.

Cask Loading

In the previous section, it was shown that even if a LIFE engine reduces the amount of waste generated per unit of energy produced, the radiotoxicity and activity associated with this waste are greater—unless burnup above 99% are achieved—and provide waste management challenges. A more comprehensive comparison is provided by determine the storage requirements for the high level waste arise from each cycle. This will be accomplished by finding the optimal HLW stored in canisters, and by determining the number of canisters required. This measure combines the volume of waste with its radioactive hazard features.

First, the tools developed for this study were benchmarked against available results. A PWR case with burnup of 28 GWd and 4.0 wt% ^{235}U enrichment was analyzed via depletion in Origen-S followed by analysis via the MATLAB script. The same optimal solution was found in the literature, with 528 kg of HLW and 1505 kg of glass per canister. The test case feasibility solution and the benchmarked solution are available in Figure 25 and Figure 26. It can clearly be seen that the intersections of constraint 1 and 7 form the optimal solution.

With the code validated, test cases with burnup from 30.150 % FIMA to 99.441 % FIMA were tested for LIFE fueled with used PWR fuel and test cases with burnup from 30.013% FIMA to 94.177 % FIMA for LIFE fueled with thorium. Decay cooling times before loading between three and forty years were tested for both fuels. Several sample solution spaces are given. Figure 27 gives an optimal solution for thorium fuel with no THOREX extraction. The molybdenum trioxide constraint and mass constraint give the optimal cask loading. Figure 28 gives the solution space for used PWR fuel in LIFE that has been reprocessed via PUREX. The intersection of constraint 4, constraint 6, and constraint 1 form the optimal solution. These three constraints were the most commonly constraining. The plutonium constraint (constraint 5) and sodium dioxide constraint (constraint 7) were never constraining for LIFE. The volume constraint (constraint 2) and mass of glass frit (constraint 3) were only constraining for non-reprocessed used nuclear fuel for LIFE and several thorium cases with THOREX reprocessing.

Table 6 contains data for optimum solutions after cooling of five years. There is less total waste when reprocessing is applied. Amount of waste stored per container tends to be larger for smaller burnups. Figure 29, Figure 30, Figure 31, and Figure 32 compare data from Table 6. Figure 29 shows the large increase of total HLW per initial tHM of LIFE relative to reprocessed PWR. PWR fuel with reprocessing, at 50 GWd/tHM offers the greatest waste reduction per initial mass of heavy metal. This is due to the large amounts of uranium and plutonium that can be removed that comprise a higher fraction of the waste. It also shows the increase in total HLW for higher burnup. Figure 30 shows the comparable levels of waste when normalized per GWd for LIFE and LWR. This is because of increased energy gained from deep-burn in LIFE. It also shows the decrease in HLW per GWd as total burnup increases. Figure 31 gives the number of canisters required to store one initial tonne of HLW waste. Since this is dependent on both the cask loading optimal solution and total HLW, there is no clear relationship between burnup and number of cask. In general, thorium fuel required similar numbers of canisters regardless of reprocessing and used PWR fuel required fewer canisters with PUREX. Figure 32 shows the comparable levels of canisters needed per GWd between LIFE and LWR. It also shows a clear decrease in number of canisters required as burnup increases.

In order to eliminate decay heat as a constraint, the waste was allowed to cool for longer periods of time until the constraint (4) was not limiting. This allowed some of the shorter lived isotopes to decay away and decrease overall heat emission. This meant that the optimal solution was constrained by constraint 1 (total mass of container) and constraint 3 (mass fraction of the

glass frit) or constraint 4 (molybdenum trioxide wt %). Cooling times required are given in Figure 33. It was found that the decay heat constraint can be eliminated for all systems with acceptable cooling time—40 years or less. LIFE fueled with used PWR required longer cooling times relative to thorium. Higher burnups tended to require less, or no, additional cooling beyond five years. Tabular date is given in Table 7. Higher burnups tended to have overall better performances in the categories of total waste and number of canisters required. To aid analysis, data from Table 7 is graphed and compared. Figure 34 shows the total HLW normalized per initial tHM after additional cooling. Total HLW is independent of decay constant, so these values are the same as before additional cooling time (seen in Figure 29 and Figure 30). Figure 36 shows the number of canisters required to store the waste per initial tHM. Despite the longer cooling time, PWR reprocessed with PUREX fuel was much more efficiently stored per initial tHM There is a clear increase in number of canisters needed with burnup, in order to accommodate higher levels of waste. In Figure 37, there is a decrease in number of canisters needed. The maximum canister savings for the thorium fuel was 1.5 canisters per initial tHM, but the maximum canister loading savings for the used nuclear fuel for LIFE was 3.6 canisters per initial tHM.

Figure 35 shows the total HLW normalized per GWd, respectively after additional cooling. The increase in energy produced per canister is graphed in Figure 38. Nearly all LIFE fuels required fewer canisters than the LWR reprocessed fuel per GWd. The main benefit of the longer cooling time can be seen in Table 8 where there were both increases in energy content per canister in GWd), which is graphed in Figure 38. Optimized cooling time led to increases in energy content in LIFE fuels so that they were higher than for the PWR, except for lower burnups of LIFE used PWR fuel. The burnup required for increased performance over the PWR is 70% FIMA. The benefit was greatest for the LIFE system fueled with used PWR fuel, as it tended to have more short lived fission products. However, at higher burnups, the decay heat tended was not normally constraining and the additional cooling time did not affect the optimum solution.

Reprocessing and removal of fission products and uranium and plutonium offered both benefits and disadvantages. Firstly, it reduced the total level of high level waste, so there was less HLW to store. However, by decreasing the overall waste to store, it increased the molybdenum trioxide fraction, another constraint. Heat emission per unit volume increased, leading to a lower threshold for constraint 4. This meant that less HLW waste could be stored per canister. However, for nearly all cases, the reprocessing led to less overall canisters, despite the decrease in the amount of waste stored per canister. Negative effects from heat emission were mitigated by longer optimized cooling times.

There are several limitations to this section of the study. Firstly, LIFE spent fuel is unlikely to be reprocessed using the PUREX or THOREX method, as there is already high burnup from LIFE. However, some processing is necessary and the assumption of PUREX or THOREX allows for a better comparison, and allows for calculation of glass frit mass needed. THOREX is also an experimental procedure and would require different processing chemicals. For simplicity and comparison, it was assumed that the process chemicals were similar. Additionally, it was assumed that the amount of process and corrosion chemicals required was linear proportional to the mass of HLW. Finally, heavy metals were extracted via the PUREX or THOREX processes were not accounted for in final waste disposal. Those heavy metals would still need to be disposed of in some form, even if they were refabricated into fuel and reused.

Table 4: Burnups analyzed for LIFE engine

Used PWR Fuel		Thorium Fuel	
FIMA (%)	Burnup (GWd/tHM)	FIMA (%)	Burnup (GWd/tHM)
50.147	490.8	50.138	478.6
70.528	688.1	70.059	671.7
90.045	879.5	90.007	862.7
99.441	971.8	94.177	901.3

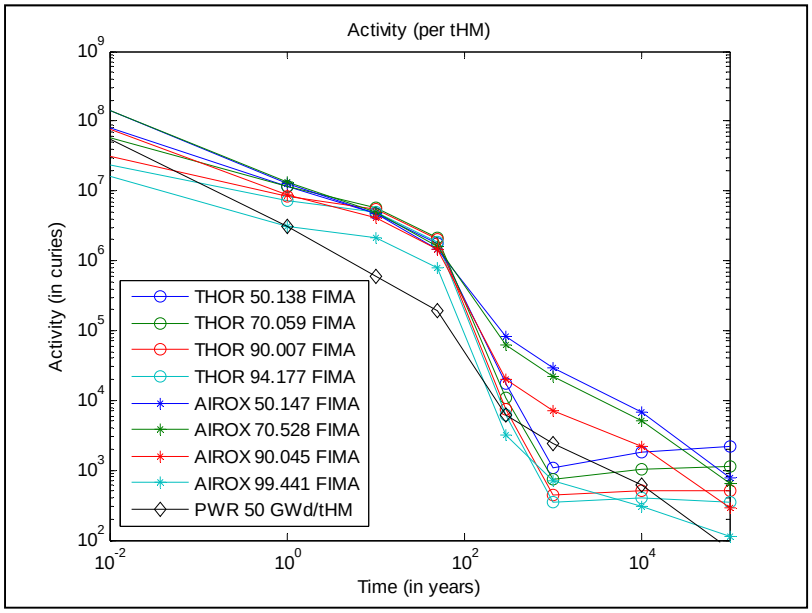

Figure 5: Activity variation for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR (normalized per tHM)

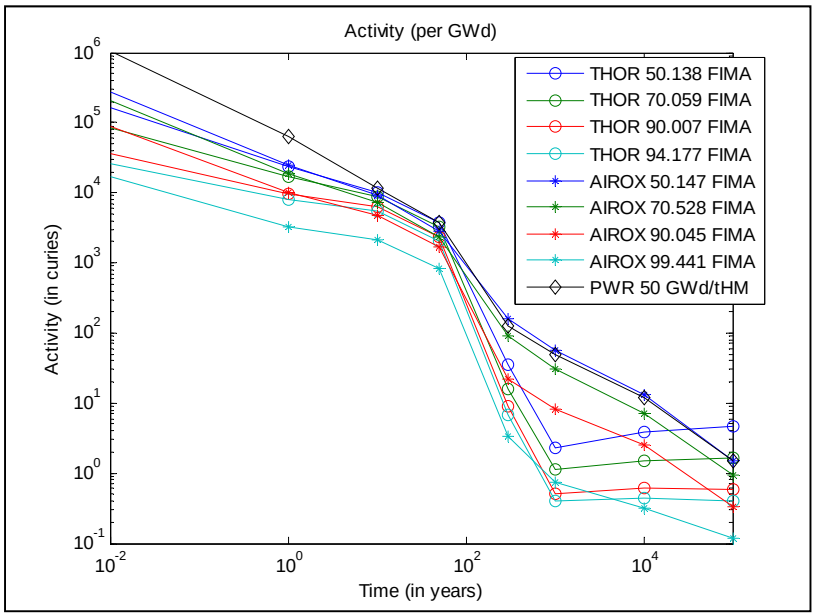

Figure 6: Activity variation for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR (normalized per GWd)

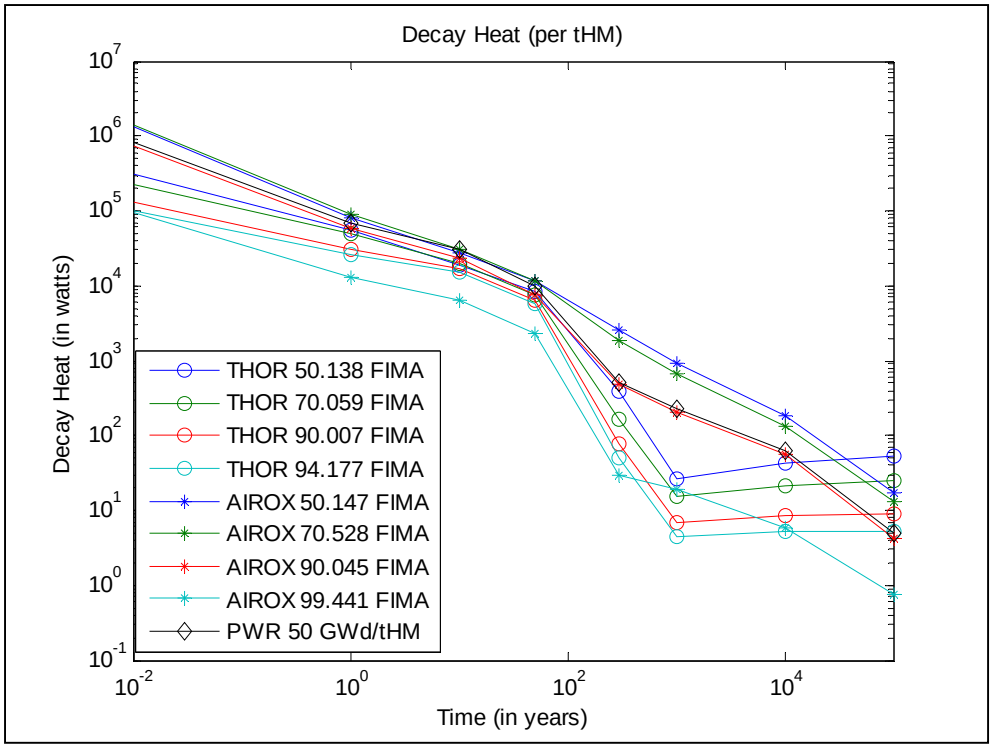

Figure 7: Decay heat variation for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR (normalized per tHM)

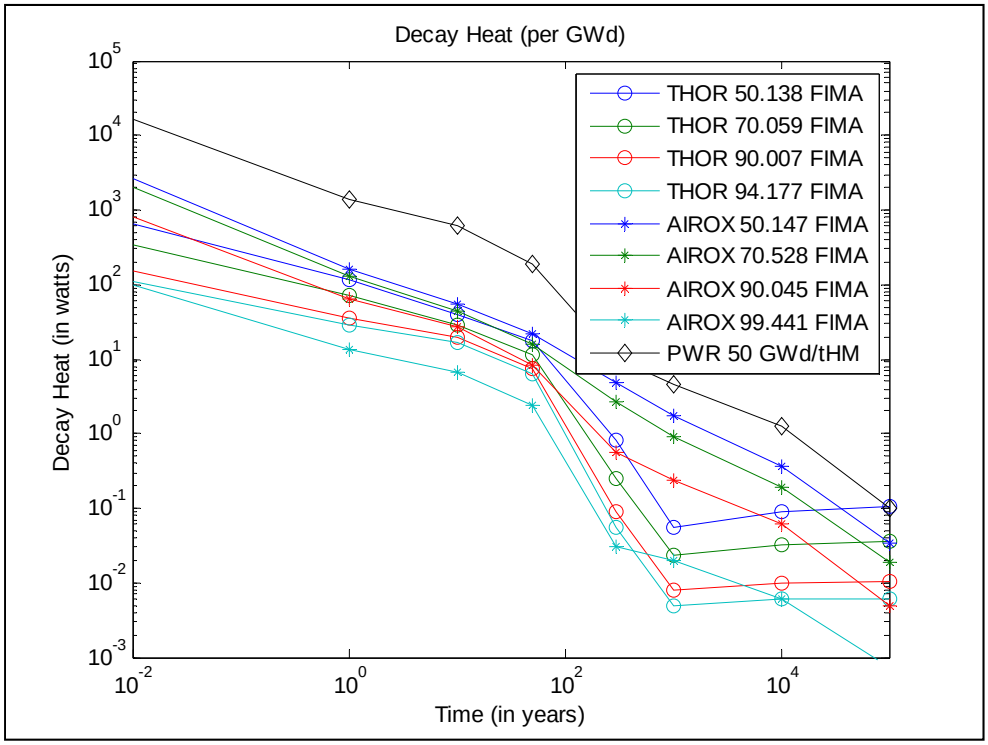

Figure 8: Decay heat variation for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR (normalized per GWd)

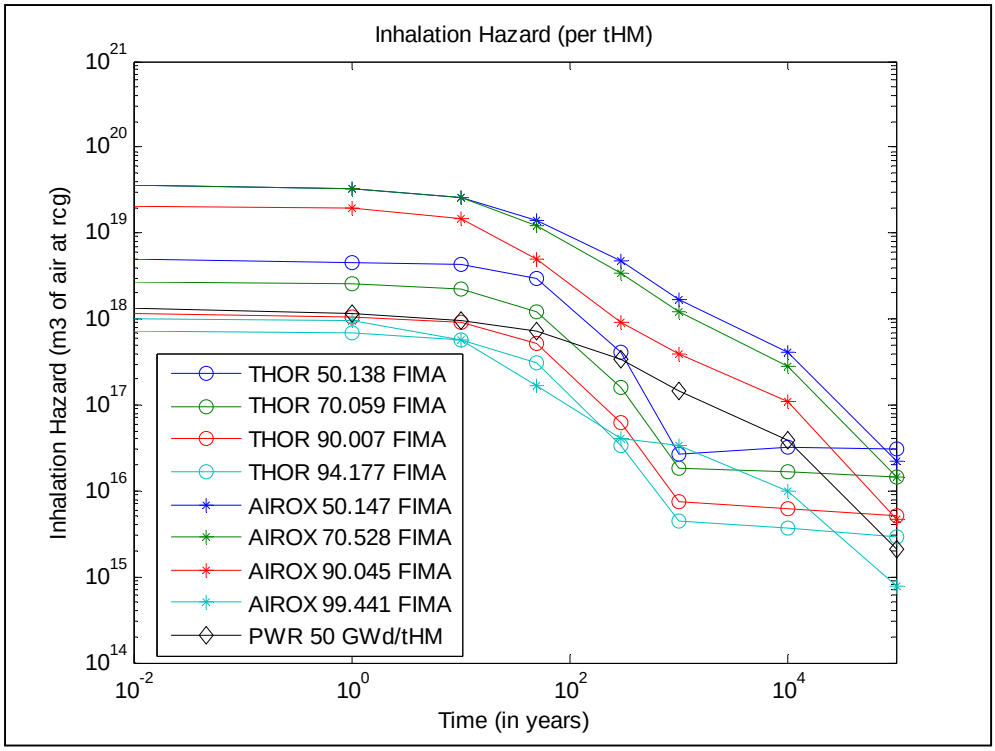

Figure 9: Inhalation hazard variation for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR (normalized per tHM)

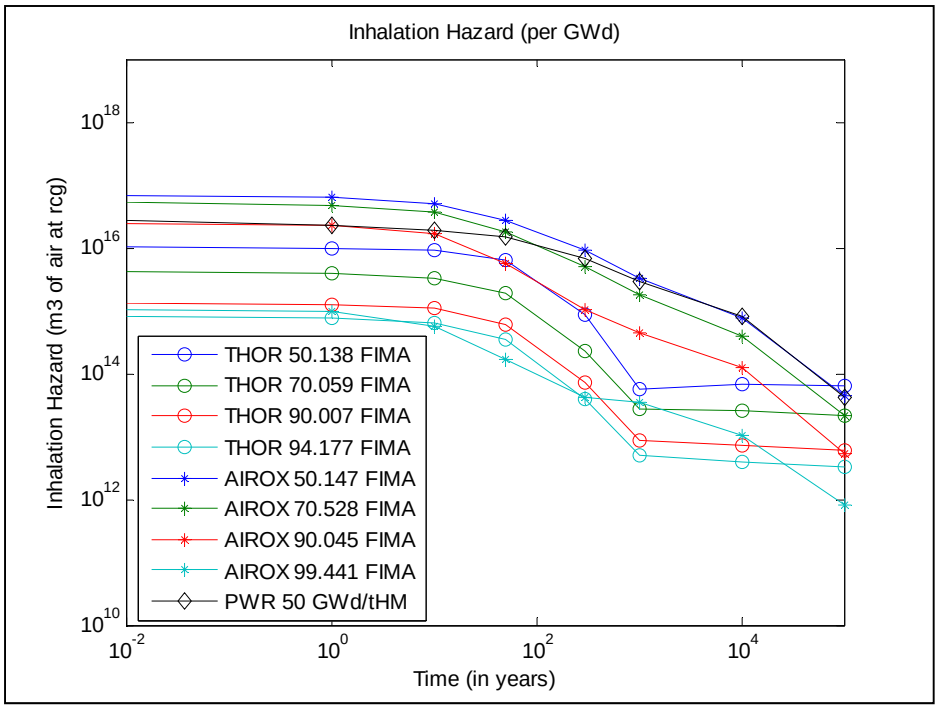

Figure 10: Inhalation hazard variation for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR (normalized per GWd)

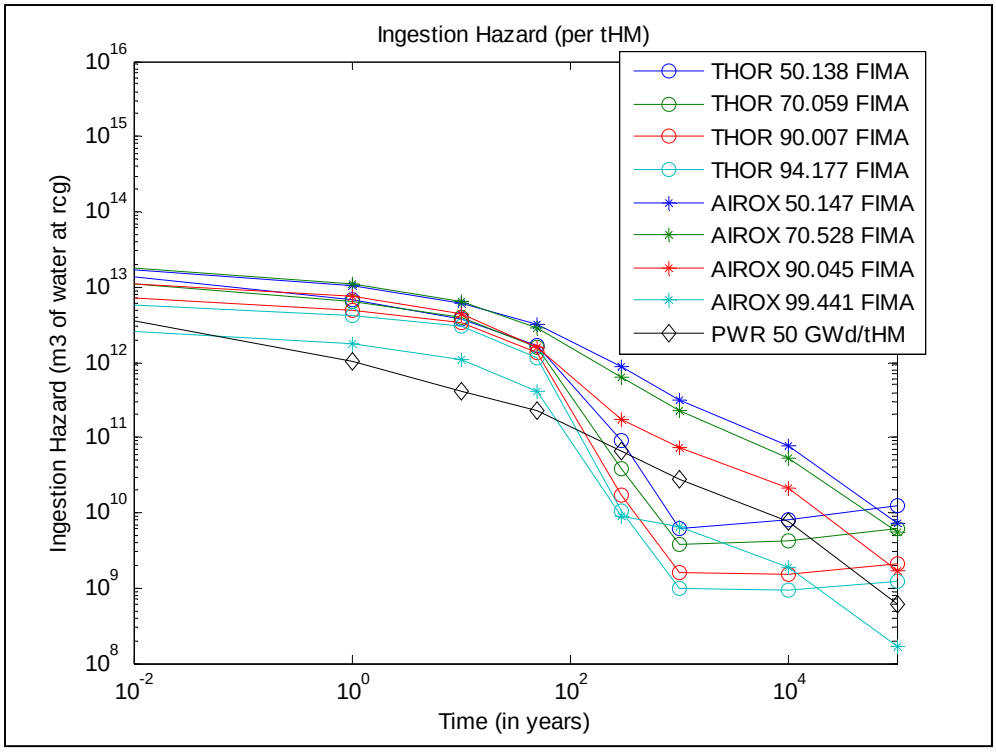

Figure 11: Ingestion hazard variation for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR (normalized per tHM)

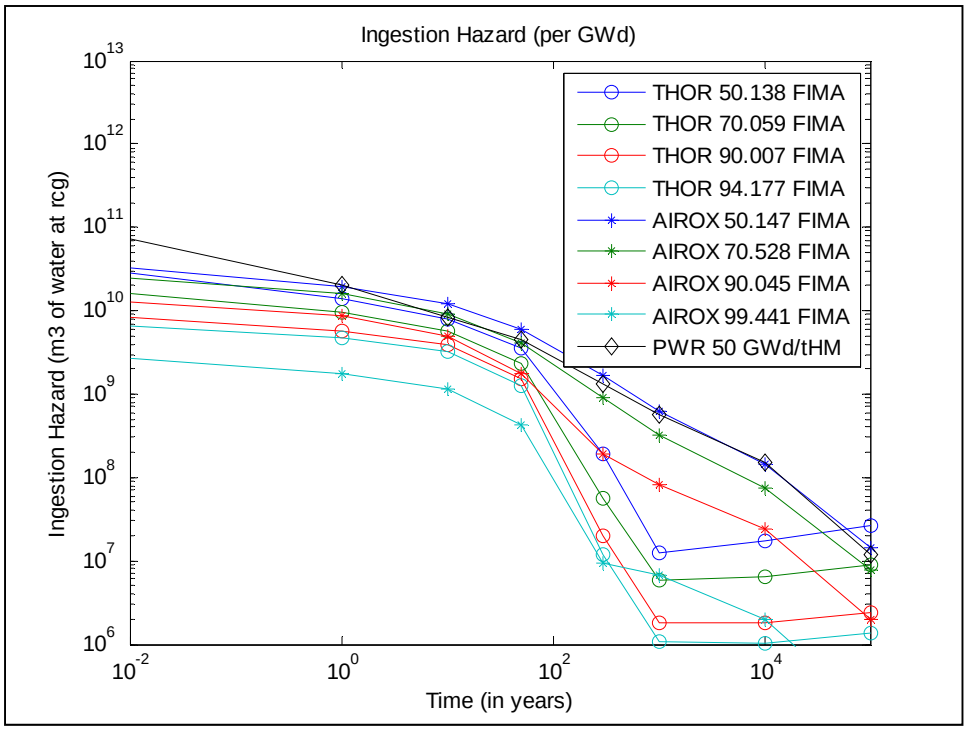

Figure 12: Ingestion hazard variation for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR (normalized per GWd)

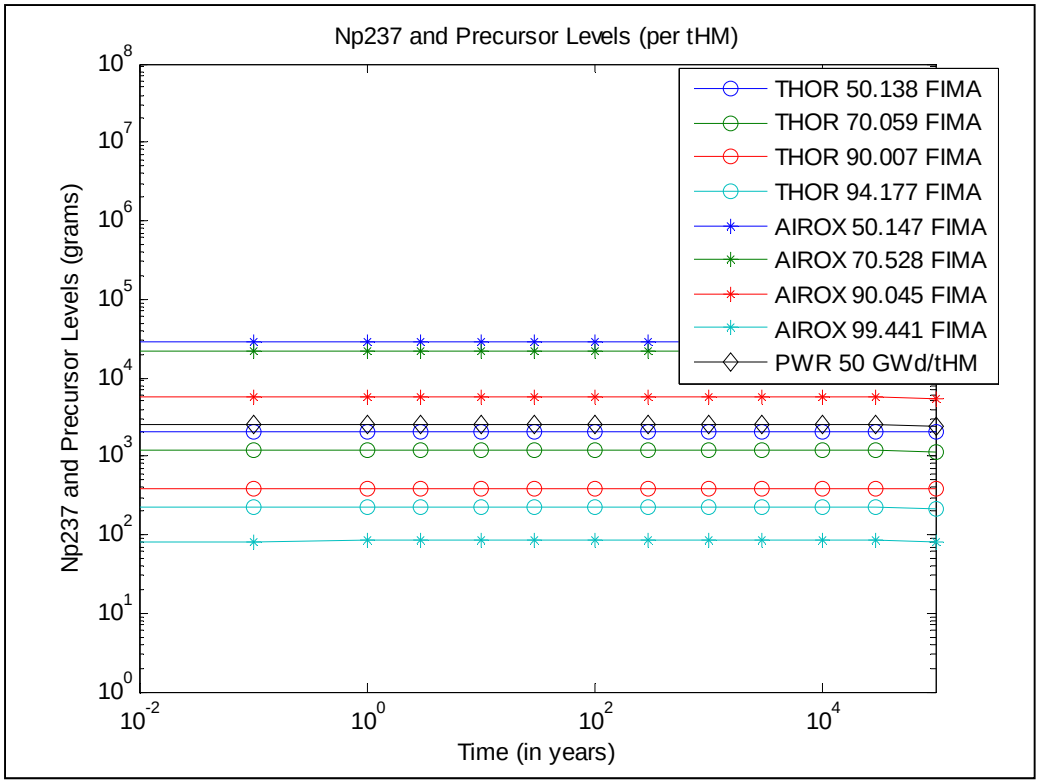

Figure 13: Np237 and precursor levels for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR (normalized per GWd)

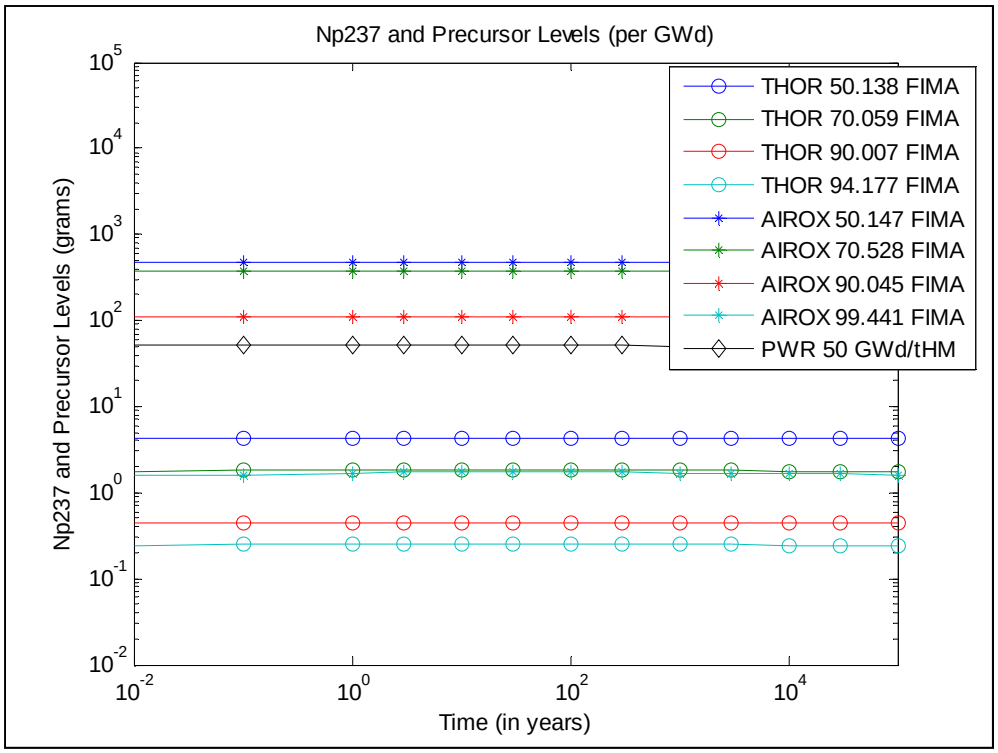

Figure 14: Np237 and precursors for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR (normalized per GWd)

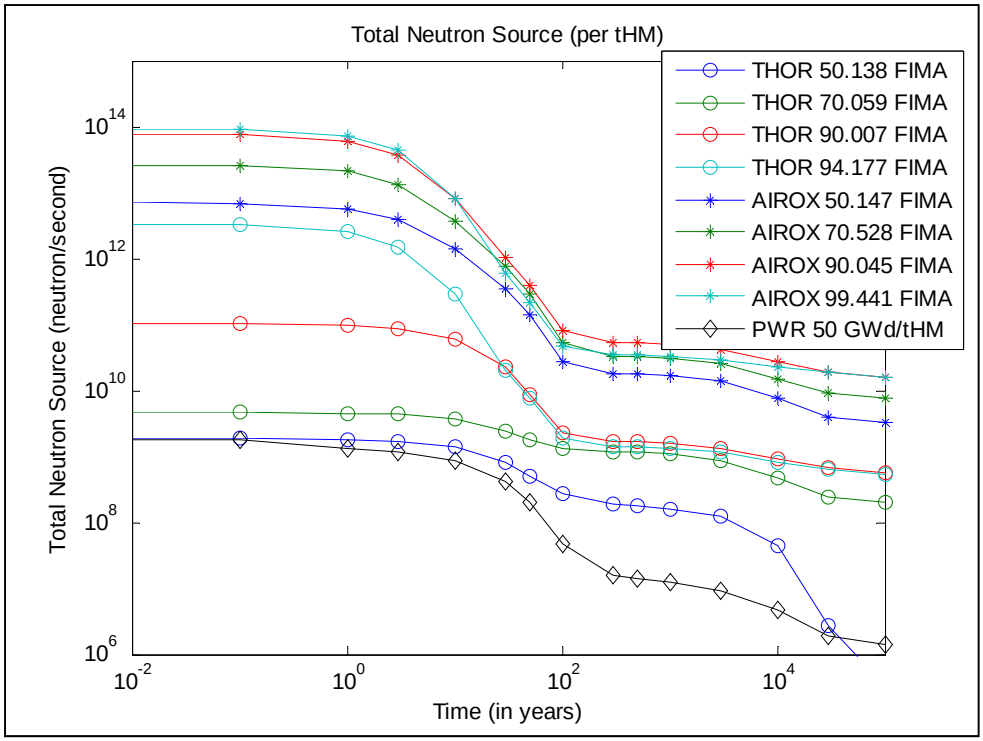

Figure 15: Total neutron source for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR (normalized per tHM)

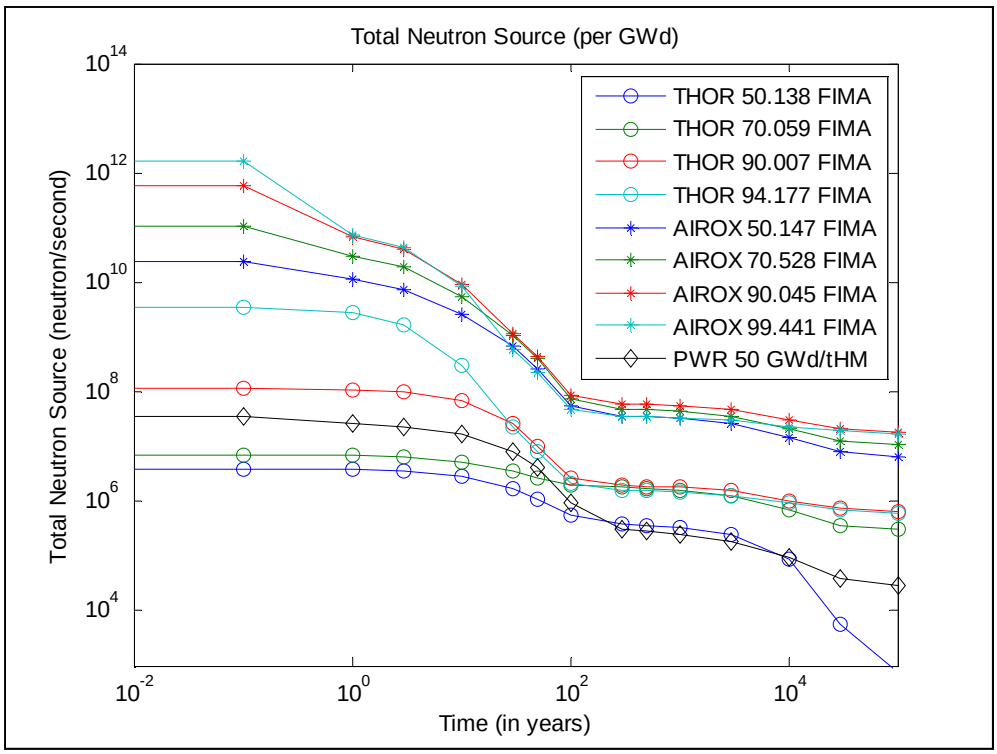

Figure 16: Total neutron source for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR (normalized per GWd)

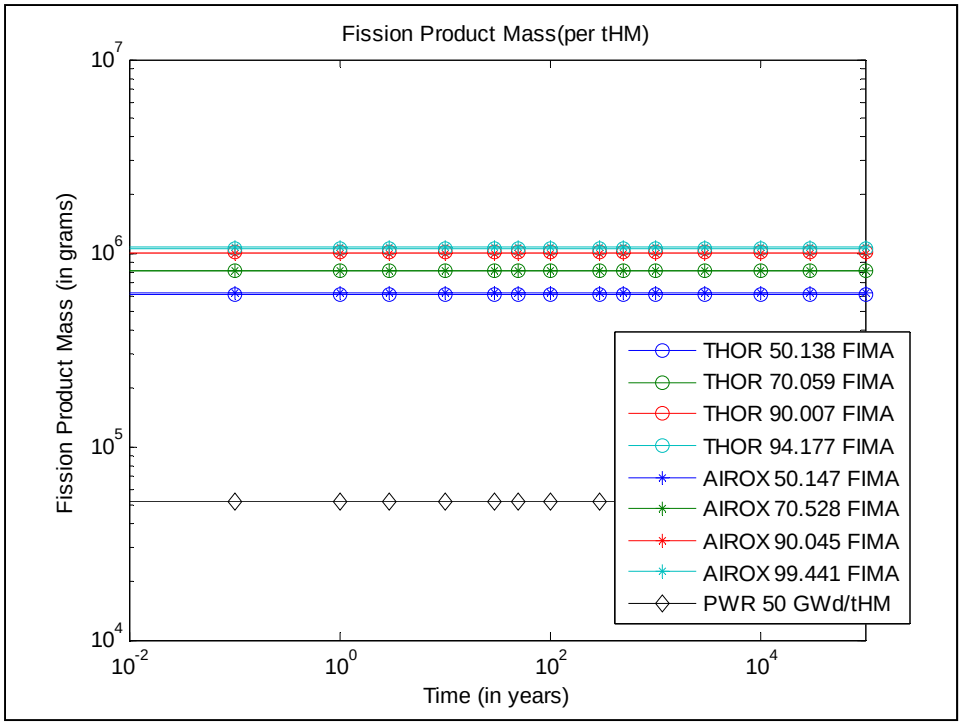

Figure 17: Fission product mass for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR (normalized per tHM)

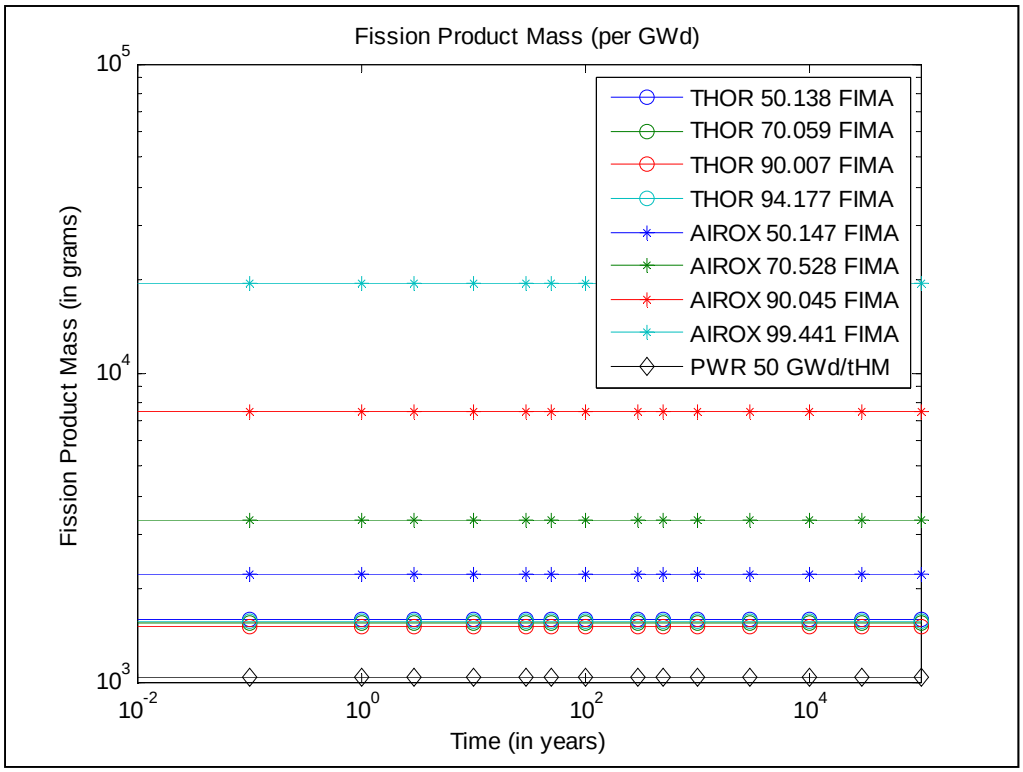

Figure 18: Fission product mass for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR (normalized per GWd)

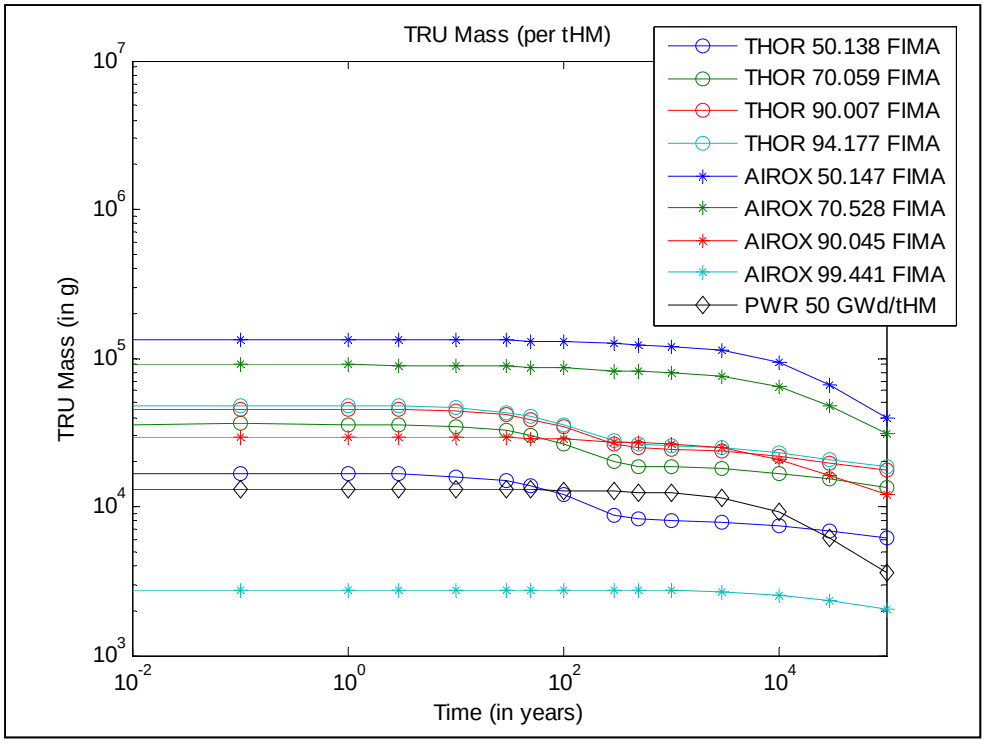

Figure 19: TRU mass for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR (normalized per tHM)

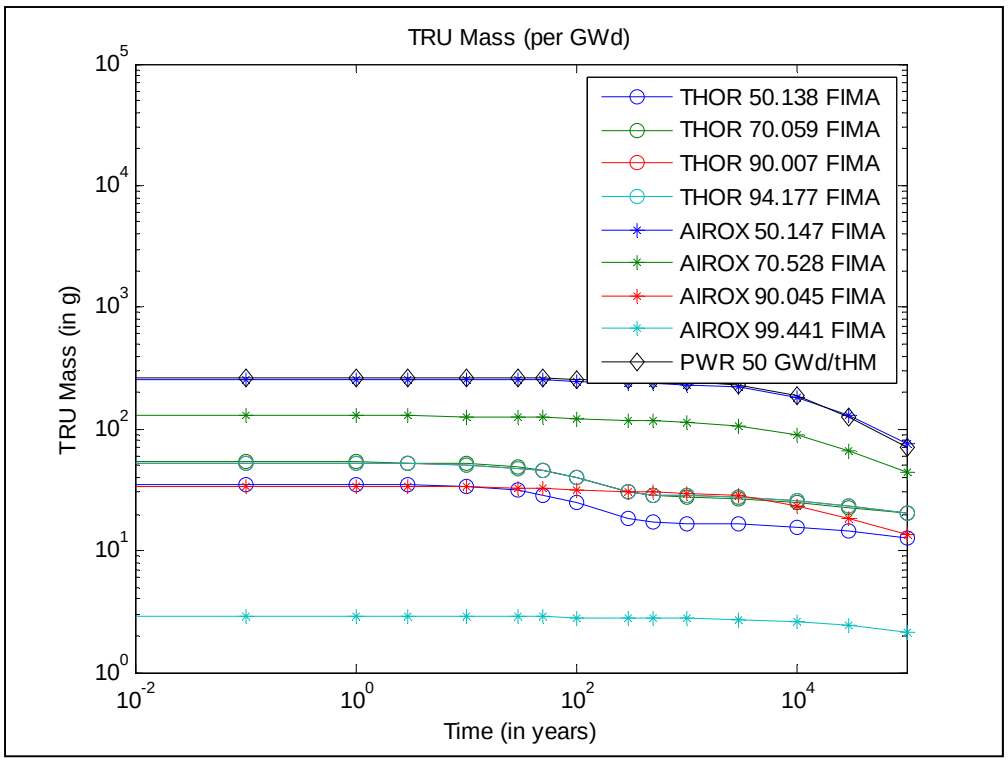

Figure 20: TRU mass for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR (normalized per GWd)

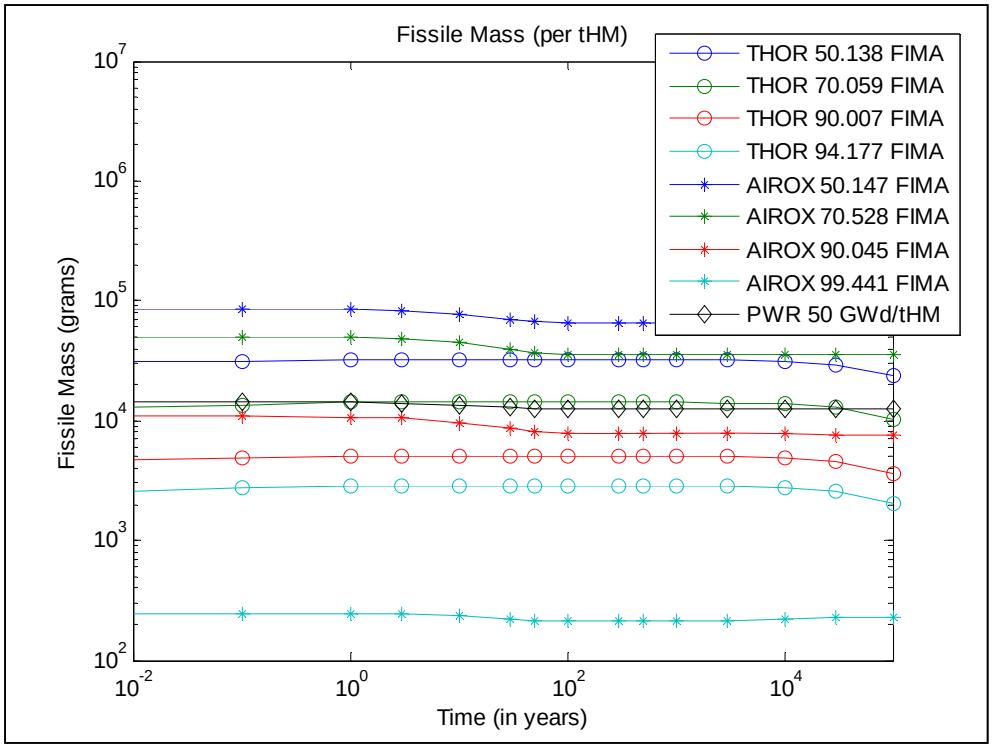

Figure 21: Fissile mass for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR (normalized per tHM)

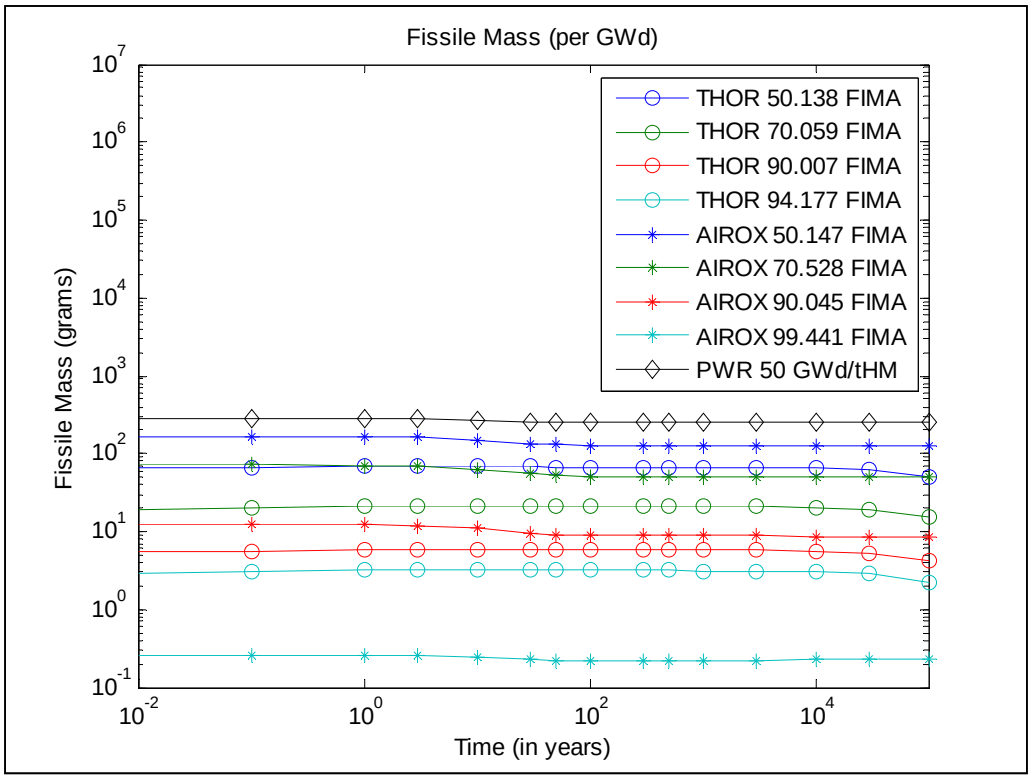

Figure 22: Fissile mass for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR (normalized per GWd)

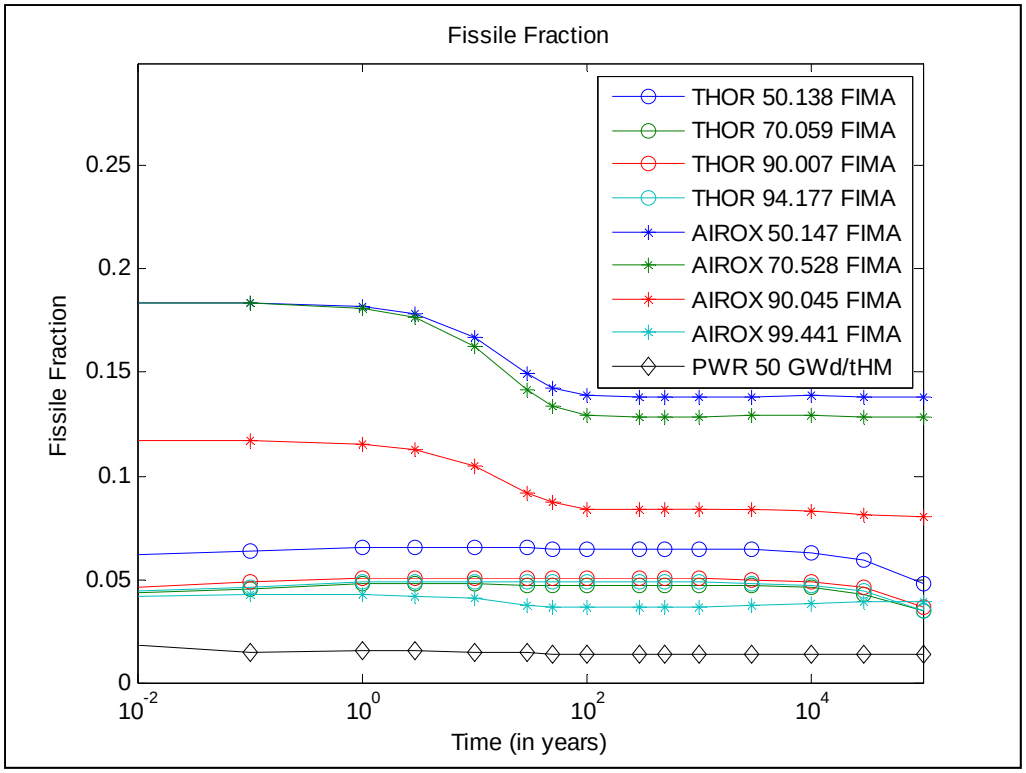

Figure 23: Fissile fraction for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR

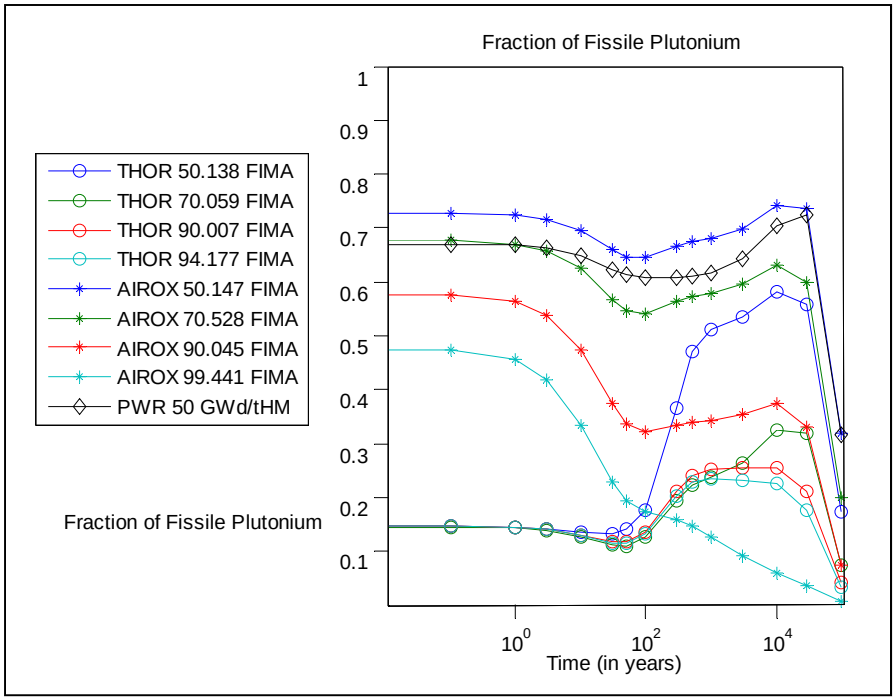

Figure 24: Plutonium fraction for LIFE fueled with either AIROX reprocessed fuel or thorium compared to a traditional 50 GWd/tHM PWR

Table 5: Rank of various parameters related to repository performance

	Per tHM			Per GWd		
	Used PWR LIFE fuel	Thorium	PWR	Used PWR LIFE fuel	Thorium	PWR
Activity	2	3	1	1	1	3
Decay Heat	3	1	2	2	1	3
Inhalation Hazard	3	1	2	2	1	3
Ingestion Hazard	3	2	1	2	1	3
Np-237 and Precursors	3	1	2	3	1	2
Total Neutron Source	1	2	3	1	2	3
Fission Product Mass	2	2	1	3	2	1
TRU Mass	3	2	1	1	1	3
Fissile Mass	3	1	2	1	1	3
Fissile Fraction	3	2	1	3	2	1
Total	26	17	16	19	13	25

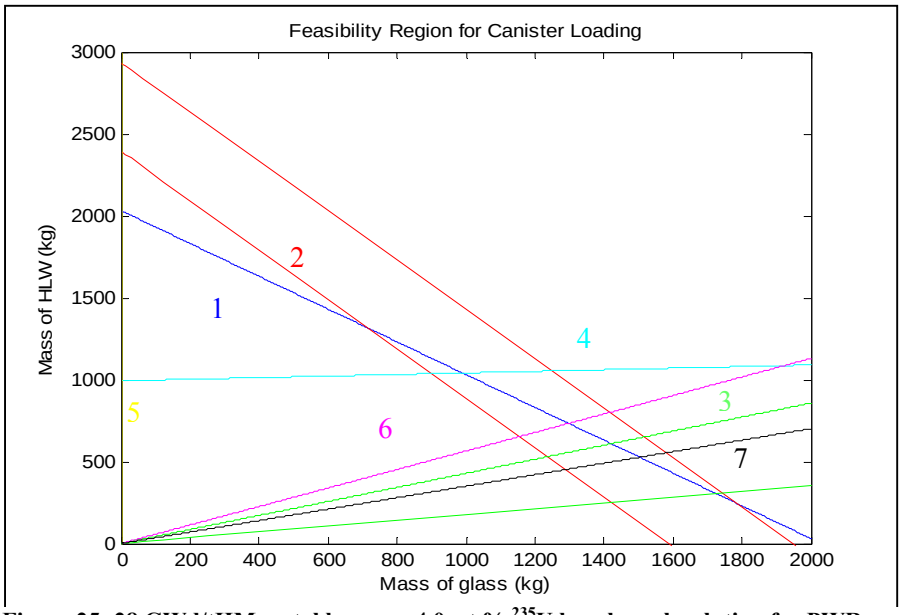

Figure 25: 28 GWd/tHM metal burnup, 4.0 wt % ^{235}U benchmark solution for PWR

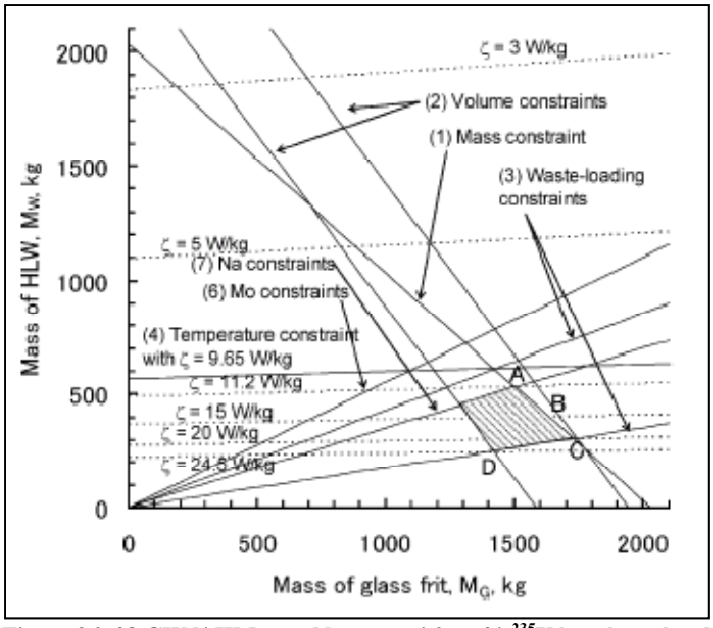

Figure 26: 28 GWd/tHM metal burnup, 4.0 wt % ^{235}U benchmark solution for PWR from Ahn

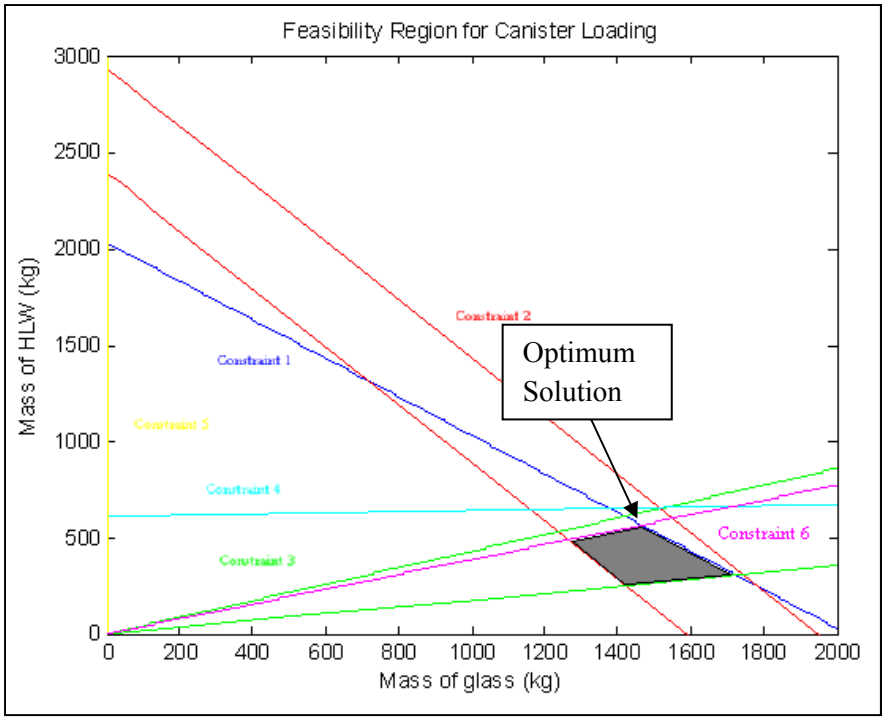

Figure 27: Feasibility Solution for BU = 90 % FIMA and cooling of 5 years for LIFE with thorium fuel (THOREX not used)

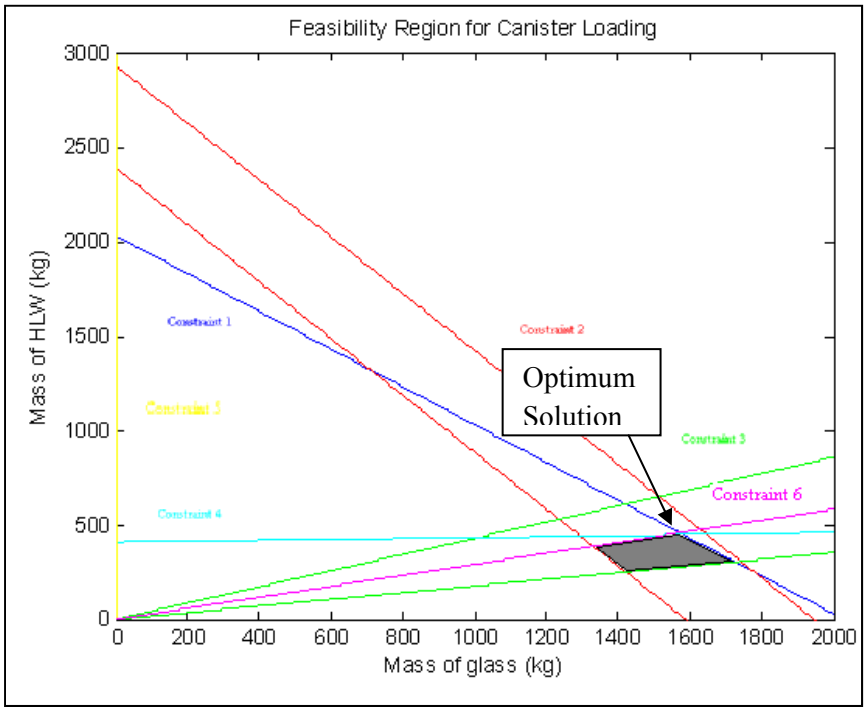

Figure 28: Feasibility Solution for BU = 80 % FIMA and cooling of 20 years for LIFE fueled with used PWR fuel (PUREX used)

Table 6: Key statistics for cask loading. The optimal solution of mass of HLW and glass in the container are give, as well as the number of canisters required for loading, normalized per tHM and per GWd. Cooling times were five or ten years before solidification.

Fuel Type	PUREX?	FIMA (%)	Mass of HLW (per canister) (kg)	Mass of glass (per canister) (kg)	Number of canisters (per tHM)	Number of canisters (per GWd)
LIFE (used PWR fuel)	No	30.510	435.0	1598.5	3.13	1.06E-02
LIFE (used PWR fuel)	No	50.147	265.5	1504.5	5.70	1.16E-02
LIFE (used PWR fuel)	No	60.265	254.5	1439.5	5.98	1.02E-02
LIFE (used PWR fuel)	No	70.528	249.0	1412.0	6.12	8.90E-03
LIFE (used PWR fuel)	No	80.196	252.0	1429.0	6.08	7.77E-03
LIFE (used PWR fuel)	No	90.045	343.0	1690.0	4.48	5.10E-03
LIFE (used PWR fuel)	No	99.441	506.0	1527.0	3.04	3.13E-03
LIFE (used PWR fuel)*	Yes	30.510	268.5	1524.5	2.33	7.86E-03
LIFE (used PWR fuel)*	Yes	50.147	259.5	1471.5	3.48	7.08E-03
LIFE (used PWR fuel)	Yes	60.265	260.5	1475.5	3.84	6.54E-03
LIFE (used PWR fuel)*	Yes	70.528	266.5	1507.5	4.13	6.00E-03
LIFE (used PWR fuel) *	Yes	80.196	280.5	1591.0	4.23	5.41E-03
LIFE (used PWR fuel)	Yes	90.045	276.5	1568.5	4.60	5.23E-03
LIFE (used PWR fuel)	Yes	99.441	443.0	1590.0	3.04	3.13E-03
LIFE (thorium)	No	30.013	610.0	1423.0	2.52	8.80E-03
LIFE (thorium)	No	50.138	501.0	1532.5	3.11	6.50E-03
LIFE (thorium)	No	60.130	491.5	1542.5	3.20	5.56E-03
LIFE (thorium)	No	70.059	508.5	1525.5	3.12	4.63E-03
LIFE (thorium)	No	80.036	538.0	1495.0	2.96	3.84E-03
LIFE (thorium)	No	90.007	566.5	1476.5	2.83	3.27E-03
LIFE (thorium)	No	94.177	546.0	1487.0	2.93	3.25E-03
LIFE (thorium)	Yes	30.013	333.0	1701.0	2.04	7.13E-03
LIFE (thorium)	Yes	50.138	318.0	1715.0	2.77	5.79E-03
LIFE (thorium)	Yes	60.130	337.5	1696.0	2.90	5.06E-03
LIFE (thorium)	Yes	70.059	369.5	1345.0	2.92	4.34E-03
LIFE (thorium)	Yes	80.036	445.0	1588.0	2.64	3.45E-03
LIFE (thorium)	Yes	90.007	452.5	1580.5	2.82	3.27E-03
LIFE (thorium)	Yes	94.177	450.0	1583.0	2.93	3.25E-03
PWR (5.0 wt %)	Yes	50 GWd/tHM	546	1487	0.188	0.00375

* Cooling time was ten years because no solution existed for five years cooling—decay heat constraint.

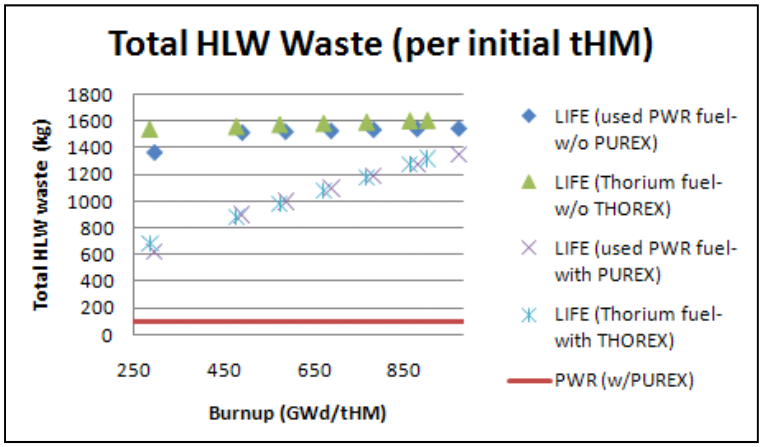

Figure 29: Total HLW waste generated per initial tHM (decay time of five years)

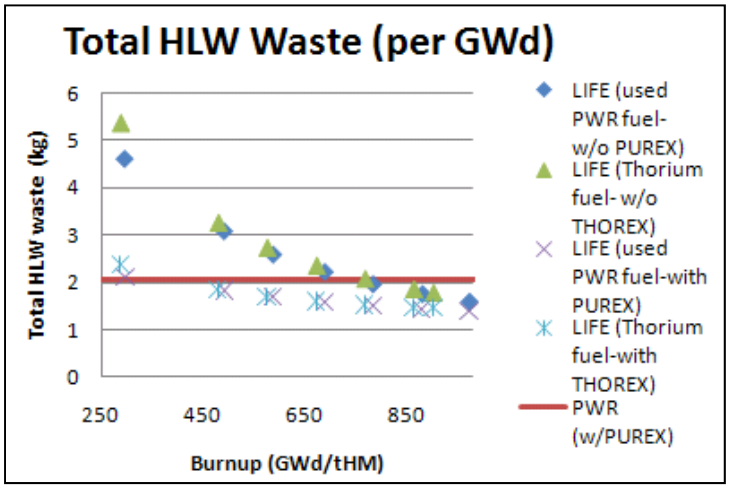

Figure 30: Total HLW generated per GWd (decay time of five years)

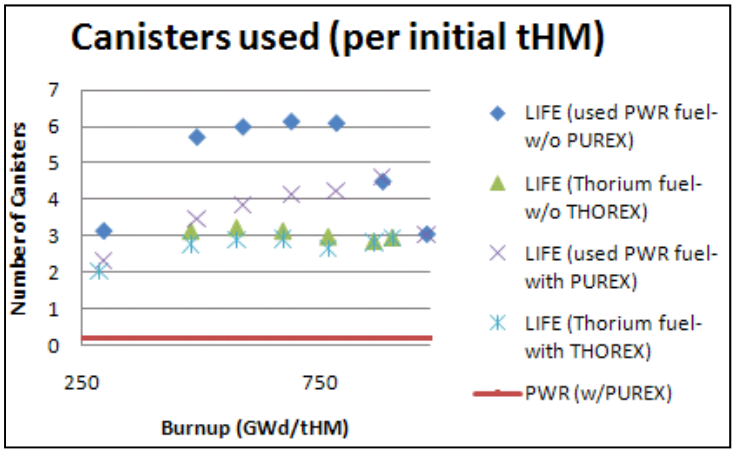

Figure 31: Fraction of canister needed to store HLW per initial tHM (decay time of five years)

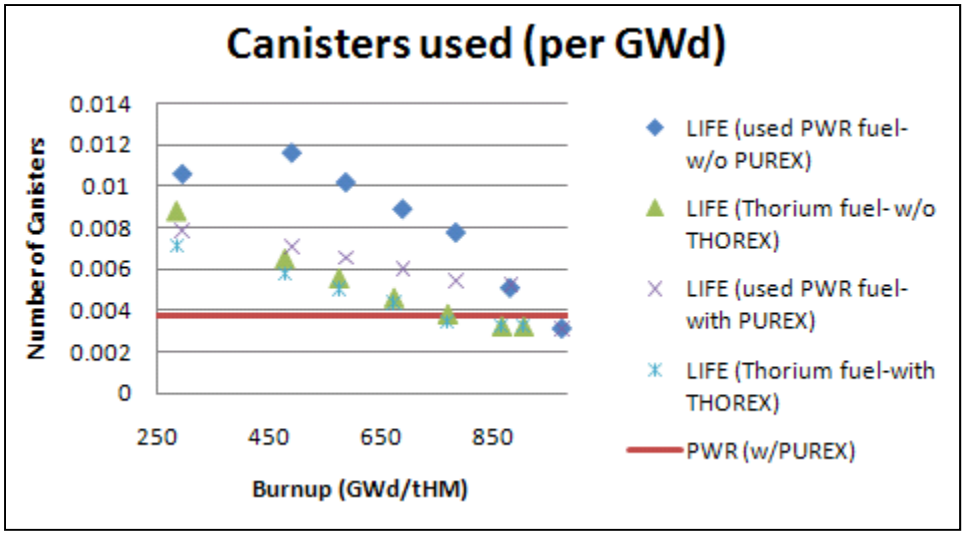

Figure 32: Fraction of canister needed to store HLW from a GWd (decay time of five years)

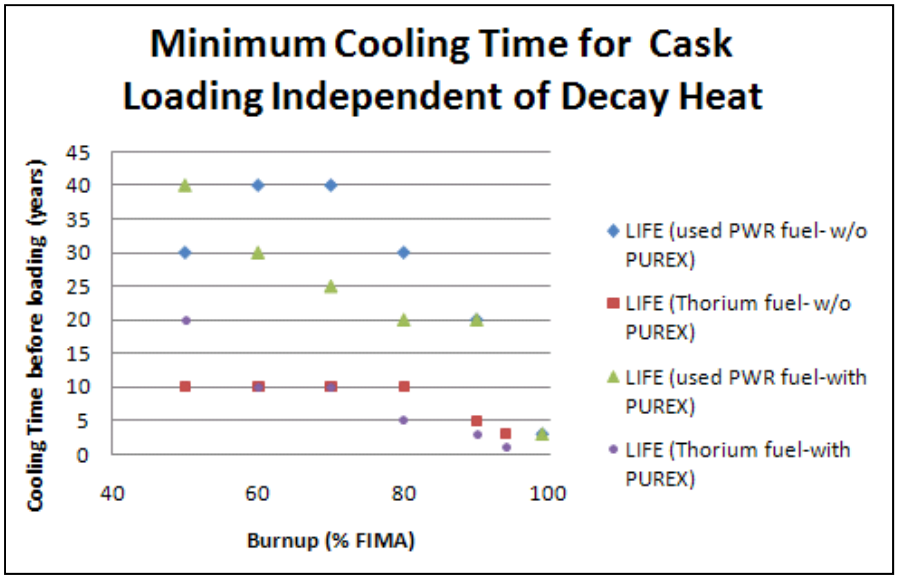

Figure 33: Minimum cooling time required for cask loading independent of decay heat

Table 7: Key statistics for cask loading with optimized cooling times. The optimal solution of mass of HLW and glass in the container are give, as well as the number of canisters required for loading, normalized per tHM and per GWd.

Fuel Type	PUREX?	FIMA (%)	Mass of HLW (per canister) (kg)	Mass of glass (per canister) (kg)	Number of canisters (per initial tHM)	Number of canisters (per GWd)
LIFE (used PWR fuel)	No	30.510	610.0	1423	2.23	0.00755
LIFE (used PWR fuel)	No	50.147	610.0	1423.0	2.48	0.00504
LIFE (used PWR fuel)	No	60.265	610.0	1423.0	2.49	0.00424
LIFE (used PWR fuel)	No	70.528	610.0	1423.0	2.50	0.00363
LIFE (used PWR fuel)*	No	80.196	592.5	1441.5	2.59	0.00331
LIFE (used PWR fuel)*	No	90.045	539.5	1494.5	2.86	0.00325
LIFE (used PWR fuel)*	No	99.441	506.0	1527.0	3.04	0.00313
LIFE (used PWR fuel)*	Yes	30.510	558.5	1474.5	1.13	0.00383
LIFE (used PWR fuel)*	Yes	50.147	527.0	1506.0	1.73	0.00352
LIFE (used PWR fuel)*	Yes	60.265	521.0	1512.0	1.93	0.00328
LIFE (used PWR fuel)*	Yes	70.528	476.0	1557.0	2.31	0.00336
LIFE (used PWR fuel)*	Yes	80.196	459.5	1574.5	2.59	0.00331
LIFE (used PWR fuel)*	Yes	90.045	445.5	1587.5	2.86	0.00325
LIFE (used PWR fuel)*	Yes	99.441	443.0	1590.0	3.04	0.00313
LIFE (thorium)	No	30.013	610.0	1423	2.55	0.00534
LIFE (thorium)	No	50.138	610.0	1423	2.57	0.00447
LIFE (thorium)	No	60.130	610.0	1423.0	2.58	0.00447
LIFE (thorium)	No	70.059	610.0	1423.0	2.59	0.00385
LIFE (thorium)	No	80.036	610.0	1423.0	2.61	0.00339
LIFE (thorium)*	No	90.007	565.5	1467.5	2.83	0.00327
LIFE (thorium)	No	94.177	546.0	1487.0	2.93	0.00325
LIFE (thorium)*	Yes	30.013	610.0	1423.0	1.12	0.00390
LIFE (thorium)*	Yes	50.138	552.5	1480.5	1.60	0.00334
LIFE (thorium)*	Yes	60.130	512.5	1520.5	1.91	0.00333
LIFE (thorium)*	Yes	70.059	484.5	1548.5	2.23	0.00331
LIFE (thorium)*	Yes	80.036	465.5	1567.5	2.53	0.00330
LIFE (thorium)*	Yes	90.007	452.5	1580.5	2.82	0.00327
LIFE (thorium)*	Yes	94.177	450.0	1583.0	2.93	0.00325

* Constrained by MoO_3 content

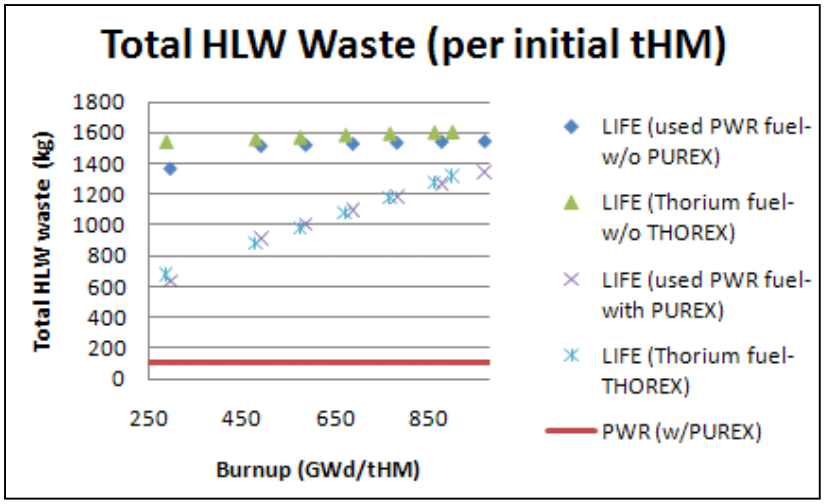

Figure 34: Total HLW waste for optimized cooling times

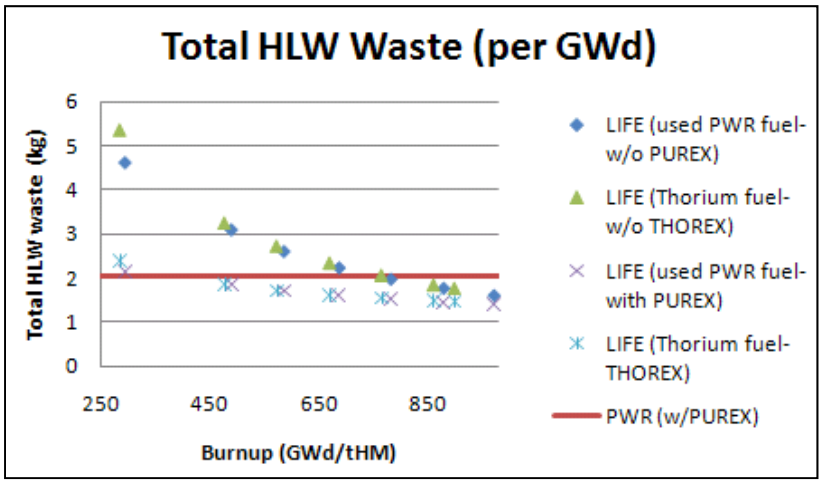

Figure 35: Total HLW (per GWd) for optimized cooling time

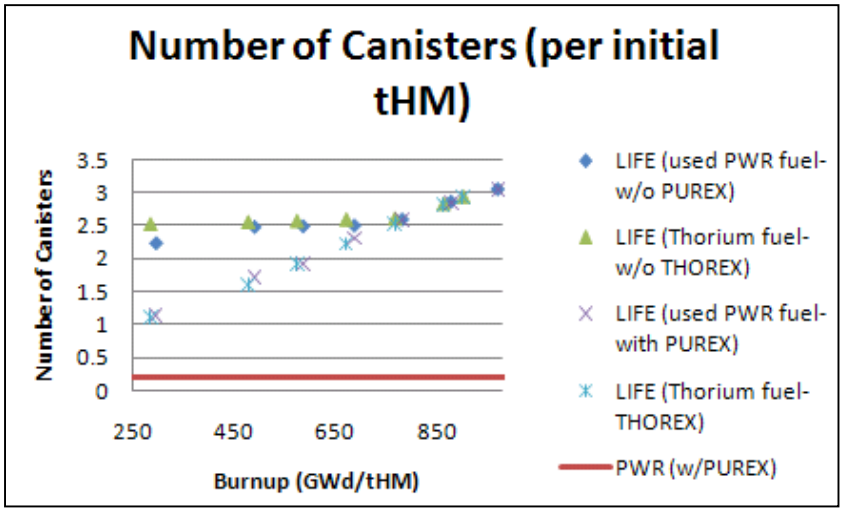

Figure 36: Number of canisters (per tHM) for optimized cooling time

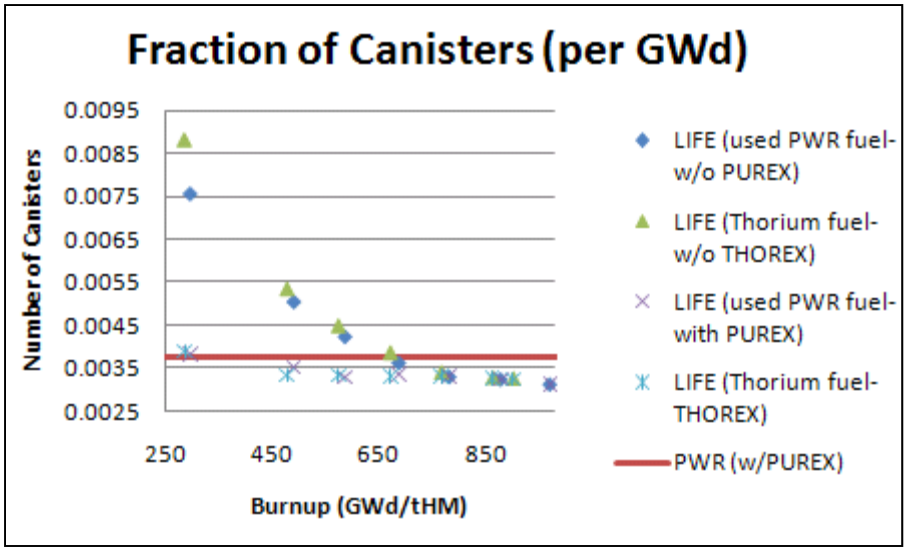

Figure 37: Number of canisters (per GWd) for optimized cooling time

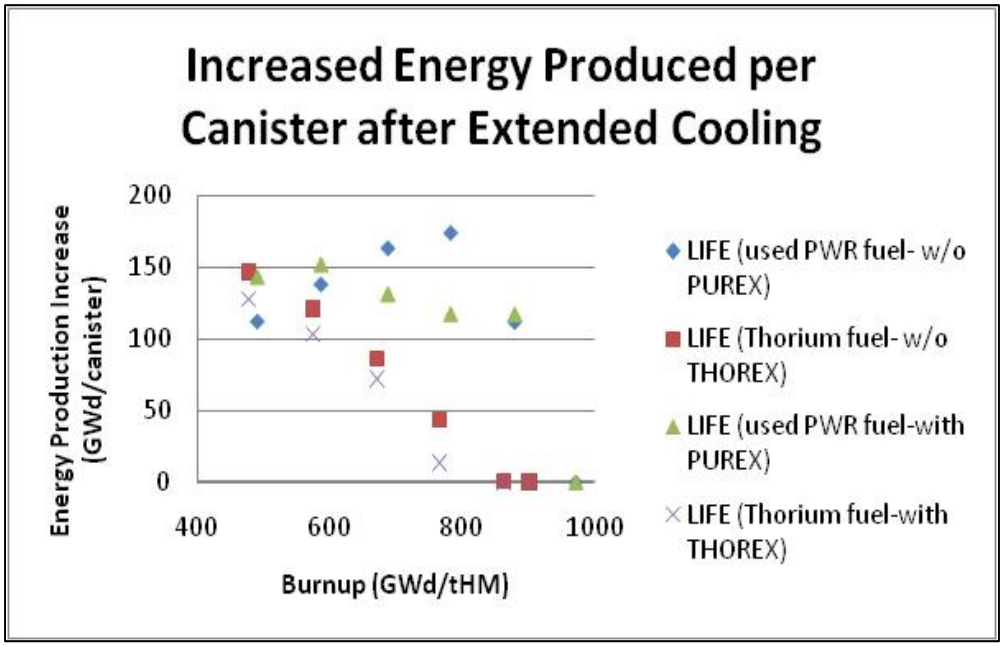

Figure 38: Increased energy production per canister after optimized cooling time

Table 8: Energy content per canister

LIFE (used PWR fuel)				LIFE (thorium fuel)			
PUREX?	Burnup (GWd/tHM)	Energy Content (GWd/Canister)	Energy Content After Optimized Cooling (GWd/Canister)	THOREX?	Burnup (GWd/tHM)	Energy Content (GWd/Canister)	Energy Content After Optimized Cooling (GWd/Canister)
No	491	86	198	No	479	155	213
No	587	98	236	No	575	180	224
No	688	112	275	No	672	216	260
No	783	129	302	No	767	260	295
No	880	196	308	No	863	306	306
No	972	319	319	No	901	308	308
Yes	491	141	284	Yes	479	173	382
Yes	587	153	305	Yes	575	198	300
Yes	688	167	298	Yes	672	230	302
Yes	783	185	302	Yes	767	290	303
Yes	880	191	308	Yes	863	306	306
Yes	972	319	319	Yes	901	308	308
PWR				Yes	50	267	267

CONCLUSIONS:

This study determined the repository performance of spent nuclear fuel from LIFE and compared to that of discharged fuel from LWR. For LIFE two fuel options were considered: (1) used fuel from LWR recovered through a dry process (AIROX); (2) thorium. The burnup level was varied between 25% and 99% FIMA for LIFE systems, while it was fixed at ~5% FIMA (50 GWd/tHM) for LWR. It was assumed that the HLW arising from each fuel cycle is conditioned and vitrified before disposal. Conditioning might or might not be preceded by PUREX or THOREX reprocessing.

The repository performance was expressed in number of canisters required to store HLW from the production of one unit energy (1 kWh). The maximum possible HLW waste load per canister was determined using linear programming techniques that allowed combination of canister design and regulatory constraints. In order to reduce the number of required canisters, spent fuel was allowed to cool long enough that decay heat was not a constraint. It was found that 40 years or less serve to the purpose.

It was found that LIFE, besides increasing resource utilizations, reduces repository space requirements, compared to LWR, when burnup reaches beyond 70% FIMA, even if no reprocessing is applied. Assuming burnup of 50% FIMA, if PUREX reprocessing is applied, LIFE spent fuel requires a maximum of 1.47E-10 canisters starting from used fuel and 1.39E-10 canisters from thorium per kWh (0.147 and 0.139 TWh per canister, respectively). A LWR requires 1.56E-10 canisters per kWh (0.156 TWh per canister). The required number of canisters decreases with fuel burnup. If uranium and plutonium are not separated from LIFE spent fuel then a maximum of 2.10E-10 canisters are required in the used fuel case and 1.96E-10 canisters in the thorium case per kWh (0.210 and 0.196 TWh per canister, respectively).

The smallest optimal solution values for HLW per canister were from the LIFE system fueled with AIROX reprocessed fuel. It benefited the greatest from the increased cooling time. An exception to this is at very high burnups of 99.417% FIMA, where the heat content was very low. Thorium fuel performed better for shorter cooling time, and both LIFE fuels behaved comparably when allowed to cool for long periods of time before solidification. Reprocessed fuels tended to perform better than non reprocessed fuels.

This study also determined the main properties (activity levels, decay heat, radiotoxicity, neptunium-237 and precursor levels, total neutron source levels, product mass, TRU mass, fissile mass, fissile fraction, and fissile plutonium fraction) of the spent fuel from each cycle as a function of time after discharge. Of particular importance to repository performance are radiotoxicity and neptunium-237 and precursor levels. Ingestion levels tended to be higher for LIFE, unless high burnups are reached. Neptunium-237 and precursor levels were higher for LIFE fueled with used LWR fuel, but much lower for LIFE fueled with thorium. Low radiotoxicity and neptunium-237 and precursor levels would reduce environmental impact. For these properties, rankings were made qualitatively based on the graphed results; the average performance for all burnups was realized. Some burnups had better or worse performance with regard to specific parameters. Further work could involve weighting certain parameters as more important than others. For instance, radiotoxicity may have more impact than fissile fraction in decision-making. Also, a method for more qualitatively ranking the data could be implemented.

However, a major exception to the general rules is the behavior of the used PWR fuel for LIFE at very high burnup. This, along with the thorium fuel at high burnup, minimized almost every category most effectively, for both normalizations. Given that the casks loaded with the

highest burnup fuel have the maximum energy content, the very high burnups offer significant repository benefits over lower burnup and used PWR fuel.

Several limitations for both components of the study should be noted. For the cask loading optimization, LIFE spent fuel is unlikely to be reprocessed using the PUREX method, as there is already high burnup from LIFE. However, some processing is necessary and the assumption of PUREX allows for a better comparison, and allows for calculation of glass frit mass needed. Additionally, it was assumed that the amount of process and corrosion chemicals required was linear proportional to the mass of HLW. Finally, heavy metals were extracted via the PUREX process for the commercial used fuel that was not also extracted for the LIFE system. Those heavy metals would still need to be disposed of in some form, even if they were refabricated into fuel and reused. Extraction was not modeled in the property comparison part of the study.

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APPENDIX

Matlab Script for Linear Programming

LPsolution.m

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%  LPSolution.m
%
% This script calls function LPsetup2.m and sets up and solves
% for the optimal solution for cask loading for thorium.
% It can be easily modified to analyze PWR and AIROX-reprocessed
% LIFE fuel, or any LIFE fuel that Origen-S depletion for decay
% cooling times have been analyzed for. Method is adapted from
% Ahn and Cheon's paper "Optimization of HLW loading in a
% vitrified from"
%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

clear all
clc

%counting variables for loops
n = 1;
i = 1;

% Burnups (for thorium LIFE fuel)
BU = [9.537e+01
1.921e+02
2.867e+02
3.821e+02
4.786e+02
5.746e+02
6.717e+02
7.669e+02
8.627e+02
9.013e+02];

inputnumber = input('What burnup position?\n'); % burnup position in BU
matrix
% used to call relevant excel input file with data from origen-s depletion
if inputnumber == 10
    input1 = 94; %refers to excel sheet
else
    input1 = inputnumber *10; %refers to excel sheet
end
BUlife = BU(inputnumber,1); %burnup to be analyzed
Mlife= 17.29405; %inital mass for LIFE system (from tbrinventory.txt from
tape 7s)

%main loop- allows for multiple cooling times or reprocessing conditions to
%be analyzed at one time
while i ~= 2
```

```
    [zeta xWPU xMoO3 xWNa20 xGNa20 TotalHLW coolingtime] = LPsetup2(input1);
%calls function to calculate parameters
    Vc = .823; %volume of canister in m3
    maxPu = 2.5; % max plutonium content
    MG = 0:.5:2000; %used to graph constraints- mass of glass
    zetamatrix = xlsread('LibrariesforLP.xls', 'zeta'); % calls library
containing interpolation values
    figure(n)
    constraint1 = 2033-MG;
    plot(MG, constraint1) %constraint 1
    title('Feasibility Region for Canister Loading') %plots figure
    xlabel('Mass of glass (kg)')
    ylabel('Mass of HLW (kg)')
    axis([0 2000 0 3000])
    hold on
    constraint2 = 2393.7-1.505*MG; %calculates constraint 2
    plot(MG,constraint2, 'r') %constraint 2
    fplot('2932.3-1.505*x', [0 2000], 'r') %constraint 2
    fplot('.1765*x', [0 2000], 'g') %constraint 3
    constraint3 = .4286*MG;
    plot(MG, constraint3, 'g') %constraint 3

    %Calculating constraint 4 from Zeta (via interplation)
    if zeta < zetamatrix(1,1)
        fprintf('It is defintely not a constraint!  You win!\n')
        K1 = -1;
        K2 = -1;
    elseif zeta < zetamatrix(2,1)
        K1 = (zeta - zetamatrix(1,1))/(zetamatrix(2,1)-
zetamatrix(1,1))*(zetamatrix(2,2)-zetamatrix(1,2))+zetamatrix(1,2);
        K2 = (zeta - zetamatrix(1,1))/(zetamatrix(2,1)-
zetamatrix(1,1))*(zetamatrix(2,3)-zetamatrix(1,3))+zetamatrix(1,3);
    elseif zeta < zetamatrix (3,1)
        K1 = (zeta - zetamatrix(2,1))/(zetamatrix(3,1)-
zetamatrix(2,1))*(zetamatrix(3,2)-zetamatrix(2,2))+zetamatrix(2,2);
        K2 = (zeta - zetamatrix(2,1))/(zetamatrix(3,1)-
zetamatrix(2,1))*(zetamatrix(3,3)-zetamatrix(2,3))+zetamatrix(2,3);
    elseif zeta < zetamatrix (4,1)
        K1 = (zeta - zetamatrix(3,1))/(zetamatrix(4,1)-
zetamatrix(3,1))*(zetamatrix(4,2)-zetamatrix(3,2))+zetamatrix(3,2);
        K2 = (zeta - zetamatrix(3,1))/(zetamatrix(4,1)-
zetamatrix(3,1))*(zetamatrix(4,3)-zetamatrix(3,3))+zetamatrix(3,3);
    elseif zeta < zetamatrix (5,1)
        K1 = (zeta - zetamatrix(4,1))/(zetamatrix(5,1)-
zetamatrix(4,1))*(zetamatrix(5,2)-zetamatrix(4,2))+zetamatrix(4,2);
        K2 = (zeta - zetamatrix(4,1))/(zetamatrix(5,1)-
zetamatrix(4,1))*(zetamatrix(5,3)-zetamatrix(4,3))+zetamatrix(4,3);
    elseif zeta < zetamatrix (6,1)
        K1 = (zeta - zetamatrix(5,1))/(zetamatrix(6,1)-
zetamatrix(5,1))*(zetamatrix(6,2)-zetamatrix(5,2))+zetamatrix(5,2);
        K2 = (zeta - zetamatrix(5,1))/(zetamatrix(6,1)-
zetamatrix(5,1))*(zetamatrix(6,3)-zetamatrix(5,3))+zetamatrix(5,3);
    elseif zeta < zetamatrix (7,1)
        K1 = (zeta - zetamatrix(6,1))/(zetamatrix(7,1)-
zetamatrix(6,1))*(zetamatrix(7,2)-zetamatrix(6,2))+zetamatrix(6,2);
        K2 = (zeta - zetamatrix(6,1))/(zetamatrix(7,1)-
zetamatrix(6,1))*(zetamatrix(7,3)-zetamatrix(6,3))+zetamatrix(6,3);
```

```
    else
        fprintf('Zeta is too high for a feasible solution to exist :( Try
letting it cool some more. Wah wah\n')
        K1 = 0;
        K2 = 0;
    end
    constraint4 = MG*K1+K2; %plots constraint4 (heat)
    plot(MG,constraint4, 'c')
    constraint5 = maxPu*Vc/xWPU*MG; %constraint 5(plutonium)
    plot(MG, constraint5, 'y')
    constraint6 = (.02 / (xMoO3-.02))*MG; % constraint 6 moly
    plot(MG, constraint6, 'm')
    constraint7 = (.1- xGNa20)/(xWNa20-.1)*MG; %constraint 7 sodium
    plot(MG, constraint7, 'k')
    hold off
    %%finds intersection point of optimal point
    %%% *******IMPORTANT********
    %% YOU ***MUST*** change the constraints to find the intersection
    %% based on the specific feasibility solution.  This is NOT
    %% done automatically.
    [row col] = size(constraint1);
    for i = 1:1:col
        if abs(constraint4(i) - constraint1(i)) < .5
            MGlass = MG(i);
            MWaste = constraint4(i);
        end
    end
    Enormal =  (BUlife * Mlife); %energy normalization
    fprintf('Optimum loading of a canister %.2d kg of HLW and %.4d kg of
glass\n', MWaste, MGlass)
    NumCanisters = [TotalHLW/MWaste TotalHLW/MWaste (7.81e4/1000)/585
(7.81e4/1000)/585]; %per MTU for LIFE and PWR ref. Ahn
    Wastegen = [TotalHLW/Mlife TotalHLW/Enormal (7.81e4/1000)
(7.81e4/1000)/28 BUlife];
    NumCanistersn = [NumCanisters(1)/Mlife NumCanisters(2)/Enormal
NumCanisters(3) NumCanisters(4)/28];
    n = n + 1;
    i = input('Type 1 to continue the analysis for a different cooling
time\nType 2 to end process\n');
    output = [Wastegen NumCanistersn MWaste MGlass]; %useful variable that
outputs normalized total waste generated and canisters required
end
```

LPsetup2.m

```
function [zeta xWPU xMoO3 xWNa20 xGNa20 TotalHLW Time] = LPsetup(sent)
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% LPsetup2
%
% This function is used to calculate5 parameters nescessary for linear
programming
% analysis of maxium loading of HLW from LIFE.  Parameters calculated are
% zeta (decay heat/kg), xWPU (weight fraction of plutonium), xMoO2
% (moly-oxide fraction), xWNa2O (sodium dioxide fraction), and xGNA20
% (assumed to be 0).  Method is adapted from Ahn and Cheon's paper
"Optimization of HLW
% loading in a vitrified from"
%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
sent = int2str(sent); %changes input to string to import from excel
[Amount Nuclides] = xlsread('canisterinputsTHORcheck.xls', sent); %reads
initial compositions

% Processing options
i = input('Type 1 for PUREX Reprocessing or 2 for THOREX: \n');
if (i == 1)||(i ==2);
    [Amount Nuclides]= PUREX(Amount, Nuclides, i); %calls processing function
PUREX.m
end

[OxidationState Nuclidestest] = xlsread('LibrariesforLP.xls',
'Nuclidestest'); %gets library information about Nuclides
HalfLives = xlsread('LibrariesforLP.xls', 'HalfLives'); %gets more library
information about nuclides
[rowN colN] = size (Nuclides);
[rowT colT] = size (Nuclidestest);
[rowA colA] = size (Amount);
[rowH colH] = size (HalfLives);
conversion = 1.602e-13; % conversion for W/MeV
NA = 6.022e23; %Avogadros number
xWPU = 0; %initialize weight fraction of plutonium variable, xPU
xMoO3 = 0; %initialize weight fraction of moly trioxide variable, xMoO3
Time = input('Please input the cooling time: \n'); %designates time of
cooling before vitrification

for i = 1:1:colA
    if Time == Amount(1, i)
        AmountNew (:, 1)= Amount(:, i); % creates col vector with just data
to be analyzed
    end
end

for i = 2:1:rowN  % converts name to atomic number for nuclide and adds in
oxidation number in to the growing matrix NewNuclides
    count = 0;
    for j = 1:1:rowT
     tester(1) = Nuclides(i);
     if strcmp (tester(1), Nuclidestest(j))
```

```
            NumberNuclides(i, 2) = Amount(i,1);
            NumberNuclides(i, 3) = Amount(i,2);
            NumberNuclides (i, 1) = OxidationState(j,1);
            NumberNuclides (i, 4:5) = OxidationState (j, 2:3);
            count = 1;
        end
    end
    if count == 0
        display(tester(1))
    end
end



for i = 2:1:rowN %adds halflife, decay constant, and decay energy data to
NumberNuclides
    for j = 1:1:rowH
        if NumberNuclides(i, 1:3) == HalfLives(j,1:3)
            NumberNuclides(i, 6:8) = HalfLives(j, 4:6);
        end
    end
end

NuclideMatrix = [NumberNuclides, AmountNew];
%concatenates the matrices with data about composition
NuclideMatrix (: , 10) = NuclideMatrix(:,9)./
NuclideMatrix(:,2).*1./NuclideMatrix(:,4).*(NuclideMatrix(:,4).*NuclideMatrix
(:,2)+16*NuclideMatrix(:,5));
%stoichiometry calcualtion of oxide form
NuclideMatrix(rowN+1,9) = (sum(NuclideMatrix(:, 9))-5);
%total inital composition
NuclideMatrix(1, 10) = 0;
NuclideMatrix(rowN+1,10) = (sum(NuclideMatrix(:, 10)));
%total oxide composition

%check for failed nuclide upload- these would have to be manually added ot
%the relevant libraries
for i = 2:1:rowN
    if NuclideMatrix (i, 1)== 0
        fprintf('The following element does not exist in the library: \n')
        disp(Nuclides(i))
        fprintf('\n')
    elseif NuclideMatrix (1:3) == [0 0 0]
        fprintf('This element has a nuclide is not in the library:')
        disp(Nuclides(i))
        fprint('\n')
    end
end

%assumed process chemicals. this should be constant- atomic A and z
%designated
%these process chemicals are ONLY valid for thorium. based of of ahns paper
%and processing required for tHM for PWR. you must change for any other
%analyis
Process = [23 11 426540.8   573164.2; 31 15 7483.506 20946.2;56 26 79976.4
114252; 58 28 20946.2   26658.8; 54 24 20755.78 30276.78];
```

```
Processtotal = [sum(Process(:,3)) sum(Process(:,4))];
%grandtotals of oxygen and total
Grandtotals = [(NuclideMatrix(rowN+1, 10)-NuclideMatrix(rowN+1, 9)+
sum(Process(:,4))-sum(Process(:,3))); (sum(Process(:,4))+
NuclideMatrix(rowN+1, 10))];

NuclideMatrix(:,11) = NuclideMatrix(:,9)/Grandtotals(2); %fractional
compostion
NuclideMatrix(:,12) = NuclideMatrix(:,10)/Grandtotals(2); %fractional oxide
composition
%calulates individual zeta
NuclideMatrix(:,13) = conversion * NA * NuclideMatrix (:,8).* NuclideMatrix
(:,7).* NuclideMatrix(:, 11)./(NuclideMatrix(:,2)/1000);
NuclideMatrix(1, 13) = 0;
NuclideMatrix(rowN+1,13) = sum(NuclideMatrix(2:rowN,13)); % total zeta

%calculates xWPU and xMoO3
for i = 1:1:rowN
    if NuclideMatrix(i, 1) == 94;
        xWPU = NuclideMatrix(i,11) + xWPU;
    elseif NuclideMatrix(i,1) == 42
        xMoO3 = xMoO3 + NuclideMatrix(i,12);
    end
end

TotalHLW = Grandtotals(2)/1000;
xWNa20 = Process (1, 4)/Grandtotals(2);
xGNa20 = 0;
zeta = NuclideMatrix(rowN+1,13);

--------------------------------------------------------------------------
```

PUREX.m

```
function [NewAmount NewNuclides] = PUREX(Amount, Nuclides, thorchoice)

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% PUREX.m
%
% This function applys reprocessing assumptions to input data.
% For PUREX, uranium and plutonium are removed (minus assumed mass escaped
% into the waste stream as well as gaseous fissioin products.
% For THOREX, U, Pu, and th are removed (minus escape into the waste
% stream) as well as the gaseous fission products.
%
% This function is called by LPsetup2.m
%
% % %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

[rowN colN] = size(Amount);
NewAmount = zeros(rowN,1); %new matrix with new masses

%applies PUREX
if (thorchoice ==1)
    for m = 1:1:rowN
        if (strcmp(Nuclides(m,1), 'pu')) %removes Pu
            NewAmount(m, 1:2) = Amount(m, 1:2);
            NewAmount (m,3:colN) = .2966/100*Amount(m, 3:colN);
        elseif (strcmp(Nuclides(m,1), 'u')) %removes U
            NewAmount(m, 1:2) = Amount(m, 1:2);
            NewAmount (m,3:colN) = .604/100*Amount(m, 3:colN);
        elseif (strcmp(Nuclides(m,1), 'xe'))||(strcmp(Nuclides(m,1),
'ne'))||(strcmp(Nuclides(m,1), 'rn'))||(strcmp(Nuclides(m,1),
'i'))||(strcmp(Nuclides(m,1), 'kr'))||(strcmp(Nuclides(m,1), 'he'))
            NewAmount(m, 1:2) = Amount(m, 1:2); %removse gaseous Fission
products
            NewAmount (m,3:colN) = zeros(1, colN-2);
        else
            NewAmount(m, 1:2) = Amount(m, 1:2);
            NewAmount (m,3:colN) = Amount(m, 3:colN);
        end
    end
else %applies THOREX conditions
    for m = 1:1:rowN
        if (strcmp(Nuclides(m,1), 'pu')) %removes Pu
            NewAmount(m, 1:2) = Amount(m, 1:2);
            NewAmount (m,3:colN) = .2966/100*Amount(m, 3:colN);
        elseif (strcmp(Nuclides(m,1), 'u')) %removes U
            NewAmount(m, 1:2) = Amount(m, 1:2);
            NewAmount (m,3:colN) = .604/100*Amount(m, 3:colN);
            elseif (strcmp(Nuclides(m,1), 'th')) %removes th- ***.700% is an
assumption, this process is not fully developed***
            NewAmount(m, 1:2) = Amount(m, 1:2);
            NewAmount (m,3:colN) = .7/100*Amount(m, 3:colN);
        elseif (strcmp(Nuclides(m,1), 'xe'))||(strcmp(Nuclides(m,1),
'ne'))||(strcmp(Nuclides(m,1), 'rn'))||(strcmp(Nuclides(m,1),
'i'))||(strcmp(Nuclides(m,1), 'kr'))||(strcmp(Nuclides(m,1), 'he'))
            NewAmount(m, 1:2) = Amount(m, 1:2); %removes xe
```

```
            NewAmount (m,3:colN) = zeros(1, colN-2);
        else
            NewAmount(m, 1:2) = Amount(m, 1:2);
            NewAmount (m,3:colN) = Amount(m, 3:colN);
        end
    end
end
NewNuclides = Nuclides;
```
