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Neutronic Analysis of Molten Salt Fast Reactor Utilizing Different Initial Fuel Loading

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Abstract: ***Molten salt reactors have the capability of operating in the thermal, epithermal, and fast neutron spectra and can also use different fuels to produce fission. These reactors utilize the thorium fuel cycle using molten fluoride or chloride salts as coolants. In this work molten salt fast reactor is simulated using MCNP6. Three initial fuels are studied, ^{233}U, ^{235}U, ^{239}Pu. The model is used to evaluate the flux distribution in the core and blanket, as well as safety parameters namely Doppler and density coefficients. The initial breeding ratio is also estimated. Burnup is performed for a period of six month. During the Burnup, the variation in effective multiplication factor is estimated. Moreover, material evolution during the period of burnup is studied for the three types of fuel.***

Keywords: Molten Salt Reactor, MCNP6, Breeding Ratio, Material Evolution

1. Introduction

The Generation-IV International Forum (GIF) identified the molten salt reactor (MSR) concept as one of the reference nuclear systems, to be considered for future deployment [1]. In a molten salt reactor, the fuel is dissolved in a molten fluoride or chloride coolant. The concept started by the molten salt breeder reactor project [2], then extensive studies n which different core arrangement, reprocessing methods and salt compositions were investigated, resulting the innovative molten salt fast reactor (MSFR) [2-6].the MSFR is different from older molten salt reactor in that it contains no graphite moderator.

In addition to the reduced cost of fuel fabrication compared with solid-fuelled reactors, liquid fuel is insensitive to radiation damage that can limit fissile and fertile material utilization, it is also possible to remove fission products continuously as well as adding makeup fuel as needed, which eliminates the need for providing excess reactivity, and employ a homogeneous isotopic composition of fuel in the reactor. The MSFR, with a fast neutron spectrum and operated in the thorium fuel cycle, may be started either with ^{233}U, ^{235}U, ^{239}Pu and/or transuranic elements (TRU) as initial fissile load [2-6].

Molten salt reactors have the capability of operating in the thermal, epithermal, and fast neutron spectra and can also use different nuclear fuels to produce fission. They rely on a thorium blanket to breed ^{233}U as illustrated in the following equation:

$$^{232}Th + {}^{1}n \xrightarrow{Capture} {}^{233}Th \xrightarrow{\beta\text{-}Decay} {}^{233}Pa \xrightarrow{\beta\text{-}Decay} {}^{233}U \qquad (1)$$

^{233}Pa is extracted by an onsite chemical processing system along with any other fission products. ^{233}Pa has a 27 day half-life before it decays to ^{233}U which and can be extracted and reinserted into the core.

The MSFR plant consists of the fuel circuit, the intermediate circuit and the power conversion circuit. In this work we are concerned with the first circuit; this circuit contains the fuel salt during power generation and includes the core cavity, pump and heat exchangers. This circuit is modeled using MCNP6 [7] and, cross section data used from the Evaluated Neutron Data File library, ENDF/B-VII.1 [8]. Three types of fuel are used as a starter; ^{233}U, ^{235}U, ^{239}Pu. Comparison between these fuels includes flux distribution in core and blanket, breeding ratio, feedback coefficient including density coefficient and Doppler coefficient, as well as kinetic parameters (effective delayed neutron fraction, and neutron generation time). Burnup is performed for six month to estimate the amount of isotopes need to be compensated for or removed from the core during this period.

Reactor Description

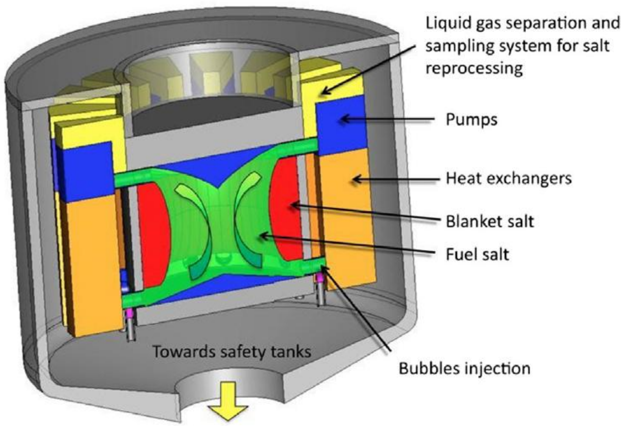

Figure 1: A Schematic Diagram of the MSFR

The reference MSFR is a 3000 MWth reactor which utilizes fluoride salt and the thorium fuel cycle. The fuel is reprocessed as part of the normal reactor where a small fraction of the molten salt is reprocessed for fission product removal and then returned to the reactor [2].

The core of the MSFR is a cylinder with the diameter equal to the height, surrounded radially by a fertile blanket, and a boron carbide layer. Reflectors are provided radially and axially in the form of a Ni-based alloy. Safety tanks are located under the core where salt draining system allows emptying the core for maintenance or in case of emergency. A sketch of the fuel circuit layout is presented in Figure 1.

The fuel salt is composed of LiF, 77.5 mole%, and a mixture of heavy nuclides $(HN)F_3$ and $(HN)F_4$ (for 22.5 mole%), the heavy nuclides initially composed of fertile thorium and fissile matter. This mixture is proposed in the frame of the EVOL project (Evaluation and Viability Of Liquid fuel fast reactor system) [6]. The MSFR can be operated with widely varying fuel compositions, thanks to its online fuel control and flexible fuel processing: its initial fissile load may comprise ^{233}U, ^{235}U-enriched natural uranium (between 5% and 30%), or the transuranic (TRU) elements currently produced by PWRs. This fuel salt composition of the MSFR with 22.5 mol% of heavy nuclei leads to a fast neutron spectrum in the core, as shown in figure 2, where the fast neutron spectrum of the reference MSFR is compared to the spectra of two solid-fuel reactors: a sodium-cooled fast neutron reactor (SFR) and a thermal pressurized water reactor (PWR).

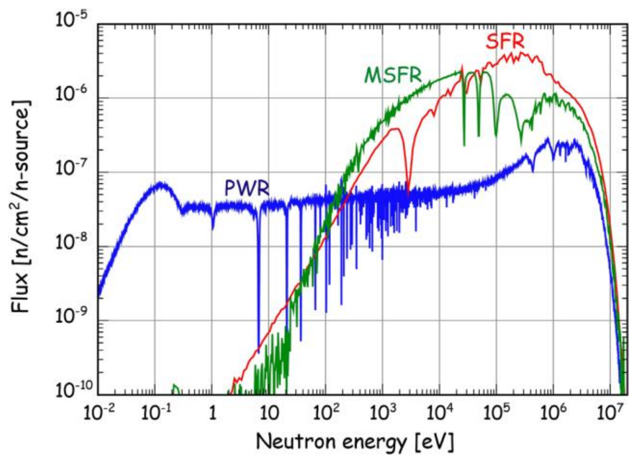

Figure 2: Fast neutron spectra of the reference MSFR (green curve) and of a sodium -cooled fast neutron reactor (SFR- red curve) compared to the thermal spectrum of a pressurized water reactor (PWR - blue curve) [2]

The fertile blanket serves as radial reflector and as a neutron shield to protect the external components of the fuel loops (pipes, heat exchangers). In addition to this protection function. The salt in the blanket is of the same type as the one in the core but with 22.5 mol% of ^{232}Th and without any initial fissile material. The fertile blanket is used to improve the breeding capabilities of the reactor, since the thorium present in the fertile salt is exposed to the core neutron flux, it will generate the ^{233}U fissile element; this ^{233}U is extracted completely in six month. In both the fuel and the fertile blanket salt, lithium is enriched in ^{7}Li up to 99.999. The blanket have an external layer of B_4C on the outer wall to further reinforce the neutronic shielding.

The structural materials surrounding the core have to bear a high neutron flux coupled with high temperatures. For these components nickel Hastelloy [2] is used, this Ni-based alloy contains W and Cr and is detailed in table 1

Table 1: Composition of Ni-Based Alloy Used as Reflector in MSFR

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

Model and Calculation Procedure

Geometry and Model

The model chosen to be studied here is the model of the EVOL project [2, 6]. An Axial-symmetric representation of the MSFR primary circuit, used here, with dimension is shown in figure 3. In this model input and output channel as well as heat exchangers and pumps are modeled as fuel with the same composition as the core.

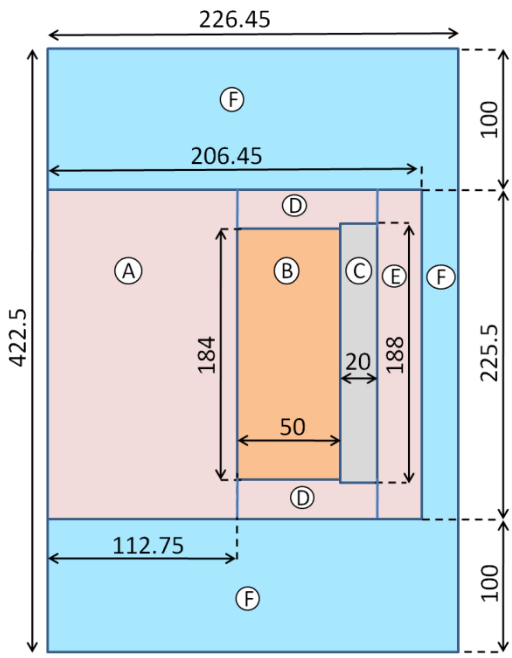

Figure 3: Axial-symmetric representation of the MSFR primary circuit (A: core; B: blanket; C: B_4C shield; D: input and output channels; E: representation of heat exchangers and pumps; F: reflector)

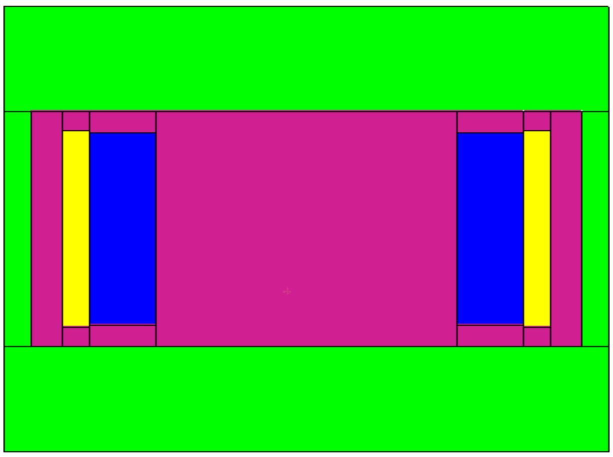

Figure 4: MCNP Model of MSFR

MCNP6 Monte Carlo code is used to construct a model for the MSFR, the model is illustrated in figure 4. 10 million neutron histories were used to perform the calculations, 20000 neutron per cycle and 500 active cycles. Cross section data are from the Evaluated Neutron Data File library, ENDF/B-VII.1. KOPTS card is used to estimate kinetic parameters like delayed neutron fraction and neutron generation time. Bunrup is performed for six months in 10 steps.

Initial Fuel Loading

In this work three types of initial loadings are considered; ^{233}U, ^{235}U, and ^{239}Pu. The mass fractions for each type of fuel, with the accompanying salt, are illustrated in table 2. These values were proposed by Green [9] in a study of initial fuel loading for MSFR.

Table 2: Initial Fuel Mass Fraction (wt%)

Isotope \ Initial Fuel	Th-^{233}U	Th-^{235}U	Th-^{239}Pu
^{233}Th	51.37	47.16	47.51
^{233}U	7.04	--	--
^{235}U	--	11.29	--
^{239}Pu	--	--	11.56
^{19}Fl	35.58	35.54	34.88
^{7}Li	6.015	6.01	6.05
^{6}Li	6×10^{-5}	6×10^{-5}	6×10^{-5}

Material Density

The physical properties of fuel salt will affect the operating temperature of the reactor. The salt melting point is 565 °C while the temperature of structural material performance is limited to 800°C [2]. The fuel salt temperature in this simulation is set at 700 °C. The density of fuel salt can be estimated from the following equation [2]:

$$\rho(gm/cm^3) = 4.094 – 8.82\times10^{-4}\,(T_{(K)} - 1008) \qquad (2)$$

The densities of various materials, used in this study, are given in table 3.

Table 3: Densities of Various Materials Used in the Model

Material	Density (gm/cm^3)
Fuel salt	4.1249
Blanket	4.1249
B_4C shield	2.52
Ni-Based Alloy	10

Numerical Results

Model Validation

The model was validated using data from a benchmark [2], the multiplication factor resulting from MCNP6 model was compared to the result of the benchmark, and the results are shown in table 4.

Table 4: Comparison of multiplication factor with previous study

Present study	Previous study
1.02182	1.02141

Flux Distribution

The flux distribution for each energy group was also calculated using 442 energy groups ranging form 1E-10 to 100 MeV [9], and the results are shown in figure 5 for ^{233}U initial loading, figure 6 for ^{235}U initial loading, and figure 7 for ^{239}Pu initial loading.

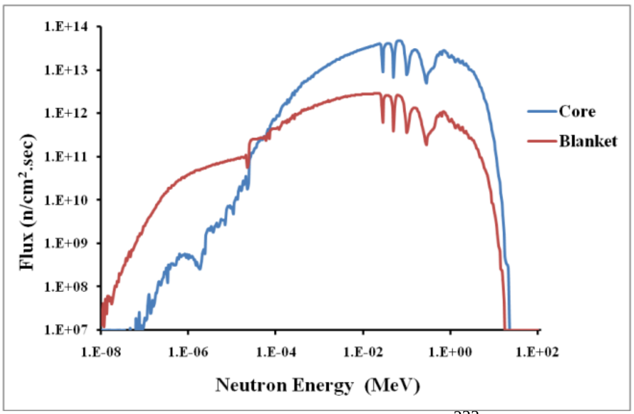

Figure 5: Neutron flux spectrum of the ^{233}U-operated MSFR

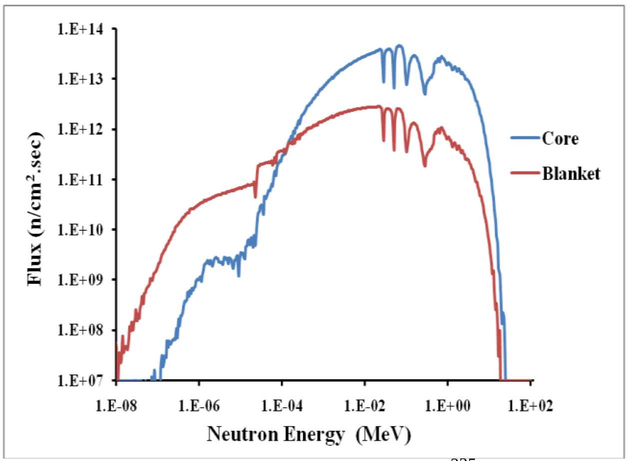

Figure 6: Neutron flux spectrum of the ^{235}U-operated MSFR

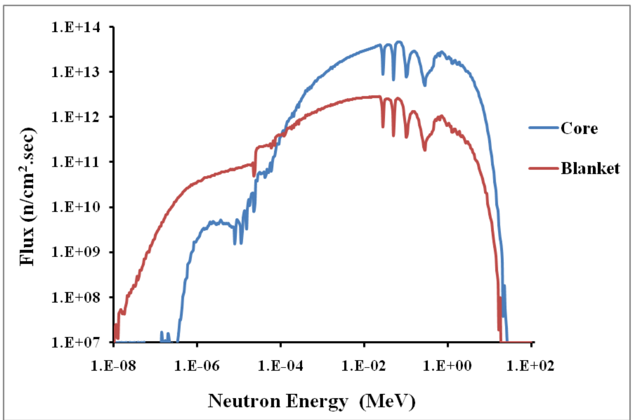

Figure 7: Neutron flux spectrum of the ^{239}Pu-operated MSFR

It can be seen from these figures the similarity in behavior which result in similar operating conditions. The flux depressions seen between 10 keV and 1 MeV are due to parasitic absorption at resonance energies of ^{19}F, present in the fuel; figure 8 illustrates the absorption cross section of ^{19}F, ^{6}Li, and ^{7}Li.

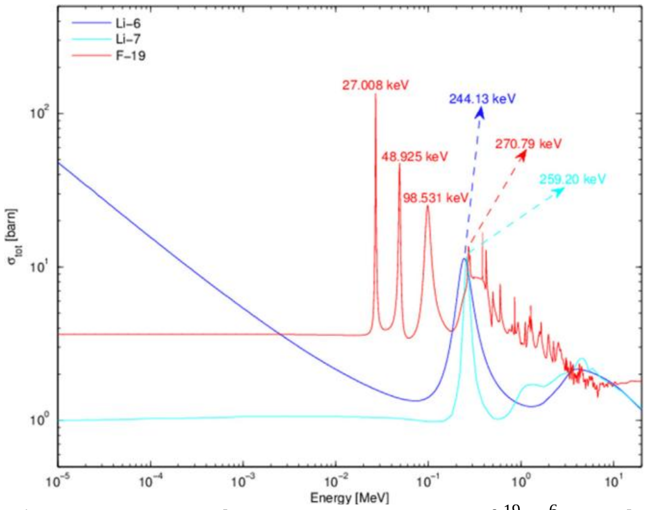

Figure 8: Neutron absorption cross section of ^{19}F, ^{6}Li, and ^{7}Li [2]

To study the distribution of flux in the reactor a mesh tally superimposed on the model geometry was introduced to estimate the flux distribution in the reactor regions. The result is shown in figure 9.

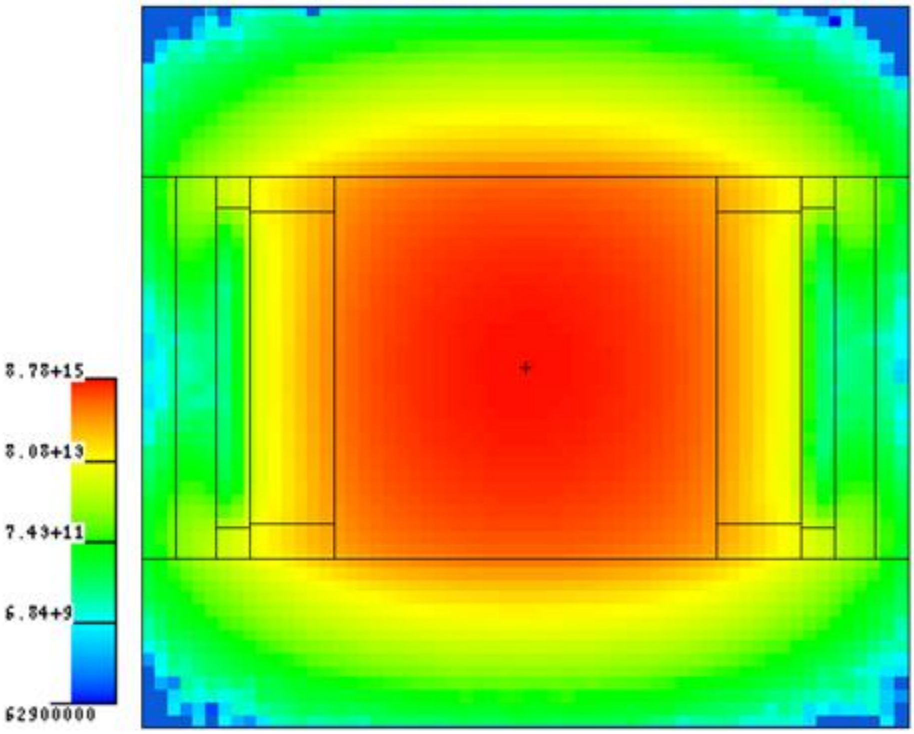

Figure 9: Neutron flux distribution in MSFR

Thermal feedback coefficients

The Doppler coefficient was estimated by a comparison of two Monte Carlo runs with fuel temperature at 900 and 1200 K. The density coefficient (or void coefficient) was calculated by reducing the fuel density by 5% (from nominal value), then calculate the corresponding temperature from equation 2. The results are shown in table 5. It can be seen that the ^{233}U starter fuel have the best safety parameters followed by ^{235}U then ^{239}Pu.

Table 5: Doppler and Density Coefficients (pcm/^{o}K)

Coefficient	^{233}U	^{235}U	^{239}P
Doppler	-4.15	-3.2	-2.82
Density	-3.9	-3.5	-3.04
Total	-8.08	-6.07	-5.86

Breeding Ratio

The initial breeding ratio (BR) is calculated using the formula [2]:

$$BR = \frac{Capture\ \ Rate\ \ in\ Th{-}233}{(Capture\ \ Rate + Fission\ \ Rate\,)\ in\ initial\ \ fuel} \tag{3}$$

An F4 tally [7] was introduced to calculate the capture and fission rates for the required nuclides, and perform the calculations using equation 3. The results are shown in table 6. The results shows that 239Pu starter core has the highest breeding ratio followed by 233U and finally 235U.

Table 6: Breeding ratio for each type of initial fuel

^{233}U	^{235}U	^{239}P
0.949	0.637	0.984

Kinetic parameters

To estimate the kinetic parameters KOPTS card of MCNP6 [10], which calculates the adjoint weighted kinetic parameters effective delayed neutron fraction (β_{eff}) and neutron generation time (Λ) in a single run, was used for each type of fuel the results are shown in table 7. Λ is much smaller for plutonium starter fuel than uranium starter, that is because of the larger thermal absorption cross sections in Pu, the slower neutrons are preferentially absorbed in comparison to U fuel resulting in a shorter prompt neutron lifetime , and hence shorter mean generation time.

Table 7: Kinetic parameters fo various initial fuels

Parameter	^{233}U	^{235}U	^{239}P
B_{eff}(pcm)	311	787	206
Generation time (μsec)	1.01795	0. 773	0. 752

Burnup Results

Burnup calculations were performed for six month in 10 time steps to evaluate the change in multiplication factor as well as the fissile material evolution in core and blanket.

The change of multiplication factor with burnup is shown in figure 10. It can be seen that with no compensation for burned fuel the multiplication factor will decrease. However for the ^{239}Pu starter the value of K_{eff} decreases to 1.0327, which means that, at the end of six month period this core is still capable of achieving criticality with no fuel compensation. On the contrary, K_{eff} decreases to 0.99524 for ^{233}U starter and to 0.99772 for ^{235}U starter; which means that compensation will be needed for these core at about 90 days as shown in figure 8. The material evolution is discussed in the following section.

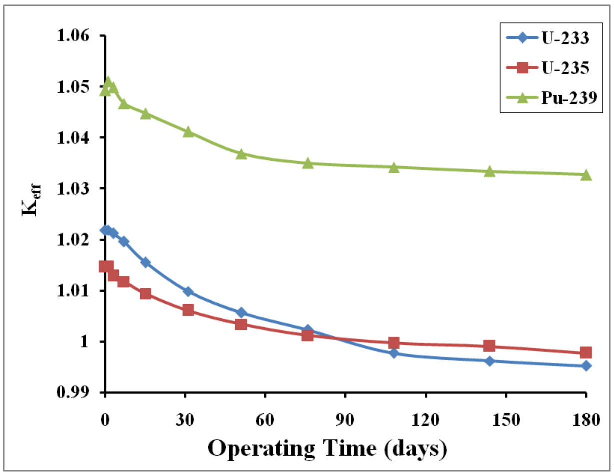

Figure 10: Change in Effective Multiplication Factor with Burnup

Material Evolution

The isotopes evolution in core for ^{233}U, ^{235}U, and ^{239}Pu initial fuels are shown in figure 11, 12 and 13 respectively. For the core with ^{233}U starter, the ^{233}U is reduced by only 3% due to buildup from thorium transmutation. ^{233}Pa is produced from ^{232}Th transmutation as a step to produce ^{233}U (Eq. 1). Other than that, only isotopes of uranium are produced with the largest production for ^{234}U which can absorb neutron to become ^{235}U. The amount of ^{234}U produced, in a 233U starter core, is 89kg, which is the largest compared to the amount produced in the other two cores.

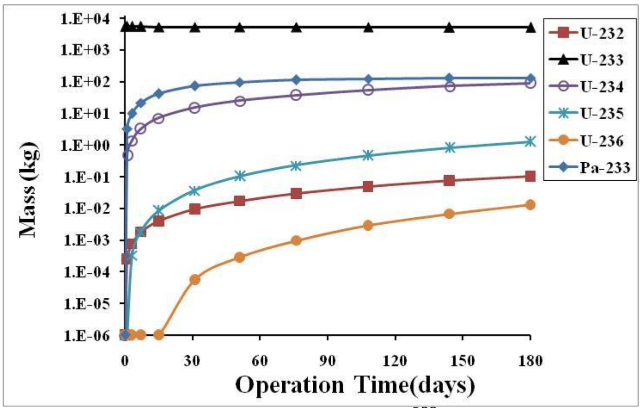

Figure 11: Isotopes Evolution for ^{233}U Starter Core

On the other hand, in ^{235}U starter core, ^{235}U is reduced by about 8.7%, while an amount of 357 kg ^{233}U is produced in 6 month. Other isotopes include uranium, ^{238}Pu, ^{239}Pu, ^{237}Np, ^{238}Np and of course ^{233}Pa. Except for ^{233}U and ^{236}U other isotopes are produced in very small amounts.

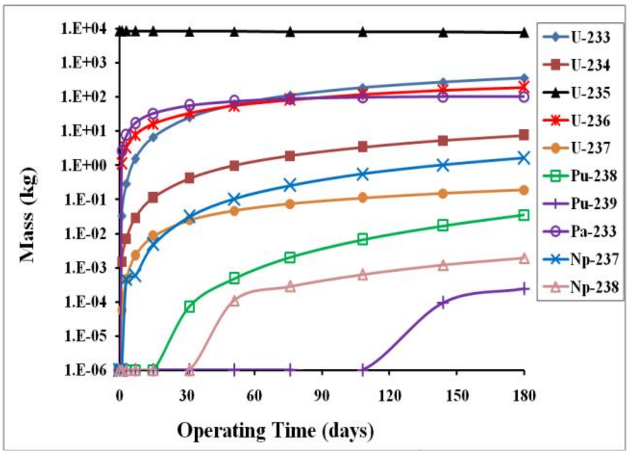

Figure 12: Isotopes Evolution for ^{235}U Starter Core

The ^{239}Pu, in ^{239}Pu starter core, is reduced by 9.3%, and an amount of 420kg of ^{233}U is produced. As seen in figure 11 only ^{233}U, ^{233}Pa, ^{240}Pu are produced in considerable amounts. Other isotopes include ^{234}U, ^{235}U, ^{238}Pu, ^{241}Pu, and finally the minor actinides ^{237}NP, ^{241}Am, and ^{242}Cm.

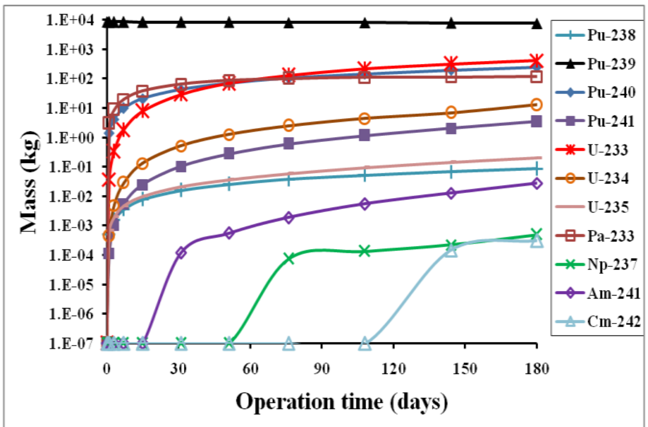

Figure 13: Isotopes Evolution for ^{239}Pu Starter Core

Generally, isotope evolution in the blanket of the three cores behave similarly, figure 14 gives an example for ^{233}U starter blanket. The amount of ^{233}U bred in ^{233}U starter core was about 57 kg, 52kg for ^{235}U starter, and 58 kg for ^{239}Pu starter, ^{233}Pa is normally produced in the process. These small differences in ^{233}U may be attributed to the difference in flux level in the core. Other uranium isotopes produced, but with small amounts, are ^{234}U and ^{235}U.

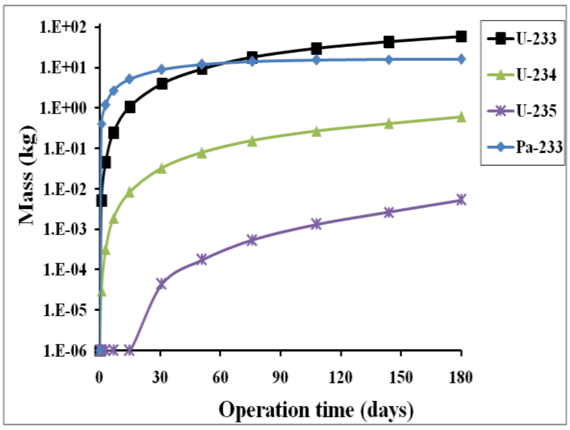

Figure 14: Isotope Evolution in the blanket

Figure 15 illustrates the consumption of ^{232}Th during the period of burnup. Thorium was reduced by about 1.2 % for all types of fuel.

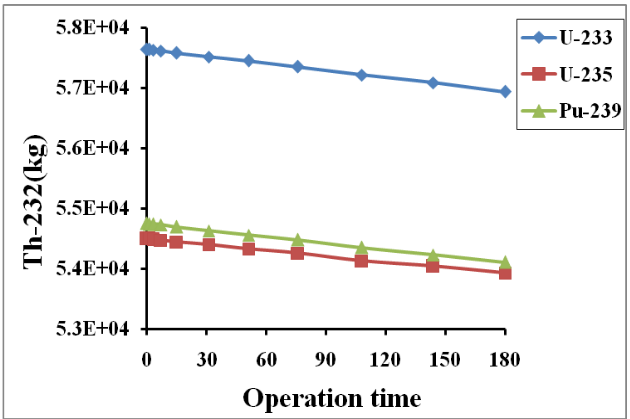

Figure 15: Consumption of ^{232}Th for Each Type of Fuel (Core+Blanket)

2. Conclusions

In this paper, a model to simulate MSFR was prepared using MCNP6. Three types of initial fuel loading were studied, ^{233}U, ^{235}U, and ^{239}Pu .The model was validated using a previous study and found acceptable. The study included flux distribution, Doppler and density feedback coefficients, kinetic parameters and initial breeding ratio .It was found that the three types of fuel are capable of achieving operational safety, with ^{233}U starter has the best safety parameters. The results also included material evolution during six month of burnup. It was found that, the core with ^{239}Pu starter has the largest production of ^{233}U and will last longer than the other two cores before it needs fuel compensation. Isotope evolution in the blanket of the three cores behave similarly, with ^{239}Pu core has the highest ^{233}U production. During six month 1.2% of thorium needs to be compensated for in the core and blanket.

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