Increasing the fuel cycle length of a PWR by means of a homogeneous uranium, thorium and plutonium fuel design

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It all starts here ™

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Abstract

Keywords:

Pressurized Water Reactor, simulations with MCNP, MCNP 6.1 Beta, homogeneous, homogeneous fuel design, thorium fuel, plutonium fuel, reactor grade plutonium, fuel burnup, fuel cycle length, fuel life time

In this study a new homogeneous fuel pellet was designed for a Pressurized Water-cooled Reactor (PWR), aimed at increasing its fuel cycle length. The standard 4.5 wt. % Low Enriched Uranium (LEU) fuel pellet of the South African Koeberg Pressurized Water-cooled Reactor (PWR) was taken as reference. The aim was to alter the isotopic composition of a geometrically standard fuel pellet, in order to increase the fuel cycle length of the core and capacity factor, ultimately improve the profitability of the plant.

The fuel cycle length is dependent of the burnup level of the fuel and is determined by the rate at which the infinite neutron multiplication factor (k_∞) decreases. The fuel cycle ends when k_∞ has decreased to the point that the core becomes sub-critical, thereby terminating the sustainable fission chain reaction.

The aim was to increase the fuel cycle length by increasing the enrichment of the fresh fuel and/or reducing the rate of decline of k_∞ with burn-up. The chosen constraints include that the fuel economy should be uncompromised by the aforementioned measures, all safety limitations for the fuel rods, such as the maximum power density and all anti-nuclear weapons proliferation limits on the isotopic composition of the fresh and spent fuel should be adhered to.

A particular constraint was the assumption that k_∞ at the beginning of life (BOL) for the fresh fuel rod should not exceed that of the fresh reference fuel rod. The neutronic performance of each fuel design was simulated by creating a model for an infinite fuel pin in MCNP 6.1 Beta. This was done by surrounding a section of the fuel rod with the appropriate volume of water, which is again boxed in by reflective boundaries on all sides. The geometries of the fuel pin, fuel rod and surrounding blocks of water were kept unchanged, i.e. only the isotopic composition of the fuel pellets was altered.

As a point of departure the enrichment of the LEU Koeberg reference was increased to the predetermined upper limit of 5 a/o ^{235}U, this is the highest enrichment that is available on the international market. This of course increased k_∞ for the fresh fuel to above the maximum limit i.e. that of the reference 4.5 a/o ^{235}U infinite fuel pin. k_∞ was then restored to the upper limit by diluting the LEU with thorium - 232 and/or adding natural boron, a well know neutron poison/absorber to the fresh fuel pellets. It was found that replacing all $^{238}UO_2$ in the LEU with an equivalent amount of ThO_2 substantially reduced the initial k_∞ for the fresh fuel.

This is mainly due to the fact that ^{232}Th has a much higher radiative, as well as total capture cross section in the thermal energy spectrum, compared to ^{238}U. Further investigation also indicated that ^{232}Th undergoes less fast fissions reactions than ^{238}U, contributing to the higher initial infinite neutron multiplication factor (k_∞). However, homogeneous mixing, e.g. equal volumes, of ^{232}Th and ^{238}U reduces k_∞ even further, and resulted in a substantial increase in total neutron captures in both of the aforementioned. One possible explanation for this phenomena, is the reduced resonance escape probability in the epithermal energy spectrum, due to the summation of all the captures resonances peaks. Therefore only 2% ^{232}Th was sufficient to reduce k_∞ for the 5 a/o LEU fuel composition to that of standard 4.5 a/o LEU fuel currently implemented in Koeberg. The logic behind the addition of natural boron was that the ^{10}B will largely burn away within months, which means that the boron will not place a substantial drag on the neutron economy of the latter parts of the fuel cycle.

An alternative approach was to determine the feasibility, of reactor grade plutonium, and MOX fuel, as a substitute, or as supplement for the standard UOX fuel composition.

The changes in fuel performance, caused by to the modifications to the isotopic composition of the fresh fuel pellets, were analysed in terms of the neutron reaction rates of the predominant fissile and fertile isotopes. Preliminary burnup data suggest that some of these fuel designs are viable substitutes for currently implemented Low Enriched Uranium (LEU) fuel designs.

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It is with great appreciation that, I offer the work contained in this document to my Father in heaven, whom has provided me with the abilities to successfully complete this endeavour. I will always hold the following close to my heart: “because I know the plans I have for you, declares the Lord, plans for a future, and to prosper”.

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Nomenclature

ACRONYMS AND ABBREVIATIONS

Abbreviation or Acronym	Definition
Am	Americium
a/o %	Atom fraction enrichment percentage
at.%	Atom fraction percentage
B	Boron
^{212}Bi	Bismuth
BOC	Beginning of Cycle
BOL	Beginning of Life
BP	Burnable Poison
C	Carbon
Cr	Chromium
DU	Depleted Uranium
EOL	End Of Life
Fe	Iron
Gd_2O_3	Gadolinia
GT-MHR	Gas Turbine Modular Helium Reactor
HEU	Highly Enriched Uranium
GWd	Gigawatt days
GWd/t_{HM}	Gigawatt days/ton heavy metal

Abbreviation or Acronym	Definition
HM	Heavy metal
HTGR	High Temperature Gas-cooled Reactor
H_2O	Water
HWR	Heavy Water Reactor
IAEA	International Atomic Energy Agency
k_∞ / K_∞	Infinite neutron multiplication factor of a reactor fuel and moderator mixture
k_{eff} / K_{eff}	Neutron multiplication factor of a finite reactor core, also called the eigenvalue.
LEU	Low Enriched Uranium. Unless stated otherwise, the chemical composition of the LEU fuel in this dissertation is UO_2.
LMFBR	Liquid Metal Fast Breeder Reactor
LWBR	Light Water Breeder Reactor
LWR	Light Water Reactor
^7Li	Lithium-7
LOCA	Loss of Coolant Accident
MCNP	Monte Carlo N-Particle code
MOX	Mixed Oxide
MSBR	Molten Salt Breeder Reactor
MWd	Mega Watt days
MWd/kg HM	Mega Watt days per kilogram Heavy Metal
Np	Neptunium

Abbreviation or Acronym	Definition
NU	Natural Uranium
O_2	Oxygen
PWR	Pressurised Water Reactor
PHWR	Pressurized Heavy Water Reactor
Pu	Plutonium
RMC	Reactor Modulating Code
RPu	Reactor Grade Plutonium (PWR)
SG	Steam Generator
Sn	Tin
ThC_2	Thorium carbide
ThF_4	Thorium tetrafluoride
^{208}Tl	Thallium
Th-OX	Thorium Oxide
$ThSiO_4$	Thorite
U	Uranium
UC_2	Uranium Carbide
UF_4	Uranium Tetrafluoride
UF_6	Uranium Hexafluoride
UN	Uranium mononitrate
UO_2	Uranium Dioxide

Abbreviation or Acronym	Definition
UOX	Uranium Oxide
woBA	Without Burnable Absorbers
wt.	Weight fraction
Xe	Xenon
Zr	Zirconium
η	Number of fission neutrons produced per neutron absorbed in the fissile fuel nuclides.

Chapter 1. Introduction

Overview

In this dissertation, a comprehensive analysis was done, on the isotopic characteristics of various fissile and fertile materials. The knowledge basis obtained from the isotopic and neutronic interactions during burnup, played a crucial role in the fuel optimization process. Various fuel cycle optimization techniques were investigated, and applied to standard fuel compositions, aimed at increased fuel cycle lengths, without geometric alterations to the reactor. The discernment gained, was applied to conceptualize a design that could be implemented in a real reactor. The information presented in this study, summarises the contrivances applied to conceptually increase the fuel cycle length of the fuel.

1.1 Background

The fuel composition of a Pressurized Water- cooled Reactor (PWR), is usually determined during the conceptual design phase of the project. Most of the reactors currently in operation, have inefficient fuel designs, and significant enhancements with regard to, fuel cycle length are possible. Koeberg nuclear power station in South Africa, currently operates on an 18 month fuel cycle length, but due to inefficient fuel design, the reactor power often has to be decreased after 16 months, to sustain a fission chain reaction, for the remained of the designed fuel cycle length.

In a scenario where the fuel composition performs poorly, a significant financial strain is created due to the loss of income, and may eventually lead to premature decommissioning of the plant as a result of, decreased profitability.

There are numerous techniques that could potentially optimize the fuel cycle length of a reactor, these include modifications to the isotopic composition of the fuel, geometric alterations to the fuel rod / pellet, fuel rod packing density, alternate fuel assembly layouts and increased / decreased moderation. A very effective technique is to decrease the excess reactivity at the Beginning of Life (BOL) by adding a neutron poison, or possibly also a fertile isotope, to the fuel composition. The aforementioned will higher fissile enrichment for the fresh fuel and thus a larger fissile fuel inventory, whilst breeding extra fissile material during burnup, in the case of the addition of a fertile isotope, may result in extended fuel cycle length.

1.2 Problem statement

The nuclear power sector in South Africa received increased popularity after publication of the Integrated Resource Plan for Electricity (IRP 2010) and its 2012 update. The resource plan placed emphasis on the depletion rate of coal reserves and initiatives to decrease carbon emissions. With this in mind significant growth is expected for the nuclear energy sector.

The known reserves of uranium are also limited. However, it must be emphasized that uranium exploration has been very limited, due to subdued uranium prices after the Fukushima nuclear disaster, and therefore the actual uranium resource might be much larger than the presently known reserves. Nonetheless, it is imperative that research should be intensified on alternative fuel compositions for the currently implemented Low Enriched Uranium (LEU) fuel composition in the global fleet of PWRs and BWRs. Unless specified differently, the chemical composition of all LEU fuels in this dissertation will be UO_2.

In view of the above, the problem to be solved in this study is to create fuel compositions that can increase the fuel cycle length of the standard LEU fuel currently used in South Africa's Koeberg nuclear power plant. The study should focus on fuel cycles that aid in incinerating the plutonium stockpile, operate on increased burnup rates and minimise downtime. The alternatives could include newly researched fuels like thorium and compositions that utilise the current plutonium stockpile. The aforementioned could be economically beneficial, whilst having advantage with regard to a reduced environmental impact.

Fuel cycle optimization strategies should be determined, and evaluated, to demonstrate their applicability, and how further expansion, could provide even greater advance in fuel cycle length.

1.3 Research aims and objectives

1.3.1 General aims

The general aims of this study is to:

- Create commercially viable homogeneous fuel pellet compositions for South Africa's Koeberg nuclear power plant that can moderately increase the fuel cycle length of the current standard 4.5 a/o% LEU fuel, without geometric alterations to the fuel.

- Maintain all other operational, economical and safety performance parameters at their present level.

1.3.2 Specific objectives

The specific objectives of this study are to:

- Conduct a comprehensive literature study in order to form a picture of the extent of the research done on fuel optimization techniques and their applicability to the current challenges.
- Determine a trusted method to accurately evaluate conceptual fuel compositions.
- Setup numerical infinite reactor models for the Monte Carlo Neutron-Particle (MCNP) Transport Code 6.1 Beta (Goorley, 2014) stochastic simulation code, in order to analyse the neutronic and isotopic behaviour of conceptual fuel amalgamations.
- Create reference models to be used as a verification benchmarks for the accuracy of the simulation methods.
- Evaluate conceptual fuel compositions by means of full burnup simulations with MCNP. Evaluation should focus on the behaviour of the infinite neutron multiplication factors (k_∞) over time and on the commercial viability of the fuel compositions in the current reactor.
- The intended improvement of fuel performance will be targeted by:
    - increasing the uranium enrichment of the LEU fuel, while limiting the reactivity at the beginning of life (BOL) by adding burnable neutron poisons,
    - adding thorium to the LEU and
    - adding plutonium to LEU and/or thorium.

1.4 Project scope and constraints

Numerical model of the conceptual fuel compositions will be limited to simulation of an infinite reactor. This will be simulated by means of reflective boundaries placed around a small length of a single fuel rod.

Simulation of more complex full-core reactor features, such as fuel assembly details, fuels assemblies of different burn-ups from different fuel reloads, control rods, ^{10}B poison in the water and the outer structures of the core will thus be excluded from the scope of this study.

The scope excludes physically testing.

The maximum ^{235}U a/o enrichment will be limited to 5%, which corresponds to the maximum limit most commercial enrichment facilities are currently licensed to enrich to. The reason for this is to limit the study to fuel compositions that are currently commercially viable. The maximum at. % reactor grade plutonium allowable in any conceptual design will also limited to 10% of the total fuel composition, in order to guard against the occurrence of a positive void reactivity coefficient.

Burnable neutron poisons / absorbers are used extensively in nuclear reactors. It is therefore fair to assume that a conceptual design containing the aforementioned would be a feasible fuel composition. The inclusion of neutron absorbers will thus be included as a design option.

Chapter 2. Literature Study

Overview

This chapter provides fundamental background information on uranium/thorium fuel mixtures and on Mixed Oxide (MOX) fuels, consisting on any combination of plutonium, uranium and thorium. Unless specified differently, MOX fuels normally have the –dioxide chemical composition, i.e. they contain a mixture of PuO_2, UO_2 and/or ThO_2. The literature review will serve as a feasibility analysis for the implementation of the proposed fuel compositions. Reactors able to alternatively operate on thorium-based or MOX fuel-based compositions are also discussed.

2.1 Thorium – 232

The following section provides background information on thorium.

2.1.1 Introduction

Thorium (Th), has an atomic number of 90, and belongs to the metallic elements group. Thorium, was discovered by a Swedish chemist, named Jons Jakob Berzelius somewhere between 1828, and 1829 (WNA, 2011). Pure thorium, is a silvery-white color, and is very susceptible to oxidation by air, after which it becomes black (Du Toit & Cilliers, 2014).

The majority of thorium reserves are found as the mineral monazite, thorite ($ThSiO_4$), and thoriante (ThO_2). Thorium dioxide (ThO_2), has one the highest melting point, with regard to metallic oxides, at approximately 3300 ^oC, making it a very attractive isotope to use in nuclear fuel compositions (WNA, 2011; Du Toit & Cilliers, 2014)

Isotopically thorium's natural abundance consists almost 100% of only a single isotope, namely ^{232}Th. However, since some other Th isotopes are daughter products in the natural radioactive decay chains of ^{235}U and ^{238}U, thorium mined from uranium-containing ores contains small amounts of other Th isotopes, which might influence the proliferation resistance of the resulting predominantly ^{233}U mixtures from the spent fuel of Th-based fuel cycles (Serfontein and Mulder, 2014). ^{232}Th is a fertile isotope and is unlikely to undergo fission reactions in the thermal neutron energy spectrum, but will fission, with a very small microscopic cross-section, in fast neutron energy spectra. Thorium's best attribute is its ability to produce uranium–233 (^{233}U), which is

an excellent fissile fuel, especially for thermal reactors. The fertile ^{232}Th captures a neutron and by means of beta-minus decay, transmutates to ^{233}U (Du Toit & Cilliers, 2014).

2.1.2 Non-nuclear applications

Thorium has numerous commercial applications, these include: welding equipment, precision glassware, and several uses in the petroleum industry (WNA, 2011; J.K. Schults, 2009). In the 19th century, thorium was used in medical application, as contrast during X-ray procedures. In glass related applications, thorium was used as a coating material, for tungsten wire in light bulbs, this is mainly due to its extremely high melting point, and as thorium dioxide (ThO_2), in the production of superior quality glass lenses (Lamarsh & Baratta, 2012).

2.1.3 Thorium reactors

The following section depicts a summary of the current and conceptual nuclear reactors that are and will be able to operate on thorium-based fuels. ^{232}Th has a lower microscopic radiative neutron capture cross section (σ_γ) in the epi-thermal and a higher σ_γ in the thermal neutron energy spectrum than ^{238}U. Therefore ^{232}Th will bread substantial amounts of ^{233}U in thermal energy spectrum reactor. These include Light Water Reactors (LWRs), Heavy Water Reactors (HWRs), High Temperature Gas-cooled Reactors (HTGRs), Light Water Breeder Reactors (LWBRs), Molten Salt Breeder Reactors (MSBRs) and most of the conceptual designs currently being considered (IAEA, 2016; Du Toit & Cilliers, 2014).

2.1.3.1 High Temperature Gas-cooled Reactors (HTGRs)

One of the first High Temperature Gas-cooled Reactors (HTGR), was designed by General Atomic, and used graphite to thermalize neutrons, and helium to extract the heat produced during fission reactions (Galperin, et al., 1997). The aforementioned HTGR was fueled with High Enriched Uranium (HEU), and used ^{232}Th as a fertile material. The addition of ^{232}Th, helped to preserve the fissile content of the fuel, due to its ability to breed ^{233}U. The fertile and fissile isotopes were combined with carbon (C), to form (Th, U) C_2 particles (Lamarsh & Baratta, 2012).

Two geometries exist for HTGRs, namely graphite pebbles, or prismatic fuel elements. The pebble, and prismatic fuel geometries utilise fuel kernels, with various silicon

carbide, and pyrolytic carbide coatings, which are aimed at decreasing radio nuclide emissions into the working fluid.

2.1.3.2 Breeder Reactors

The term breeder reactor is coined from the primary function of these reactors and this is to breed certain isotopes for use in other reactors or for fuel for nuclear weapons. The conversion ratio for the aforementioned is usually above 2, meaning that for every one fissile nucleus destroyed, either by means of fission or radiative capture, at least one new fissile nucleus will be bred, usually from radiative capture in a fertile isotope, such as ^{238}U or ^{232}Th. If the conversion ratio is less than 1, the reactor will consume more fissile fuel than it produces. (WNA, 2011)

The term breeding is usually described in context of the reactors doubling time. This is the time interval it would take for the breeder reactor to breed a sufficient amount of fuel to double its initial fuel inventory. Obviously this extra fuel could then be used to start up another reactor. The breeding rate of a reactor (Lamarsh & Baratta, 2012) is the average number of new fissile nuclei bred per fissile nucleus consumed in the previous generation. The higher the breeding ratio and the shorter the doubling time, the more efficient the reactor will be able to breed fissile isotopes.

Due to ^{232}Th not possessing a fission cross section in the thermal energy spectrum, it will always have to be homogeneously or heterogeneously mixed with some kind of neutron source, typically the fissioning of another fissile isotope, to supply the neutrons for breeding the fissile isotope ^{233}U (Walt, 2015). The dependency on the neutron source for neutrons will gradually decrease with the addition of ^{233}U.

2.1.3.2.1 Molten Salt Breeder Reactor (MSBR)

The Molten Salt Breeder Reactor (MSBR) operates on thermalised neutrons by means of a homogeneous mixture of molten thorium salt, uranium salt and other salts. The reactor uses ^{233}U as fissile isotope and is designed to operate in extremely high temperatures (1400 ^{o}C) but at reduced pressure (WNA, 2011). The extreme operating temperatures ensure that the coolant fluid/ moderator stay in a liquid phase. This is a potentially hazardous design, especially in accident scenarios where, due to a lack of heat, the molten salt can freeze.

The Liquid Fluorine Thorium Reactor (LFTR) is an alternative design of the Molten Salt Breeder Reactor (MSBR) and utilises a liquid ^{232}Th salt blanket to breed ^{233}U (Du Toit

& Cilliers, 2014). During operation ^{233}U, is continuously reinserted into the core after the extraction process. The ^{233}U is combined with fluoride to form $^{233}UF_4$ and added to the molten salt at approximately 700^{o}C. The graphite structure of the core also serves as a neutron reflector, ultimately increasing the neutron population in the epithermal energy spectrum.

The majority of the fission products dissolve in the molten salt moderator/ coolant, from where it is collected via chemical methods (WNA, 2011). Actinide population in such a $^{232}Th/^{233}U$-based fuel cycle is much lower than in U/Pu fuel cycles. The actinides that do form are retained in the fuel and undergoes decay processes, subsequently transmutating to fissile isotopes that eventually fission and contribute to the neutron economy of the reactor.

The fertile ThF_4 breeds ^{233}U and due to the heat produced forms a soluble $^{233}UF_4$. The operators then bubble Florine gas (F_2) through the homogeneous mixture of molten salt and $^{233}UF_4$, eventually producing uranium – 233 hexafluoride ($^{233}UF_6$). The $^{233}UF_6$ gas is then collected at the top of the mixture and by means of reduction columns and hydrogen gas (H_2) reduced to $^{233}UF_4$ (WNA, 2011; Du Toit & Cilliers, 2014).

Molten Salt Breeder Reactors (MSBRs) are characteristically different from other reactor types in the sense that they do not utilise solid/ridged fuel rods, cladding material, or water as heat transfer mechanism. The heat transfer is done by the homogeneous molten salt and fuel mixture directly. The low operating pressure, in the range of 500 [kPa], is low enough that the addition of a pressurizer and/or heavy duty pressure vessel is not required (Kamei & Hakami, 2011).

2.1.4 Optimization techniques

Numerous optimization techniques exist, to increase the fuel cycle length of a nuclear reactor. This section will focus on the use of thorium, as part of, or substitute for, a standard nuclear fuel composition aimed at improving the fuel cycle length, and fuel utilization of the reactor.

2.1.4.1 Optimization by means of thorium - 232

There are various studies that evaluate the economic feasibility of ^{232}Th-based fuel compositions, but (Du Toit & Cilliers, 2014), revealed substantial detail with regard to refuelling cycle interval length, load capacity factors, and the magnitude of spent fuel depositories.

The research focused on once-through then out, homogeneously mixed, Th/U fuel compositions burned over a 24 month period, as opposed to the standard 18 month, Uranium Oxide (UOX) fuel composition, fuel cycle length.

Vital information, with regard to conversion rates of ^{232}Th to ^{233}U, and increase reactivity stability was indicated by (Du Toit & Cilliers, 2014). The aforementioned, were supported by Figure 1, which indicates the advantages of breeding ^{233}U by thermalized neutron capture of ^{232}Th, and how the addition of ^{232}Th, stabilizes the reactivity of the reactor (Du Toit & Cilliers, 2014).

The evaluated fuel compositions in Figure 1, include a standard UOX fuel composition (UOX-ref), Thorium- Mixed Oxide fuel, (Th-MOX-18), and (Th-MOX-24) burned over 18 and 24 months respectively, Thorium-Mixed Oxide with burnable absorbers (Th-MOX-BA), and a UOX fuel without burnable absorbers (UOX-woBA).

The economic evaluation, incorporated an in-depth analysis, of the financial implications relating to ^{232}Th-based fuels compositions. Subsequently the following characteristics were analysed: fuel cycle costs, material requirements, reprocessing, enrichment, manufacturing, storage of spent fuel, spent fuel disposal, and estimated total fuel cycle cost (Walt, 2015; Du Toit & Cilliers, 2014).

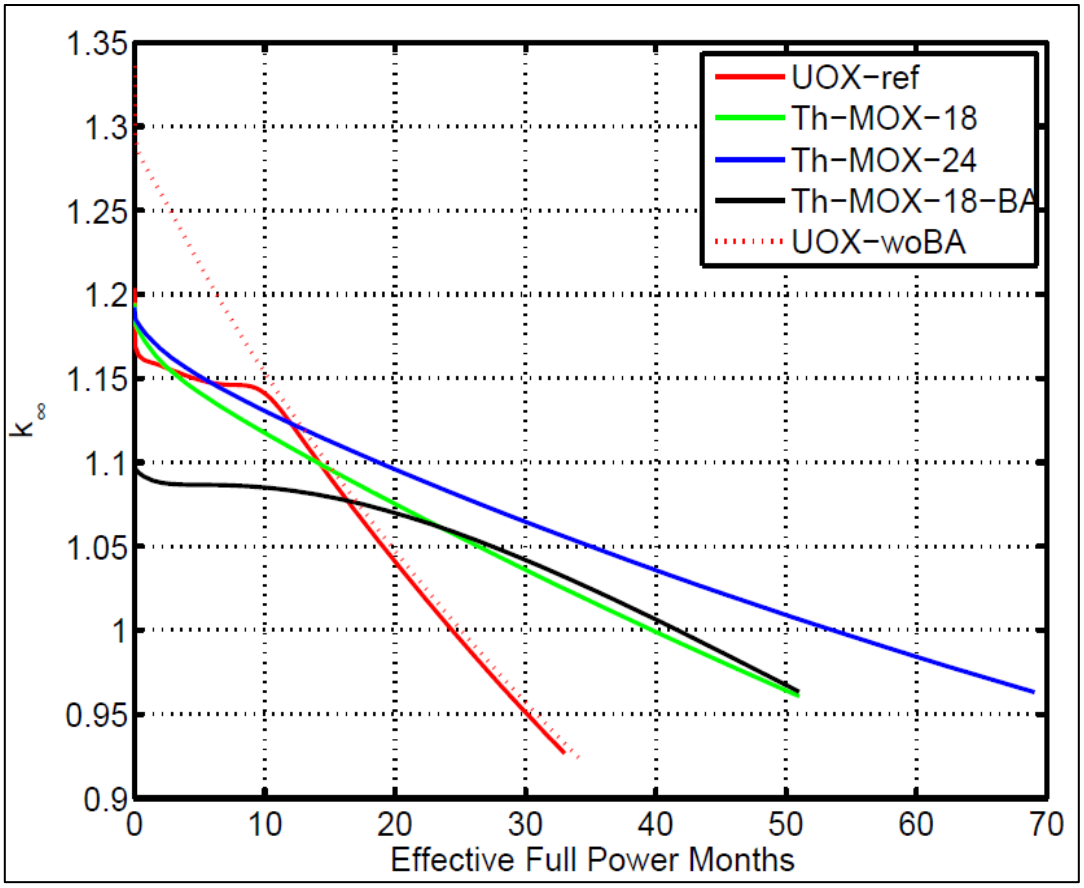

Figure 1: Infinite reactor reactivity versus full-power months for Uranium and Thorium-based fuels (Thor Energy, Norway, 2012; Du Toit & Cilliers, 2014)

Investigation of an alternate method by (Brown, et al., 2014), for optimization of the fuel utilization, included the use of uranium mononitrate (UN), as an alternative for standard UOX fuel.

The following chemical compositions: UN/U_3Si_5, UN/U_3Si_2, UN/UB_4 and UN/ZrO_2 were evaluated with numerical models, and based on the geometric, and power specifications of the Westinghouse Advanced Passive 1000 (AP1000) reactor. In above mentioned evaluation process included parameters like: fuel porosity, neutron population energy distribution, neutron capture cross sections, and neutron resonance escape probability, were taken into account during burnup. The initial reactivity, reactivity stability, and conceptual fuel compositions cycle length were also considered. The thermal conductivity [W/mK], of nitride-based fuels are significantly higher than the thermal conductivity [W/mK], of UO_2 fuel compositions (Walt, 2015; Brown, et al., 2014).

The conclusion of the results were, that the uranium mononitrate-based fuels provided increased fuel cycle lengths, and subsequently can withstand higher burnup rates (Brown, et al., 2014). The research did highlight some consideration points, one of which was the reduced burnable neutron absorber/ poisons inside the uranium mononitrate-based fuels, due to their operational energy spectrum.

The aforementioned provided the necessary information, to justify the investigation of thorium-based fuels. The use of uranium mononitrate-based fuels were chosen to be unfeasible, especially in accident situations, contrary to the use of thorium-based fuels, which have increased proliferation resistance.

2.1.4.2 Homogeneous Thorium based fuels

Conceptual thorium-based fuel compositions for nuclear reactors have been intensely researched for a number of years, and proposed designs have been made by (Herring, et al., 2001), in which the proliferation resistance cost of thorium-based fuel compositions, would suffice in converting the public opinion on nuclear energy, and more specifically the aforementioned reactor designs.

The aim of the research was to conceptualize a thorium-based fuel composition which would have decreased fabrication costs, in comparison with the standard UOX fuel compositions, increased the fuel cycle length of the fuel, increased proliferation resistance, and produced safer waste with decreased weapons risk. The research was based on a homogeneous uranium dioxide (UO_2), and thorium dioxide (ThO_2), fuel composition, with varied weight fractions (wt.), but for consistency a standard enrichment of 19.5% was used for the UO_2.

The obtained results from the numerical models done by (Herring, et al., 2001), indicated that higher burnup rates were achievable by thorium dioxide (ThO_2), uranium oxide (UO_2), this can be ascribed to the sub-critical inducing, properties of the thorium dioxide (ThO_2), which subsequently causes decreased operational temperatures in the reactor core. Decreased core temperature enables that the operation of the conceptual fuel composition at excessive burnup rates, with sufficient safety.

The implementability of homogeneous thorium-based fuels, have been extensively researched, and produced results that suggest commercial viability (Du Toit & Cilliers, 2014; Herring, et al., 2001; Galperin, et al., 1997; Thor Energy, Norway, 2012; Yamamoto, et al., 2002; Walt, 2015).

2.1.5 Advantages of thorium based fuel

Thorium dioxide (ThO_2), has higher stability, and is more resilient than UO_2 from a metallurgical, and isotopic point of view (Caner & Dancan, 2000). The proposed fuel showed increased resistance to high burnup rates. Metallic thorium-based fuels, have decreased severity during steam interactions, compared with metallic uranium fuels (Greneche, et al., 2007). Thorium dioxide (ThO_2), does not fluctuate significantly from the aforementioned stoichiometric isotopic composition, even when imperiled to air (O_2), or water (H_2O), at temperatures approaching 1727°C (Herring, et al., 2001; Du Toit & Cilliers, 2014). The burnup rate of reactors utilizing thorium-based fuel compositions, can be increased, due to the higher material melting point of 3300 ^oC. These aforementioned characteristics result in increased safety features, and optimized thermal efficiencies (IAEA, 2007).

The radioactive nuclide population of depleted thorium-based fuels, are estimated to be lower, in comparison with depleted UOX fuels. This is attributed to the decreased atomic weight of thorium, in comparison with uranium, plutonium, and the significantly smaller production rate, of minor actinides (Puill, 2002). Intensely irradiated, and depleted conceptual thorium-based fuel compositions, produced a reduced population of toxic radio nuclide, for an approximate period of 10000 years, when compared with standard UOX fuel compositions (Galperin, et al., 2000).

2.1.6 Challenges with Thorium based fuel

The higher radiative and total neutron capture cross section in the thermal energy spectrum of ^{232}Th, in comparison with ^{238}U, leads to higher capture neutron rates, which obviously leaves less remaining neutrons that can produce fissions. More captures and less fissions by definition results in reduced values of k_∞ and k_{eff}. This necessitates increased enrichment percentages in order to maintain reactor criticality for thorium-based fuel designs, for reactors operating in the thermal energy spectrum (Kanmei & Hakami, 2011). The aforementioned affects the fissile isotope conversion ratio of the fuel composition.

In terms of the fissile isotope conversion ratio, ^{238}U is advantageous in comparison with ^{232}Th (Puill, 2002). Both of the aforementioned fertile isotopes are fissionable at high energies, but ^{238}U has a much higher fast fission cross section in the high neutron energy region, compared to ^{232}Th (OECD, 2016). Since fast fissioning of fertile isotopes

produce substantially more fission neutrons per neutron absorbed (η), compared to thermal fissions of predominantly fissile isotopes, even just a small fraction of fast fissions generate a substantially larger fraction of fission neutrons. Therefore fast fissioning of ^{238}U contribute up to 8% of the total fission neutrons, compared to only 2-3% for ^{232}Th (Du Toit & Cilliers, 2014; Puill, 2002). When it comes to the conversion ratio, fast fissions of fertile isotopes are even more advantageous (Serfontein and Mulder, 2014): when fissile isotopes are irradiated with thermal or epithermal neutrons, a large fraction of these neutrons will produce fissions. For every one neutron that absorbed to cause such a fission, about 2.5 fissions neutrons will be emitted. After replacing the one neutron that was absorbed, there is thus now an excess of 1.5 neutrons, which can be captured by fertile isotopes to produce 1.5 new fissile nuclei, provided that there are no other neutron losses, which there always are. Since one of these new fissile nuclei must be used to replace the fissile nucleus that was destroyed by the fission, the theoretical maximum gain in fissile nuclei is 0.5 nuclei. However all fissile fuels have higher values of σ_γ at thermal and epithermal neutron energies than at high energies. Therefore a substantial fraction of the neutrons that are used to irradiate the fissile fuel nuclides are absorbed by means of radiative capture, for instance $^{235}U(n,\gamma)^{236}U$. Just like the fission process, this radiative capture destroys a fissile nucleus, as it changes the fissile ^{235}U into the non-fissile ^{236}U. Additionally this process reduces the number of neutrons available for fission by one and thus reduces the number of fission neutrons produced by about 2.5, which leads to a substantial reduction in the conversion ratio and thus in the conversion gain.

The effect of fast fissions of fertile isotopes, on the other hand, is much more advantageous: fast fissions produce on average more neutrons per fission than thermal or epithermal fissions. Let's assume 3.5 neutrons per fast fission for this example. So after replacing the one neutron that was absorbed to initiate the fission, a theoretical maximum of 2.5 excess neutrons remain available for breeding new fissile isotopes. However, since it was a fertile, rather than a fissile, nucleus that was destroyed by the fission, none of these 2.5 newly bred fissile nuclei have to be used to replace a destroyed fissile nucleus. Therefore the maximum theoretical gain in fissile nuclei is now 2.5 nuclei, which is 500% more than the 0.5 nuclei for the case of thermal/epithermal fissioning of fissile isotopes. This explains why a small excess in fast fissions of ^{238}U, compared to the smaller number of fast fissions of ^{232}Th, can produce a relatively large increase in the conversion ratio of the fuel cycle.

Radioactive ^{232}U is an unwanted by product of thorium-based fuel designs, due to its tendency to decays into thallium (^{208}Tl) and bismuth (^{212}Bi). The aforementioned isotopes emit gamma radiation during decay, which significantly complicates fabrication, transit, reprocessing and waste disposal procedures. Increased gamma radiation shielding is a prerequisite for all of the aforementioned procedures (Puill, 2002). However, this increased radiation also makes it quite dangerous for would-be nuclear weapons proliferators to shape the ^{233}U into a nuclear weapon (Serfontein and Mulder, 2014). In fact, this added radiation is the main factor that provides resistance against nuclear weapons proliferation for the spent fuel from Th-based fuel cycles.

2.2 MOX fuel

The following section depict all relevant information on Mixed Oxide (MOX) fuels.

2.2.1 Introduction

Nuclear reactors all over the world produce plutonium during neutron capture reactions in ^{238}U, which transmutates to ^{239}Pu and then by consecutive neutron capture reactions to ^{240}Pu, ^{241}Pu and ^{242}Pu and thereafter to the Minor Actinides, i.e. different isotopes of Am and Cm (WNA, 2011).

Of the Pu isotopes only ^{239}Pu and ^{41}Pu are fissile. Approximately half of the bred ^{239}Pu undergoes fission reactions, contributing to about one third of the total system energy (WNA, 2011). Normally about 1% of the spent LEU fuel discharged from a pressurized PWRs comprises of plutonium and about 66% of the above mentioned consists of fissile plutonium isotopes. This mixture is called reactor grade plutonium (Pu(PWR)) or civil plutonium.

An estimate of about 70 tons of Pu(PWR) is extracted from used LEU fuel per annum by means of chemical reprocessing. Some of this Pu(PWR) is then used to manufacture Mixed Oxides (MOX) fuel, which normally consist of about 8 wt% Pu(PWR) and 92 wt% depleted uranium, i.e. the waste stream from the uranium enrichment process. This MOX fuel is then inserted in MOX fuel licensed reactors, subsequently contributing in the electricity generation process (WNA, 2011). The recycling of plutonium and utilization thereof in the form of MOX fuel increases the energy extracted from the original amount of uranium by approximately 12% and recycling of uranium from the spent fuel, further increases the energy utilization to

approximately 22%. The aforementioned is based on a standard Pressurized Water-cooled Reactor with a burnup of 45 GWd/t HM.

2.2.2 MOX fuel production and implementation

The first uses of MOX fuel in thermal reactors, date back to 1963, but only became commercialized in the 1980s. To date approximately 2000 tons of MOX fuel have been manufactured, and implemented in an array of power reactors worldwide. In 2006 an estimated 180 tons of MOX fuel assemblies, were burned in over 30 MOX fuel licensed reactors, most of which were Pressurized Water-cooled Reactors (PWR), and the majority belonging to Europe (WNA, 2011).

MOX fuel is widely implemented in Europe, and Japan. Currently 40 European reactors (Belgium, Switzerland, Germany and France) are licensed to add MOX fuel to their current UOX fuel loading, and just over 30 of the aforementioned are doing so (WNA, 2011). Japan has only 10 reactors licensed to operate on MOX fuel loading, in conjunction with their UOX fuel loadings, and several do so. MOX fuel license reactors generally use MOX fuel, as about 1/3 of their total core assemblies, while some will accept up to 50% MOX assemblies (WNA, 2011).

The addition of larger core fractions of MOX fuel assemblies, would require increased moderation to achieve criticality, this is contributed to the excessive neutron capture cross sections, of the fertile plutonium isotopes, at the upper end of the thermal energy spectrum, and the beginning of the epithermal energy spectrum.

The leading nuclear capital of the world, France aims to convert all of their 900 MWe nuclear reactors to operate on a minimum of 1/3 MOX fuel assemblies. Japan also plans to increase their MOX fuel utilization, by licensing approximately 1/3 of their reactors in the near future. Advanced reactor designs by Areva, and Westinghouse, the EPR and AP1000, respectively will be able to reach criticality on a full MOX fuel core loading (WNA, 2011).

Several fast neutron reactors utilise MOX fuel, predominantly in France and Russia. However fast reactors require much higher enrichments and thus the fraction of Pu in the mix is increased drastically. MOX burning in fast reactors was first conceptualised during experimental research done in USA, Russia, UK, France, Germany, Belgium

and Japan (NP.net, 2016). Today, Russia frontrunner in fast neutron reactor conceptualization and plans to increase their fast neutron reactor fleet (WNA, 2011).

Currently the plutonium produced from spent fuel reprocessing plants surpass the depletion rate of MOX fuel in MOX fuel licensed reactors, thereby causing a growing stockpile of Pu(PWR) in countries licensed to use nuclear reactors for power generation. The above mentioned stockpiles are anticipated to exceed 250 tons, before a dramatic decrease is expected, due to increased MOX fuel licensed reactors. MOX fuel is expected to provide 5% of the worldwide demand of nuclear fuel (WNA, 2011).

2.2.3 Advantages of MOX fuel

One of the primary advantages of MOX fuel is that the fissile enrichment can easily be increased by the addition of more plutonium, contrary to uranium where the enrichment can only be increased by expensive additional uranium enrichment. This is problematic as most enrichment plants are only licensed to enrich up to 5%.

MOX fuel loadings can withstand increased burnup levels and help prolong current fuel cycle lengths, which makes it an attractive option. Since Pu extraction by chemical reprocessing of spent fuel is expensive, it will only become economically feasible if uranium prices were to increase substantially (Serfontein, 2011). MOX fuel also has it environmental benefits, as it reduces the current spent fuel stockpile and provides energy for electricity generation. Approximately seven LEU fuel assemblies are required to manufacture one MOX assembly, resulting in only about 35% of the volume, mass and cost of spent fuel disposal (WNA, 2011).

2.3 Proliferation risk

The following section depict information on the proliferation risk of certain fuel compositions.

2.3.1 Introduction

It is predominantly clear that proliferation resistance of nuclear fuel, is a fundamental parameter that has to be considered, during the conceptualization of new fuel compositions, especially in technique implemented to increase the reactors fuel cycle length. The following section depict research done on the proliferation resistance of various fuel.

Due to the high burnup rates permitted in thorium-based fuels, thorium-based fuels can increase the weapons proliferation-resistance of Pressurized Water-cooled Reactors (PWRs), in three ways (Herring, et al., 2001). The generated amount of weapons grade material will be significantly decreased in comparison with the quantity produced by other fertile materials. It is important to note that even though the generated quantity of weapons grade material is less than in standard LEU fuel compositions, the critical mass of ^{233}U, is substantially lower than that of ^{235}U, and ^{239}Pu (Serfontein & Mulder, 2014). To further prevent the aforementioned the composition can be further denatured with increased quantities of ^{238}U.

Predicted fuel cycle lengths will be substantially longer, subsequently decreasing the frequency of refuelling periods, therefore decreasing the likelihood of material diversion during refuelling procedures. Thorium-based fuel composites withstand higher burnups rates, this provide a basis for fuel cycle length spanning, up to 24 months, opposed to the current 18 month cycles, of standard LEU fuel compositions (Du Toit & Cilliers, 2014).

The presence of the various plutonium isotopes in spent fuel is undesirable for the use nuclear weapons, when fuel containing plutonium isotopes are subjected to high burnup rates, the quantity of fertile plutonium isotopes (^{238}Pu, ^{240}Pu, ^{242}Pu) increases. These aforementioned isotopes, provide increased resistant to the production of nuclear weapons (Herring, et al., 2001; Walt, 2015). The above mentioned isotopes release large amounts of spontaneous neutrons which decrease the probable yield of a nuclear weapon drastically, they also release large amounts of decay heat which makes weapon fabrication extremely difficult (Herring, et al., 2001).

The preferred plutonium isotope for use in weapons application is ^{239}Pu, due to its high fission cross section, superior neutron yield per fission neutron, considerably decreased levels of spontaneous fission reactions, spontaneous neutron production and decay heat production rate (Herring, et al., 2001; Walt, 2015). Weapons grade plutonium is manufactured by irradiating natural or depleted uranium in special plutonium production reactors to only a low neutron fluency. The aim is to produce high purity ^{239}Pu by stopping irradiation after a substantial amount of ^{239}Pu has been bred, but before the rest of the transmutation chain, from ^{240}Pu onwards, has formed substantially.

Plutonium produced in commercial reactors are, however, subjected to much higher neutron fluencies, as the burn-up and thus fuel cycle lengths are maximised. This leads to a strong increase in the presence of those isotopes in the spent fuel that is undesirable for the use nuclear weapons, i.e. ^{238}Pu and ^{240}Pu and americium-241 (^{241}Am). (Herring, et al., 2001; Walt, 2015). The plutonium content is also dependant on the following factors: neutron energy, neutron flux, fuel cycle length, frequency of the refuelling periods (Herring, et al., 2001; Walt, 2015).
^{240}Pu releases large amounts of spontaneous fission neutrons which causes imploding nuclear weapons to predetonate and thus blow itself apart before the optimum level of implosion has been reached. This decreases the energy yield of such weapons dramatically. However, even such low yield nuclear weapons, detonated in highly populated areas would cause tremendous psychological strain and terror and could thus still be effective weapons for the purposes of terrorists (Serfontein, et al., 2014)**.** Therefore a substantial level of denaturisation of ^{239}Pu with ^{240}Pu might not be a sufficient deterrent against nuclear weapons proliferation.

If a substantial fraction of ^{238}Pu is present, it will release such large amounts of decay heat, from alpha-decay of ^{238}Pu, that it will melt or even explode the plastic explosives that are normally put around the fuel shell of an implosion type nuclear weapon. This will makes weapon fabrication so difficult that it can be viewed as a sufficient deterrent against nuclear weapons proliferation (Serfontein and Mulder, 2014b), (Herring, et al., 2001).

The volume of plutonium produced per MWd, in thorium-based amalgamation fuels are approximately 3.2 times smaller than the produce observes in standard LEU fuel compositions, if burned at a uniform burnup rate of 45 MWd/kg. This can be ascribed to the much lower atom fraction (at.) of ^{238}U of only 24-28%. The second reason is the higher burnup rates, during which almost 50% of the produced ^{239}Pu undergoes fission reactions (Walt, 2015).

However, the main proliferation risk of Th-based fuels lies in the ^{233}U that can be separated from their spent fuels. In order to increase the proliferation resistance of thorium-based fuel cycles, the fraction of ^{232}U in the spent fuel should be increased. This will result in high concentrations of ^{208}Tl, a highly radioactive daughter product of ^{232}U which can emit lethal doses of high energy gamma-rays. This decreases the

manufacturing probability and increases risk of detection subsequently aiding in the proliferation resistance of the fuel composition (Serfontein & Mulder, 2014).

2.3.2 Barriers to the deployment of Thorium based fuel assemblies

Thorium-based fuel cycles are predicted to be more proliferation resistant in comparison with the standard LEU fuel compositions (Serfontein & Mulder, 2014). Nevertheless, there are obstacles that restrict the implementation of thorium-based fuel compositions in most nuclear reactors. The U/Pu fuel cycles do not share the same constraints and are therefore favoured for use in commercial reactor.

The sustainability and profitability of thorium-based fuel cycles are inversely related to that of LEU fuel cycles. At the currently decreased prices and abundance of U fuel, there is no persuasive reason to change to thorium-based fuel compositions. Thorium-based fuels have excessively high manufacturing and enrichment costs. Therefore, unless the prices of U/Pu fuel skyrocket, which is unlikely, the use of thorium-based fuels will remain uneconomical over the short term. (Walt, 2015)

The reprocessing spent thorium-based fuel cycles require the extraction of ^{233}U by means of chemical reprocessing. Unfortunately reprocessing is extremely expensive which, would also requires uranium prices to increase substantially before this option becomes economically feasible (Walt, 2015).

The radiotoxicity of spent thorium-based fuels are initially lower than that of spent LEU fuel compositions. After approximately 1000 years this radiotoxicity increases promptly and after approximately 11000 years, it exceeds the radiotoxicity of spent LEU fuels. This characteristic could potentially increase waste disposal costs significantly. (Serfontein & Mulder, 2014).

In accident scenarios, emissions of radioactive nuclides from thorium-based fuels during the first few weeks are significantly more dangerous, than that of standard LEU fuel compositions under the same circumstances. However, thorium-based fuel compositions, possess increased chemical stability, in comparison with UO_2 fuel compositions. Most radioactive nuclides might thus remain captured inside the thorium fuel. The aforementioned benefit is not infallible and nuclear regulators may not fully consider this characteristic, during licensing procedures. (Serfontein & Mulder, 2014; Walt, 2015).

2.4 Summary

Numerous techniques have been evaluated to increasing the fuel cycle length of a Pressurized Water-cooled reactor (PWR). The factual inconsistencies have been considered and adhered to, by means of extensive research, and cross referencing of principals from various similar studies. The evaluated studies can be used as a benchmark, to predict the behaviour of various conceptual fuel compositions alterations and the numerical models can be used to verify these predictions or vice.

The complications experienced by previous studies have been addressed, these include: proliferation, political, financial feasibility, manufacturing, obtainability and environmental impact.

Chapter 3. Methodology

Overview

This chapter provides, a comprehensive narrative of the strategy followed, to fulfil the feasibility prerequisites of this study. In this study, conceptual fuel compositions will be designed, and analysed for feasibility. Numerical models, enable the testing of conceptual fuel compositions, under various conditions, and help to predict the isotopic and neutronic behaviour of the fuel composite during burnup, without fabrication.

3.1 Conceptual design development

The goal of this project was to find a homogeneous fuel composition that would prolong the fuel cycle length of a standard PWR. The literature survey, was specifically compiled with this objective in mind. Therefore, the majority of the literature studied designates various methods used, to increase fuel cycle lengths. The published strategies were analysed for feasibility, and implementability.

After meticulous evaluation of the known optimization techniques, a detailed project scope was determined, aimed at increasing the fuel cycle length, of Koeberg nuclear power plants, 900 MW PWR.

This strategy was to, develop a homogeneous conceptual fuel composition, that would decrease, initial excess reactivity, improve fissile breeding rates, and provide a longer fuel cycle length than the currently implemented, LEU fuel composition. The conceptual fuel composition, should be a viable substitute for the current LEU fuel composition, without any geometric changes to the reactor, or fuel pellet.

The initial departure point was to increase the enrichment of the standard LEU fuel. This subsequently would cause excess reactivity at the Beginning of Life (BOL). The mitigation of the aforementioned could be achieved by the addition of neutron absorber / poisons directly into the fuel composition, or a fertile isotope with a high thermal neutron capture cross section could be added. The logic behind this is to increase fissile ^{235}U content of the standard LEU fuel composition, without increasing reactivity at BOL, and thereby providing extended operation.

The conceptual fuel compositions, were then further developed into a design, which could be evaluated, by means of numerical models. An important parameter is to keep

in mind, is what is achievable with regard to the scope, and what limitations should be expanded to fulfil the feasibility prerequisites, with the minimum amount of time, and resources.

The conceptual fuel compositions, were used to determine system specifications for a preliminary fuel cycle design. This design incorporates geometric, isotopic, neutronic, and thermodynamic specifications. The conceptual fuel compositions, were designed in accordance with current fuel legislation, and limitations as set by the governing body.

To model and test the new design it was necessary to determine which simulation software should be used and then reference models were created to allow better understanding of the software, to the point where it became easier to model the required design. Verification of the results was done throughout all stages of the development to improve the accuracy of each new iteration.

3.2 Use of numerical models

Utilization of numerical models enables behaviour analysis of the conceptual fuel compositions during burnup, without physical testing.

The scope of this project entails a fuel composition that could conceptually extend the fuel cycle length, it was never intended to be directly implementable. Additional research will be fundamental to determine the actual feasibility of the proposed designs.

The simulation software used in this document is MCNP 6.1 Beta. The numerical model consists of a small length of geometric standard fuel rod, cladding and surrounding water moderator.

A square control volume was used, subsequently simulating a fuel rod in a square fuel lattice. Reflective boundaries on all the outside surfaces of the geometry infinitely duplicates the numerical model in all simulated directions, effectively simulating an infinite amount of geometric identical fuel rods, with an infinite length.

To reduce computational time, the aforementioned model was geometrically simplified to a quarter control volume (1/4) model. Due to the symmetrical properties of a fuel pin, a “pizza slice”- shaped section of the fuel rod was used with reflective boundaries, effectively simulating the total circumference of the fuel pin.

3.2.1 Reference cases

Reference models were used to determine computational accuracy of the MCNP 6.1 Beta numerical models. The computed results from reference models are preferred to have a high correspondence with results from parametric similar models, obtained from studies done by other institutions.

Results from in-depth studies, on conventional and homogeneous conceptual fuel cycles simplified cross referencing of our results dramatically. Result verification of models containing burnable poisons / absorbers were also done to determine if isotopic inclusions of other isotopes still delivers results with the permitted accuracy level.

After the verification process of the generated data from the numerical reference models, a knowledge basis was obtained which aided in determining the conceptual designs isotopic composition. Some of our novel fuel compositions could not be verified against published results as not data could be found or these compositions. In such cases the modelling proses was first applied to well-known fuel compositions. These model output results were then verified against published data. Once it was established that the modelling process works correctly, the fuel composition was then changed to the desired new fuel. Based on the fact that the same modelling method was accurate for the well-known fuel compositions, it was then assumed that it could also be trusted for the new fuel composition.

When statically significant deviations in the results were noticed, literature studies was analysed to determine, if there were any factors not considered, or included in the numerical model.

3.3 Summary

The implemented strategy used to address, the concerns as stated, for this study have been explained. Ultimately the goal is to develop a conceptual fuel composition that, can produce an increased fuel cycle length, without compromising the reactors safety, or any geometric alterations to the reactor, and fuel. The various concepts, should be evaluated, and verified through numerical models.

Chapter 4. Conceptual design

Overview

Conceptual fuel compositions are proposed, as substitute for the currently implemented LEU fuel composition in Koeberg nuclear power plant. The conceptual fuel compositions, are amalgamations of various fissile and fertile isotopes, and require comprehensive research, to determine their feasibility, and implementability. This section depict the proposed conceptual compositions, and aspires to address the anticipated challenges involved with the conceptual designs.

4.1 Design Specifications

The following section, depict the conceptual fuel pellet design as simulated in MCNP 6.1 Beta.

4.1.1 Introduction

The following section describes the geometric, and material specifications applied during the fuel burnup simulations contained in this document, and aims to address any anticipated challenges. Figure 2, depict a top view of the effective simulated control volume, the control volume is square due to the cubical packing order implemented in PWRs. Reflective boundary conditions where used to reduce geometric complexity, and simulates an array of infinite fuel pins, in an infinite reactor with regard to height.

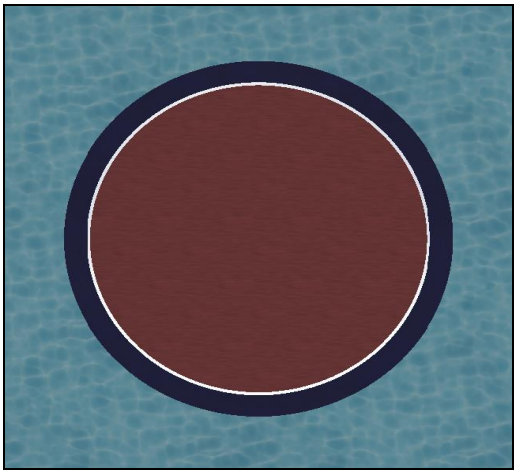

Figure 2: Top view of the control volume containing the fuel pin, helium gap, cladding material and moderator

The geometric specifications, of the effective control volume are presented in Figure 3, and Figure 4.

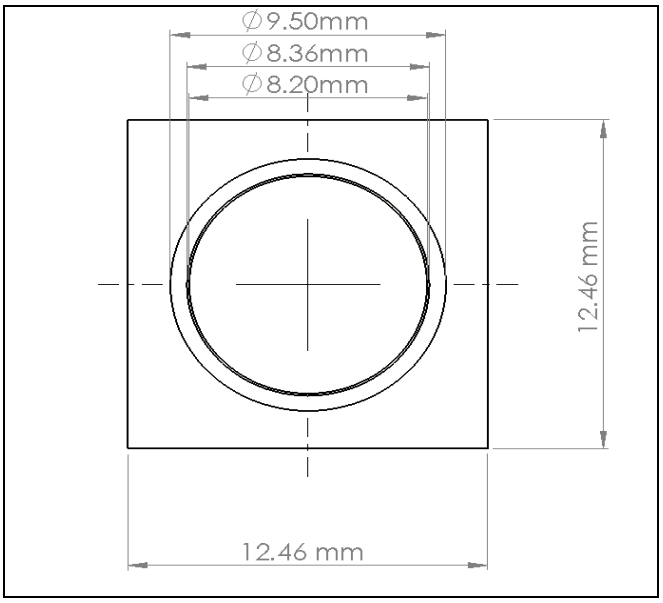

Figure 3: Top view of the geometric specifications of the simulated model

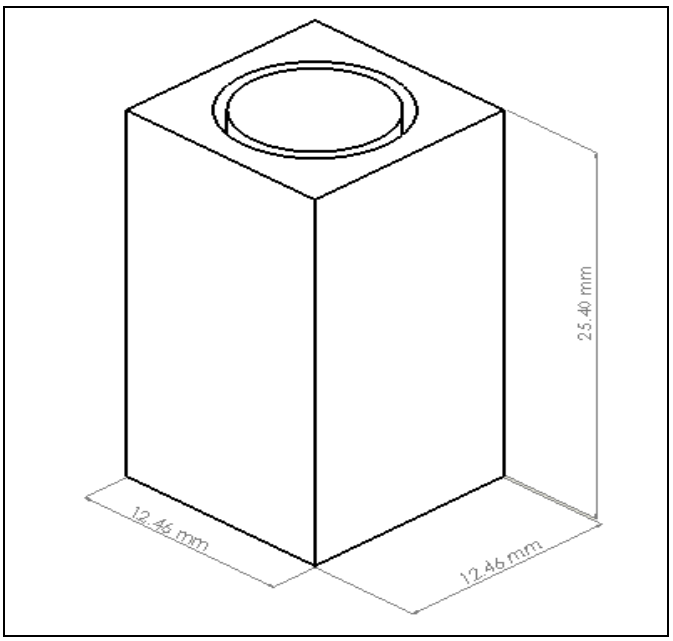

Figure 4: Isometric view of the geometric specifications of the simulated model

Due to computational limitations, the geometry of the simulated control volume had to be reduced. The symmetrical properties of the control volume, and the addition of reflective boundaries, enabled the use of a quarter model, as seen in Figure 5.

The reflective boundaries, enables the refined model to successfully simulate a full circumferential control volume, and infinite fuel pin array, by duplicating the surfaces in all the simulated directions.

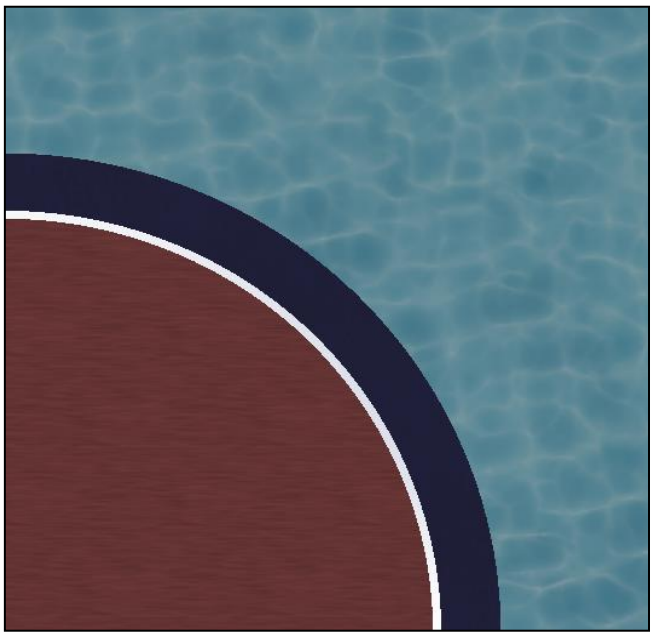

Figure 5: Top view of the quarter model control volume as simulated in MCNP 6.1 Beta

4.1.2 Material description

The material breakdown, of the quarter model control volume as depicted by Figure 6, provides an indication of the layout of the fuel pellet, cladding material, and moderator.

4.1.2.1 Fuel pellet

The fuel pellet, will be isotopically altered, to simulate various conceptual fuel compositions, thereby investigating their isotopic and neutronic interactions, during burnup. The evaluated fuel compositions will consists of LEU, MOX, and isotopic inclusion of selected isotopes. It is important to note, that all other aspects of the quarter model control volume, will be kept constant, to ensure accurate, and reliable results.

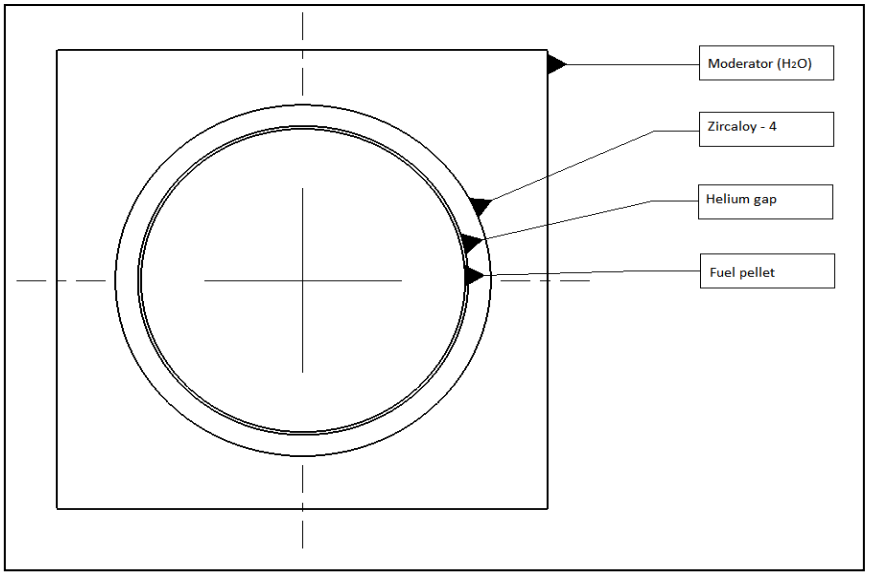

Figure 6: Material breakdown of the materials used for the simulated model

4.1.2.2 Helium gap

The fissure between, the fuel pellet and the cladding material is filled with helium, this aids in the heat transfer from the fuel pellet to the cladding material. Helium is an inert gas, and will therefore not compromise any fuel characteristics, or neutron economy.

4.1.2.3 Cladding material

The cladding material used during simulations, correspond isotopically to the composition used in currently operational PWRs. The cladding material is called Zircaloy - 4 and is an amalgamation of various isotopes of zirconium (Zr), tin (Sn), chromium (Cr) and iron (Fe). This composition aims at preventing the moderator from coming in contact with the fuel pellet, thus preventing radionuclide contamination and oxidation of the fuel pellets, while simultaneously minimising absorption of neutrons.

4.1.2.4 Moderator/coolant

The moderator is used to thermalize neutrons enabling safe reactor operation within the thermal energy spectrum. The moderator/coolant is also used to extract heat from the reactor core, subsequently reducing fuel temperatures to within operational limits. The water is used as moderator in PWRs and has to be kept under pressure to increase its boiling temperature.

4.1.3 Optimization strategy

The numerical models, will evaluate isotopic, and neutronic interactions of an infinite reactor geometry, during burnup simulations. After the result verification process, various conceptual fuel compositions can be analysed, and evaluated for feasibility, and implementability.

Conceptual homogeneous fuel amalgamations will be evaluated to determine if they are a suitable substitute, for the LEU fuel composition, currently implemented in Koeberg nuclear power plant. The feasibility of the fuel composites will be determined by analysing their ability to extend the fuel cycle length, reduce the initial infinite neutron multiplication factor (k_∞), increase fissile isotope breeding rates, reduced depletion rates of fissile isotopes.

Before the optimization process can commence, a benchmark for isotopic, and neutronic interactions, of the predominant fertile and fissile isotopes, currently found in PWRs and / or their spent fuel depositories, had to be generated. The aforementioned is achievable, by simulating a standard isotopic composition percentage, of each of the predominant fissile isotopes, in combination with each of the predominant fertile isotopes.

Koeberg nuclear power plant currently operates, on a LEU fuel composition, with an enrichment of 4.5% ^{235}U, which is below the permitted limit of 5% ^{235}U. This served as the basis, for evaluating the effect of an increased enrichment, as the primary approach, to extend the fuel cycle length.

The increased enrichment, will cause an increased initial infinite neutron multiplication factor (k_∞), and as this is a limiting parameter for feasibility, isotopic inclusions of isotopes, with high thermal neutron capture cross sections, like boron, and thorium can be used to mitigate the effect of the increased enrichment. Conceptually, the addition of the aforementioned will reduce the initial infinite neutron multiplication factor (k_∞), whilst preserving the fissile reserve of the fuel, consequently resulting in extended fuel cycle lengths. The isotopic inclusion of a fertile isotope like ^{232}Th, could be beneficial, as it will reduce, the initial excess reactivity, and breed fissile ^{233}U, which will ultimately contribute to an extended fuel cycle length.

Utilisation of spent fuel, can be increased by, analysing the feasibility of conceptual fuel compositions, containing reactor grade plutonium, or MOX fuel, as a substitute for the standard LEU fuel composition, or to be used as a supplement.

4.2 Anticipated challenges

An implementable conceptual design, requires adherence to certain isotopic, and thermodynamic characteristics that could potentially result, in adverse operational parameters. Mitigation of the aforementioned, is a fundamental practice for increased feasibility.

4.2.1 Plutonium

High concentrations of plutonium, will have adverse effects on the safety characteristics of the reactor.

4.2.1.1 Excess reactivity

Due to the higher fission cross section of ^{239}Pu and ^{241}Pu, the presence of these isotopes will increase for neutrons being absorbed to create fissioning of these isotopes, as opposed to being for instance parasitically absorbed by neutron poisons in the fission products. These Pu isotopes also have a greater neutron yield per fission neutron than any of the other predominant fissile isotopes. Subsequently the addition of fissile plutonium will cause excess initial reactivity and will require upgraded reactivity control.

4.2.1.2 Reactivity coefficients

Substantial inclusion of Pu might produce a positive void reactivity coefficient and even a positive moderator temperature reactivity coefficient. This is partly attributed to the, fission cross section peak of ^{239}Pu and ^{241}Pu near 0.3 eV in the thermal energy range. These are not permitted in commercial reactors and should thus be kept in consideration during conceptual fuel design.

4.2.1.3 Heat transfer capabilities

The thermal conductivity coefficient of plutonium, is inferior when compared with, that of other fuel options. Therefore large additions of plutonium, will reduce the extractable amount of heat from the fuel pellet to the moderator, where it is then extracted by the steam generators (SG). The decreased heat transfer capabilities, will result in higher

fuel temperatures, and a reduced neutron economy, due to excessive neutron captures in the resonance area, as a result of Doppler broadening.

4.2.1.4 Neutron economy

If large concentrations of reactor grade plutonium, known to contain large amounts of ^{240}Pu, is added to the fuel composition, drag will be placed on the neutron economy, due to the extremely high radiative neutron capture cross section resonance peak of ^{240}Pu at 1.05 eV.

Unfortunately ^{240}Pu, is not the only fertile isotope of plutonium, with a high radiative neutron capture cross section, in the thermal end epithermal energy spectrum. The radiative neutron capture cross section of all the fertile isotopes of plutonium (^{238}Pu, ^{240}Pu, ^{242}Pu) are higher than for any other known fertile isotope, with regard to neutron capture cross section in the thermal energy spectrum.

4.2.1.5 Reprocessing

Chemical reprocessing of plutonium, subsequently making it commercially implementable is a very costly endeavor, due to the low product yield and due to the high levels of radiation from the various radioactive isotopes in the Pu transmutation chain.

4.3 Summary

The conceptual designs as described above, have been simulated in MCNP 6.1 Beta, as an infinite reactor by means of reflective boundaries. A quarter sized control volume with reflective boundaries, has been developed to reduce geometric complexity, and computational time.

Challenges regarding, the composition of the conceptual fuel design, have been addressed. Furthermore, the aforementioned, have been set as objectives, thereby conceptualizing a design that mitigates the challenges as mentioned in section 4.2.1.

Chapter 5. Results

Overview

The results of numerous numerical models and tests used, as verification for the various conceptual fuel compositions. Depict the effect and detailed characteristics of isotopic substitution in known fuel amalgamations, during burnup simulations. Criticality calculations over extended burnup periods, to serve as further feasibility, and implementability analysis, of the proposed conceptual fuel compositions.

5.1 Reference models

Reference models are used to verify computational results by comparing burnup data from models found in published literature with geometric similar simulated fuel pin specifications, and power densities.

The references used for the data verification process include, the Swedish Ringhals 3 PWR which is enriched with 3.1 a/o ^{235}U and South Africa's, Koeberg PWR which has 4.5 a/o ^{235}U. The burnup data for the above mentioned were gathered from papers published by (Thor Energy, Norway, 2012) and (Du Toit & Cilliers, 2014) respectively.

Due to computational and time limitations, geometric complexity had to be reduced, ultimately resulting in reduced time duration for burnup calculations. The refined model, as specified in the Chapter 4 of this report, required an accuracy analysis to ensure dependable results. The accuracy analysis was initiated by duplicating power density, cycle length, fuel geometry, isotopic atom fraction specifications and simulating an infinite fuel pin burnup of the specified materials. The above mentioned process was applied for both of the reference cases.

The accuracy and verification process is delineated by two steps; the first step is the code verification process, were the MCNP 6.1 Beta results are compared with the data generated by another reactor modulating code (RMC) in the case of (Thor Energy, Norway, 2012) the CASMO-5 code. The second step, is verification of the generated data, by comparing burnup data from simulations done by (Du Toit & Cilliers, 2014) of a standard 17 x 17 Koeberg nuclear reactor fuel assembly, ensuring that results are statistically relevant.

5.2 Reference model detailed geometric specifications

The geometric specifications used to simulate the reference models are listed in Table 1. It is important to note that both of the cycles used as verification benchmark were comprised of a homogenous low enriched UOX fuel mixture.

Table 1: Design specifications used for reference numerical models.

	Ringhals 3	**Koeberg**
Parameter	Value and units	Value and units
Fuel pellet radius	0.4096 [cm]	0.4096 [cm]
Cladding inner radius	0.4178 [cm]	0.4178 [cm]
Cladding outer radius	0.4750 [cm]	0.4750 [cm]
Pin pitch	1.26 [cm]	1.26 [cm]
Fuel density	10.607 [g/cm^3]	10.607 [g/cm^3]
Cladding density	6.55 [g/cm^3]	6.55 [g/cm^3]
Coolant density	1.003 [g/cm^3]	1.003 [g/cm^3]
Power density	105.5 [kW/dm^3]	102.8 [kW/dm^3]
Power Output	1047 [MWe]	930 [MWe]
Enrichment	3.1 a/o ^{235}U	4.5% a/o ^{235}U

Table 2: Temperatures of relevant materials used in the reference models

Material	**Temperature [K]**
Coolant [H_2O]	600 K
Cladding [Zr_4-Alloy]	600 K
Helium gas [^{2}He]	600 K
Fuel [UOX]	900 K

The material operating temperature for the reference models are listed in Table 2. The isotopic cross section data was evaluated at the specified temperatures in accordance with the MCNP data tables.

MCNP 6.1 Beta has built in material libraries which were used for all models and were specifically developed in such a manner that each material has the isotopic composition of the isotope in highest natural abundance. The above mentioned is not relevant for scenarios where simulated materials were enriched with a specific isotopes, as stated by (Winter, 1993-2015).

5.3 Uranium dioxide (UOX) references

Two reference models were created in MCNP 6.1 Beta, both containing UO_2 with varying atom fraction enrichment percentages of ^{235}U and without the addition of any burnable poisons (BP).

5.3.1 UOX model with 3.1 a/o ^{235}U

The first low enriched UOX model contains 3.1 a/o ^{235}U corresponding to the specifications of a standard Ringhals 3 17 x 17 fuel lattice, simulated in CASMO-5 by (Thor Energy, Norway, 2012). It is important to note that (Thor Energy, Norway, 2012) did a burnup of an infinite fuel assembly, the relevance of using this reference is to analyse the accuracy of an infinite fuel pin burnup in MCNP 6.1 Beta by comparing the computed results. The data was verified on the basis of the infinite multiplication factors (k_∞) behaviour over time, during a constant power density burnup of an infinite fuel pin.

A high correspondence between the data sets will enable the assumption that it is sufficient to use infinite fuel pin burnup simulations for preliminary evaluations of various fuel compositions, and that the computed results has an ample accuracy.

The UOX-reference burnup results with the addition of some thorium-MOX fuel simulations done by (Thor Energy, Norway, 2012) are depicted in Figure 7. It is important to note that for the data verification process as described above the only data set of interest is the UOX-without Burnable Absorbers (woBA). Figure 8 depict the comparison between the UOX-woBA cycle simulated in CASMO-5 and the 3.1 a/o ^{235}U UOX reference model simulated in MCNP 6.1 Beta.

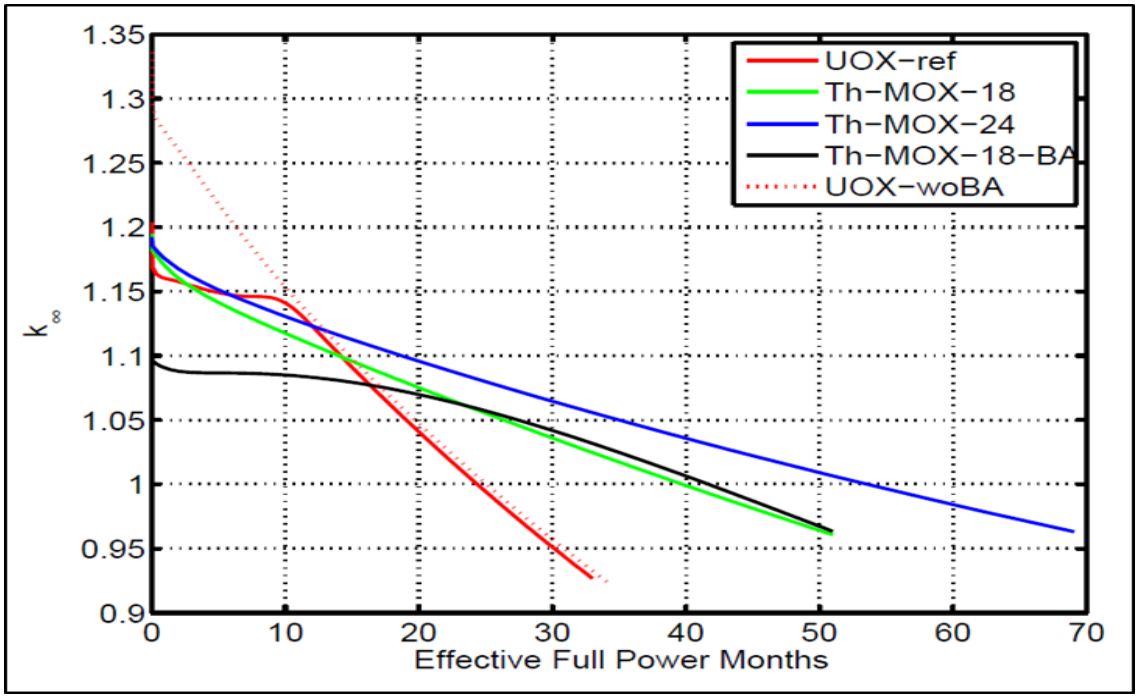

Figure 7: Dependence of the infinite multiplication factor (k∞) with respect to time during a burnup simulation by (Thor Energy, Norway, 2012).

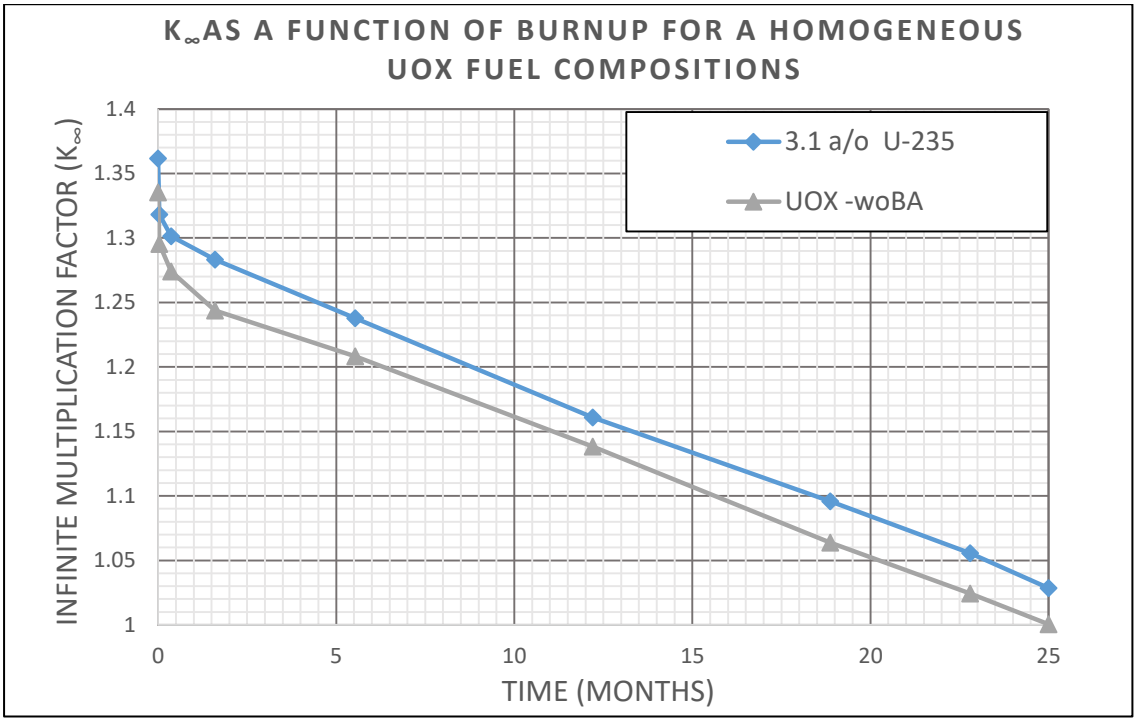

Figure 8: Comparison of the dependency of the infinite multiplication factor (k∞) with respect to time, during burnup simulations of the selected UOX reference models.

5.3.2 Discussion of results

Table 3 depict the computed infinite multiplication factor (k_∞) from the 3.1 a/o ^{235}U reference model compared with the data obtained from the UOX-woBA CASMO-5 simulations done by (Thor Energy, Norway, 2012) . To determine the percentage difference, the following formula was used:

$$Percentage\ Difference = \frac{\Delta v}{\frac{\sum v}{2}} x100 = \frac{v_1 - v_2}{\frac{v_1 - v_2}{2}} x100$$

Table 3: Comparison of the infinite multiplication factor (k_∞) values with regard to time during burnup simulations for the UOX-woBA and 3.1 a/o ^{235}U UOX reference models.

Time (Months)	k_∞ - UOX-woBA	k_∞ - 3.1 a/o ^{235}U	Percentage difference [%]
0	1.33545	1.36171	1.9472
0.033333	1.29551	1.3183	1.7438
0.366667	1.27409	1.30128	2.1115
1.6	1.24386	1.28325	3.1173
5.533333	1.20822	1.23786	2.4234
12.2	1.13835	1.16089	1.9606
18.86666	1.06382	1.09575	2.9570
22.8	1.02429	1.05549	3.0003
25	1.00040	1.02852	2.7719
Average percentage difference		**2.44815 %**	

It is apparent from the data that the simulations have a very high correspondence, with a negligible average percentage difference of only 2.44815%.

5.3.3 UOX model with 4.5 a/o ^{235}U

The second UOX model contains 4.5 a/o ^{235}U corresponding to a standard Koeberg 17 x 17 fuel lattice also coded in CASMO-5 and simulated by (Du Toit & Cilliers, 2014). The data was verified on the basis of the infinite multiplication factors (k_∞) behaviour over time, during a constant power density burnup of an infinite fuel pin.

Similar to the first UOX-woBA reference it is important to note that (Du Toit & Cilliers, 2014) also did a burnup of an infinite fuel assembly, the relevance of using this reference is to analyse the similarity of the data since (Du Toit & Cilliers, 2014) also simulated a standard Koeberg fuel cycle. A high correspondence between the data sets, will enable the assumption that it is sufficient to use infinite fuel pin burnup simulations for preliminary evaluations of higher enriched fuel compositions, and that the computed results has an ample accuracy.

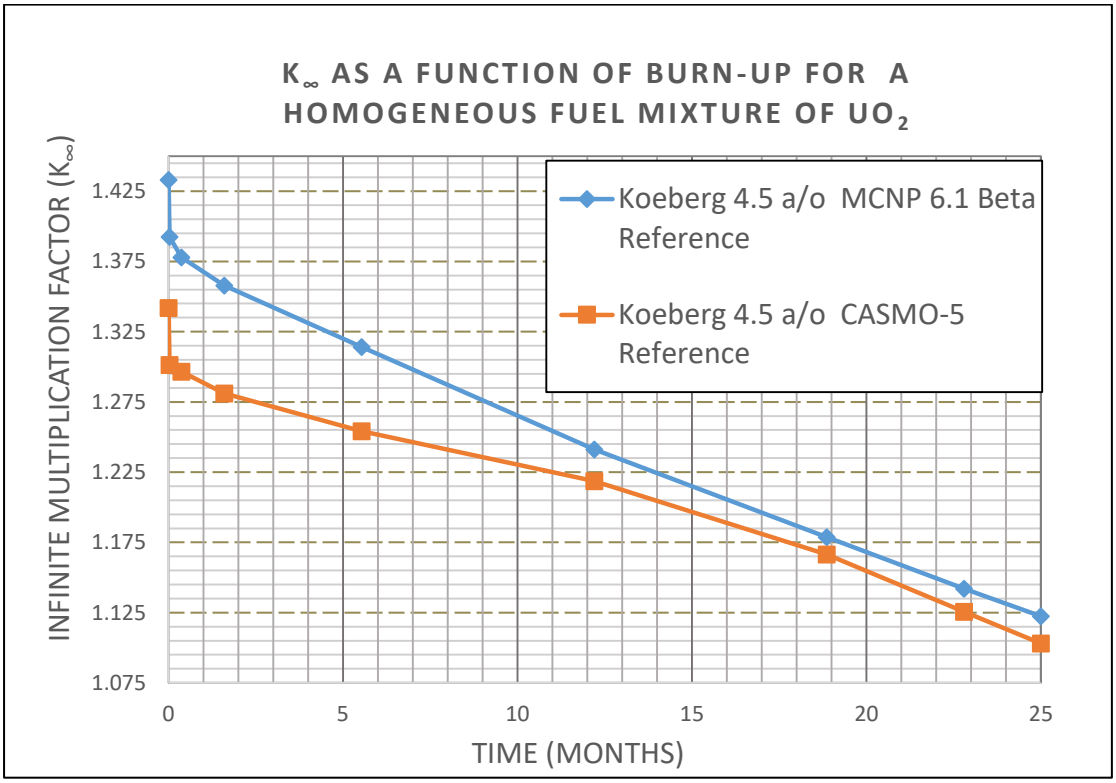

Figure 9: Comparison of the dependency of the infinite multiplication factor (k_∞) with respect to time, during burnup simulations of the selected UOX reference models.

5.3.4 Discussion of results

By analysing the burnup data in Figure 9 it is evident that burnable absorbers are present in the fuel composition, which would explain the lower initial infinite multiplication factor of the Koeberg 4.5 a/o CASMO-5 model simulated by (Du Toit & Cilliers, 2014). Further evaluation indicated that during the burnup simulations of the infinite fuel lattice 12 of the rods in the standard 17 x 17 Koeberg fuel lattice were superseded by GdO_3 and ZrB_2 rods.

Table 4 depict the computed infinite multiplication factor (k_∞) from the Koeberg 4.5 a/o ^{235}U MCNP 6.1 Beta reference model compared with the data obtained from the Koeberg 4.5 a/o ^{235}U CASMO-5 simulations done by (Du Toit & Cilliers, 2014).

Table 4: Comparison of the infinite multiplication factor (k_∞) over time due to burnup for the Koeberg 4.5 a/o ^{235}U MCNP 6.1 Beta Reference and Koeberg 4.5 a/o ^{235}U CASMO-5 Reference models.

Time (Months)	k_∞ - Koeberg 4.5 a/o MCNP 6.1 Beta	k_∞ - Koeberg 4.5 a/o CASMO-5	Percentage difference [%]
0	1.39809	1.3420	6.5679
0.033333	1.35938	1.3013	6.7737
0.366667	1.34453	1.29652	6.0916
1.6	1.32555	1.28103	5.8192
5.533333	1.28259	1.25407	4.6787
12.2	1.21402	1.21872	1.8213
18.86666	1.15621	1.16647	1.0379
22.8	1.11711	1.12559	1.4544
25	1.09793	1.103025	1.7475
Average percentage difference		**3.9991 %**	

It is apparent from the data that the simulations have a high correspondence, with an average percentage difference of 3.9991%. The average percentage difference, is

substantially higher than the 3.1 a/o ^{235}U and UOX-woBA reference case mainly due to the burnable absorbers added to the fuel assembly, which dramatically decreased the infinite multiplication factor (k_∞), for the first few months of the burnup simulation.

The effect of the burnable absorbers have completely dissipated at about 1 months into the burnup simulation. At that point, the average percentage difference becomes 2.248075% for the remainder of the 25 month burnup simulation, which can be considered as a very high correspondence between the data sets.

By comparing the average percentage difference from the two reference cases, 2.44815% without burnable absorbers, and 3.9991% with burnable absorbers, it is evident that there is also a close correspondence, between the generated data sets.

5.3.5 Conclusion

The data obtained, from the various reference simulations indicated that MCNP 6.1 Beta would suffice as an infinite fuel pin burnup modulating code, for fuel compositions consisting of various isotopes, due to the high correspondence between the published and compute results for the infinite multiplication factors (k_∞) behaviour, with regard to time, at a constant power density burnup.

The burnup data provided valuable information with regard to operational limitations of the simulated fuel cycles. By determining the infinite multiplication factor (k_∞) over a 25 month burnup period, it enabled the estimation of the point where the reactor would need to be shut down for refuelling. This point is reached when the effective multiplication factor (k_{eff}) is below 1.

The value for k_{eff} =1 was estimated as the k_∞ value at day 480 of the 4.5 a/o ^{235}U reference model simulated in MCNP 6.1 Beta. The aforementioned value k_∞= 1.205 was chosen as one of the parametrical constraints, and served as a feasibility benchmark for all conceptual fuel compositions tested in this document.

To clarify k_∞=1.205 is the lower operational limit of the reactor, for an infinite multiplication factor (k_∞) lower than 1.205 a sustainable fission reaction will not be possible thus the k_∞ value should always be greater or equal to 1.205.

5.4 Characteristics of homogeneous fuel compositions of specific fissile and fertile isotopes

The following section depict the detailed characteristics of the main fissile and fertile isotopes currently present in PWR fuel compositions.

5.4.1 Introduction

In this section, various fissile and fertile isotopes were characteristically analysed to determine which homogeneously mixed, combination of isotopes would yield the best overall result, with regard to the problem statement as specified in Chapter 1 section 1.3.2 of this document. The isotopes selected for analysis were specifically chosen, and correspond to the predominant isotopes used in currently operational pressurized water reactors and/or found in their spent fuel depositories. The aforementioned isotopes are delineated by two groups, fissile isotopes: ^{233}U, ^{235}U, ^{239}Pu, ^{241}Pu and fertile isotopes: ^{232}Th, ^{238}U, ^{238}Pu, ^{240}Pu, ^{242}Pu.

5.4.2 Methodology

To separately determine the effect of each isotope, independent homogeneous mixtures of each fissile and fertile isotope were simulated by burn-up calculations of an infinite fuel pin in MCNP 6.1 Beta. Realistically these isotopic amalgamations would feasible as it is, for instance, not possible to obtain pure ^{235}U and therefore it is not possible to manufacture a mix of pure ^{235}U and pure ^{232}Th. However, for the sake of gaining insights into each isotopes neutronic interactions in reactor conditions, such fuel compositions were simulated.

Limiting factors for isotopic enrichment of certain fissile isotopes include the legislation applicable on non-military enrichment facilities, inhibiting the a/o ^{235}U greater than 5%. For this reason, the atom fraction enrichment of each of the fissile isotopes were limited to 5% and homogeneously mixed with a single fertile isotope with an atom fraction percentage (at. %) of 95%. The geometric and power density specifications are identical to the Koeberg 4.5 a/o ^{235}U MCNP 6.1 Beta reference model.

The burnup data from the various homogeneous isotopic composition, will serve as a benchmark for expected behaviour of further more complex fuel compositions. Table 5 depict all the combinations of fissile and fertile material tested during the data acquisitioning process. All isotopic compositions were simulated as mixtures of the following chemical compositions: UO_2, ThO_2 or PuO_2.

Table 5: Benchmark isotopic compositions index

Isotopic compositions evaluated for benchmark			
Fissile Isotopes of Uranium	**Fertile Isotopes**	**Fissile Isotopes of Plutonium**	**Fertile Isotopes**
(5%)U233	(95%)Th232	(5%)Pu239	(95%)Th232
	(95%)U238		(95%)U238
	(95%)Pu238		(95%)Pu238
	(95%)Pu240		(95%)Pu240
	(95%)Pu242		(95%)Pu242
(5%)U235	(95%)Th232	(5%)Pu241	(95%)Th232
	(95%)U238		(95%)U238
	(95%)Pu238		(95%)Pu238
	(95%)Pu240		(95%)Pu240
	(95%)Pu242		(95%)Pu242

5.4.3 Nuclear data comparison

The following segment will provide a comprehensive analysis of the isotopic and neutronic interactions during burn-up simulations done in MCNP 6.1 Beta of the fuel compositions described in Table 5.

Each of the fissile isotopes with their corresponding fertile isotopes were evaluated on the following basis: infinite multiplication factor (k_∞), total number of capture and fission reactions at Beginning of Life (BOL), neutron yield per fission reaction, the fuel mixtures ability to breed fissile isotopes (breeding ratio), moderator temperature reactivity, void reactivity, and fuel temperature reactivity coefficients.

5.4.3.1 Uranium – 233

The following section depict all relevant data with regard to ^{233}U.

5.4.3.1.1 Characteristics of uranium - 233

Uranium-233 is a synthetic isotope of uranium, meaning it has no natural abundance. It is produced in nuclear reactors with Th fuel compositions as a result of neutron capture by ^{232}Th, to form ^{233}Th, which then β^- – decays to ^{233}Pa and lastly to ^{233}U. Figure 10 depict the radiative neutron capture and fission cross section (OECD, 2016) for ^{233}U in the thermal, epithermal and fast neutron energy spectrum.

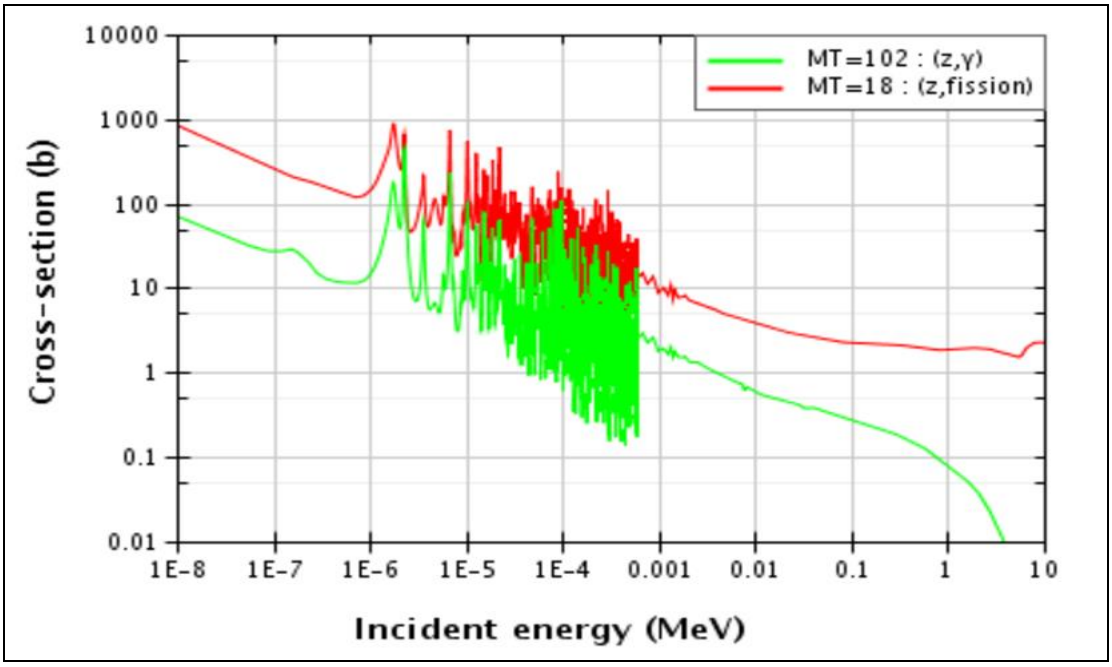

Figure 10: Radiative capture and fission cross section for ^{233}U (OECD, 2016)

From Figure 10 it is evident that ^{233}U has a higher fission than radiative capture cross section in the thermal (0.0253 – 0.5 eV), fast (100 keV – 20 MeV) and most of the epithermal (0.5 eV – 100 keV) energy spectrum. In comparison with the thermal fission and radiative capture cross sections, the fission and radiative capture cross sections in the fast energy spectrum are substantially lower. ^{233}U is the best fuel to use in thermal reactors, including Pressurized Water-cooled Reactors (PWR). This is mainly due to the fact that the thermal capture-to-fission ratio (α) of 233U is the lowest of all fissile isotopes and therefore its number of fission neutrons released per thermal neutron absorbed (η) is the highest of all readily available fissile isotopes (Lamarsh & Baratta, 2012). This also applies to PWRs, as the ^{1}H nuclei in the water thermalize neutrons very effectively and therefore produce well moderated neutron spectra. The only problem is that, unlike ^{235}U, ^{233}U is not naturally available and thus it has first to be bred from ^{232}Th before it can be used. Therefore, except where breeder reactors are used to first separately breed the ^{233}U, where after it is chemically extracted and inserted into PWR fuel, it is not possibly to have a PWR that runs on, for example, a mixture of ^{233}U and ^{238}U. More realistic is the option where the ^{233}U is bred and burned in situ by starting the fresh PWR fuel with a mixture of for instance Pu(PWR) as driver fuel and ^{232}Th as fertile fuel.

5.4.3.1.2 Neutron yield per fission neutron for ^{233}U

The fission neutron yield per fission of ^{233}U as seen in Figure 11 can be estimated at 2.498 neutrons per fission neutrons for the thermal energy spectrum, this corresponds with the 2.4968 neutrons per thermal fission neutron for ^{233}U as published by (IAEA, 2007). It is noteworthy that ^{233}U is the uranium isotope with the highest neutron yield per thermal fission neutron.

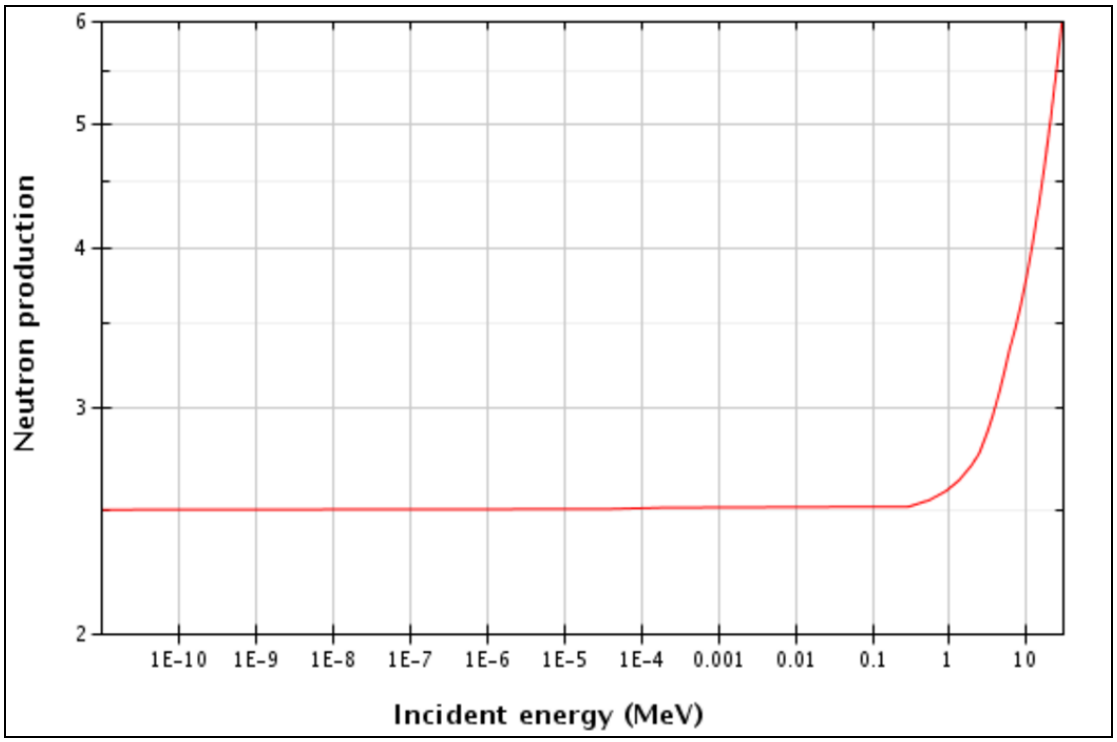

Figure 11: Fission neutrons yield per fission reaction for ^{233}U (OECD, 2016)

5.4.3.1.3 Reactivity coefficients of ^{233}U fuel compositions

Figure 12 and Figure 13 is an amalgamation of the fission and radiative capture cross sections respectively, and depict all the isotopes tested in the above mentioned fuel compositions. By analysing the portrayed data in Figure 12 and Figure 13 predictions can be made of the neutronic and isotopic behaviour of the fuel compositions during accident scenarios.

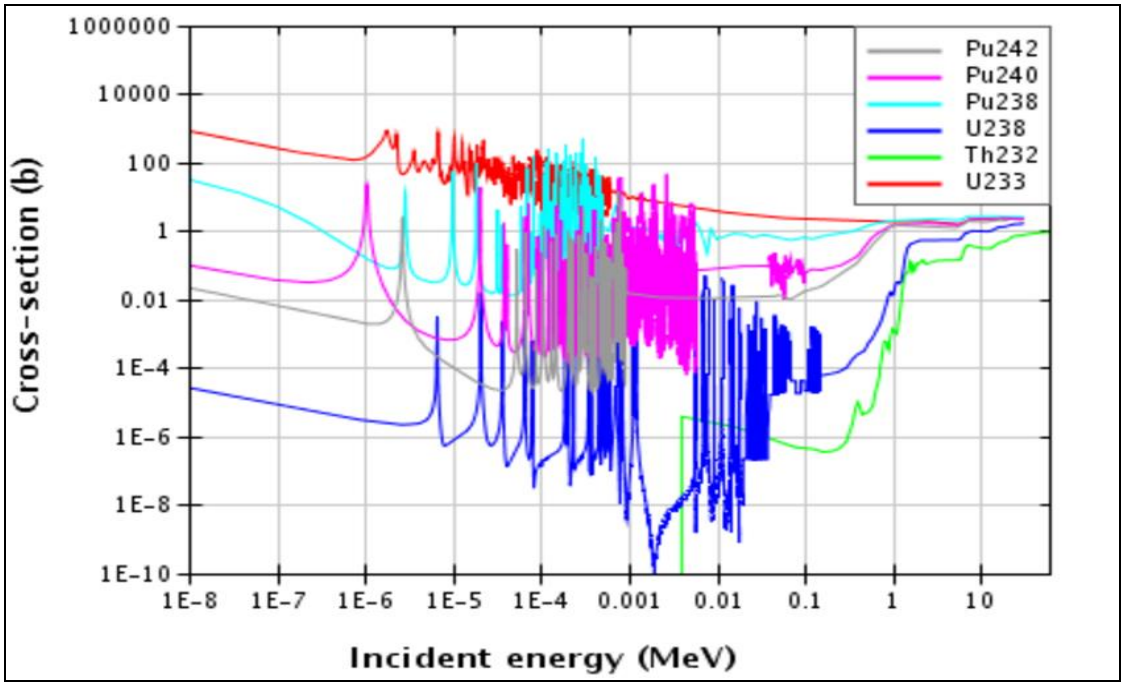

Figure 12: Fission cross sections for all the isotopes tested in the ^{233}U homogeneous fuel mixtures (OECD, 2016)

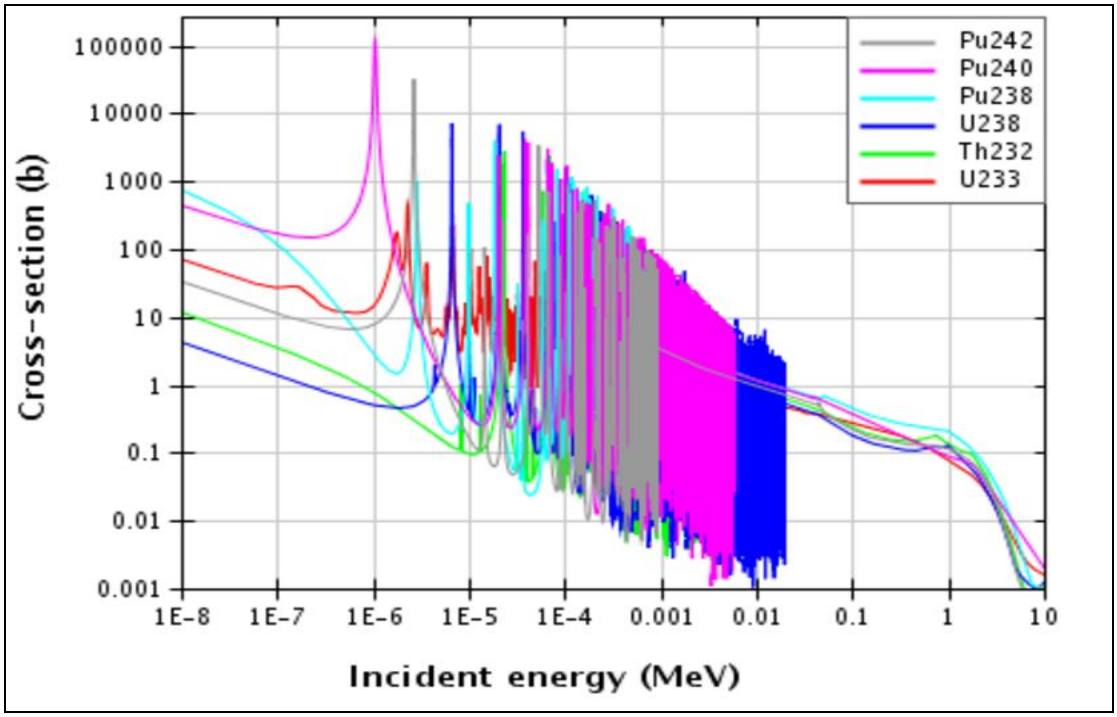

Figure 13: Radiative capture cross section for all the isotopes tested in the ^{233}U homogeneous fuel mixtures (OECD, 2016)

From the fission cross sections portrayed by Figure 12: Fission cross sections for all the isotopes tested in the ^{233}U homogeneous fuel mixtures , it is evident that in the thermal energy spectrum as the only fissile isotope ^{233}U has the highest probability of undergoing a fission reaction of all the simulated isotopes. This ensures utilization of thermal neutrons where intended and provides a level of safety with regard to unsolicited fluctuations in the infinite multiplication factor due to fissioning of unanticipated isotopes.

5.4.3.1.4 Moderator temperature reactivity coefficient

In an accident scenario; for example a partial reduction in coolant primary flow, a small to moderate increase in moderator temperature occurs and resultantly peak in the Maxwell neutron energy distribution in the moderator shifts up to higher energies. Other than in ^{235}U, this will lead to an increased fission rate in ^{233}U. See Table 3.2 of (Lamarsh & Baratta, 2012). In large concentrations, ^{233}U will thus increase the infinite neutron multiplication factor (k_∞), which could result in a positive moderator temperature reactivity coefficient, which from a safety standpoint could become problematic.

It is noteworthy to mention that for small increases in moderator temperature, and a fuel mixture with a high concentration of ^{233}U, and ^{232}Th, the predicted result will be a positive moderator temperature reactivity coefficient. This is due to the inferior capture cross section of ^{232}Th when compared with the fission cross section of ^{233}U for the 0.01 – 40 eV energy range as seen in Figure 14.

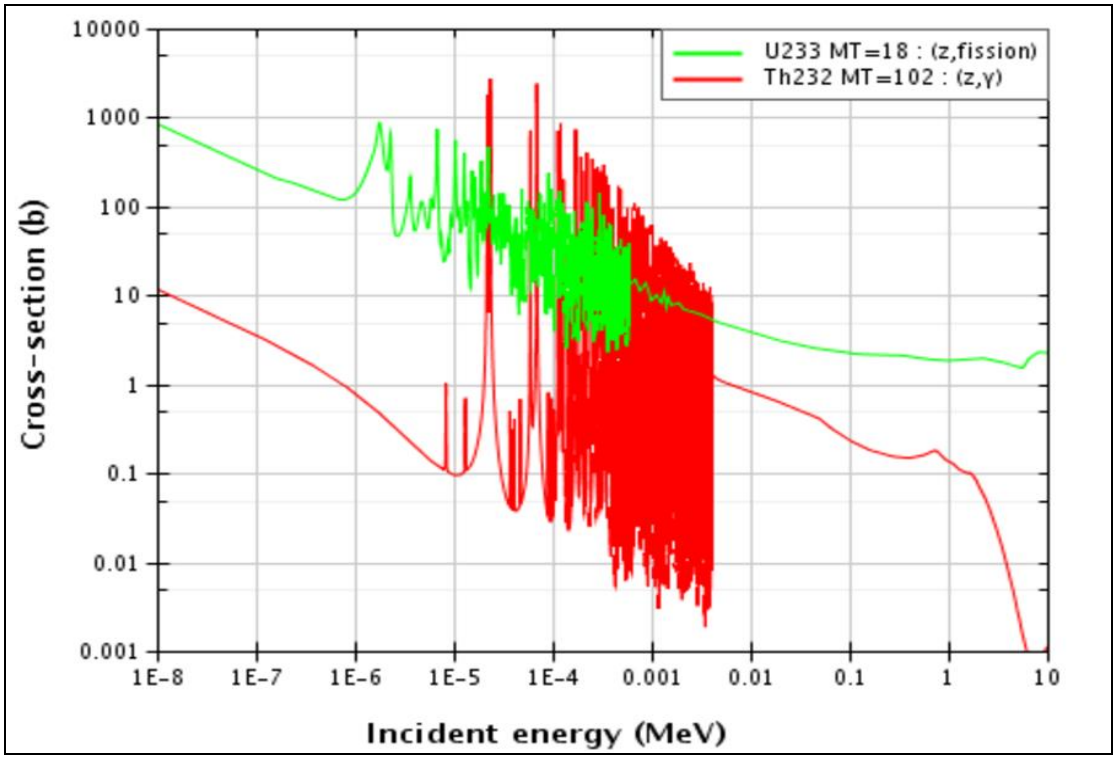

Figure 14: Comparison of the radiative neutron capture cross section of ^{232}Th and the fission cross section of ^{233}U (OECD, 2016)

5.4.3.1.5 Void reactivity coefficient

In the scenario where a void is formed in the reactor. This can be ascribed to moderator boiling (low pressure in primary loop), or insufficient heat removal due to a Loss of Coolant Accident (LOCA). Neutron thermalisation will diminish, due to a lack of moderation in the steam filled void, causing more fast fissions in the fissile and fissionable isotopes present in the fuel composition. In general faster neutrons are captured less and fast fissions yield more neutrons per fission, causing an increase in the infinite neutron multiplication factor (k_∞) with increasing void fraction, i.e. a positive void reactivity coefficient.

Mitigation of the aforementioned is possible, with the addition of isotopes with aggressive resonance capturing peaks, preferably a resonance capturing cross section spanning over a large section of the neutron energy spectrum and low fast fission cross sections.

From Figure 13, it can be concluded that the isotope that best counteracts a positive void reactivity coefficient is ^{232}Th, as it has resonance capture cross sections, spanning

over a large section of the epithermal energy spectrum. More importantly it has a much lower fast fission cross section that ^{238}U. Therefore the void-induced upshift in the energy spectrum cases less fissions in die accompanying fissile isotope in the thermal region, much more capture in the epithermal region and only a little more fast fissions, which will in most causes produce a negative void reactivity coefficient.

As seen in Figure 15, a positive void reactivity coefficient can occur in fuel compositions, containing high concentrations of ^{238}Pu and ^{242}Pu due to their small resonance capture cross sections. More importantly the fertile Pu isotopes, especially ^{238}Pu and ^{240}Pu (Figure 16), have much higher fast fission cross sections that ^{238}U and ^{232}Th.

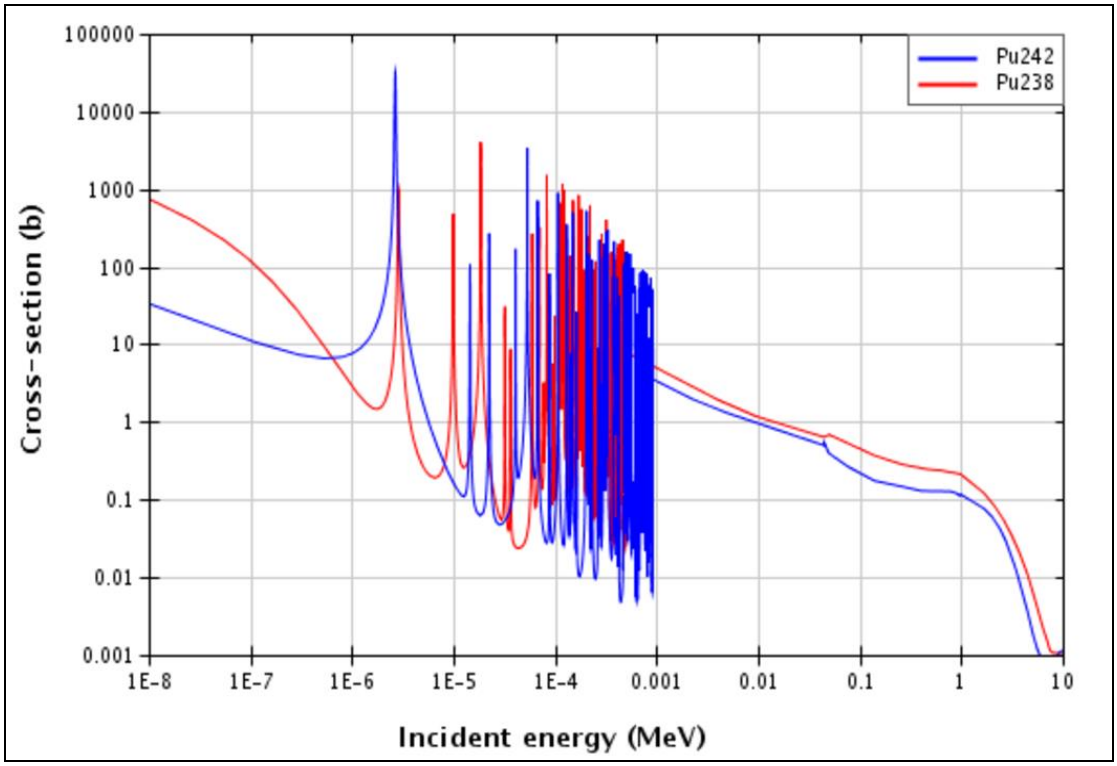

Figure 15: Radiative neutron capture cross section of ^{238}Pu and ^{242}Pu (OECD, 2016)

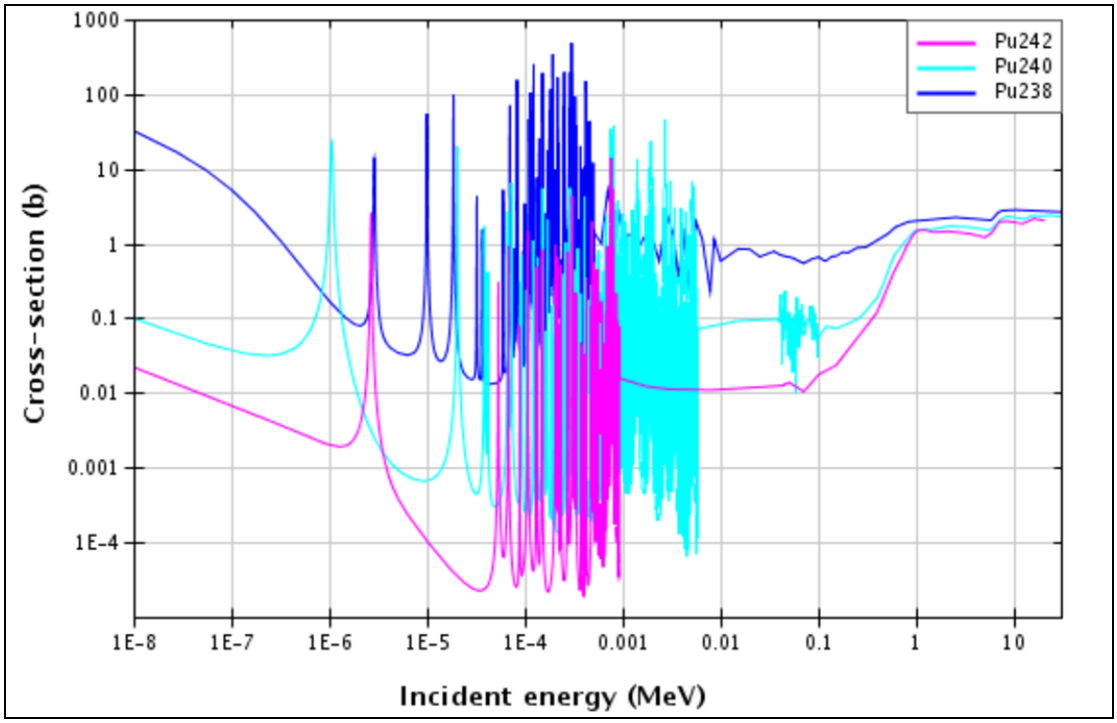

Figure 16: Fast fission cross section of ^{238}Pu, ^{240}Pu, and ^{242}Pu

5.4.3.1.6 Fuel temperature reactivity coefficient

In the scenario where an increase in fuel temperature occurs, Doppler broadening of the resonance fission and radiative capture peaks will occur. Doppler broadening decreases the neutron resonance escape probability and subsequently reduces the infinite neutron multiplication factor (k_∞). This gives the fuel composition a negative fuel temperature reactivity coefficient and thus increased inherent safety.

It is noticeable from Figure 13 that most of the capture resonance peaks have extremely high radiative capture cross sections, in the case of ^{240}Pu and ^{242}Pu as high as 140000 and 50000 barn respectively.

Fuel compositions comprised of isotopes with the same characteristics, used to mitigate a positive void reactivity coefficient can thus be used to ensure a negative fuel temperature reactivity coefficient. This can be attributed to the large resonance capture area and density of the capture peaks. PWR fuel compositions are specifically selected to utilize the phenomena of Doppler broadening, thus increasing the inherent safety of the reactor.

5.4.3.1.7 Computed results of Uranium-233 fuel compositions

The following section contains a discussion of the results acquired during burnup simulations of homogeneous mixtures of 5 a/o ^{233}U and 95 at. % of selected fertile isotopes.

The computed infinite multiplication factor (k∞) for ^{233}U fuel compositions as described in Table 5, are presented in Figure 17. The burnup data with regard to time will provide an indication of the capture, neutron energy spectrum, fission, and breeding capabilities of each homogenous fuel mixture. These results will be discussed further down after the reaction rate tables.

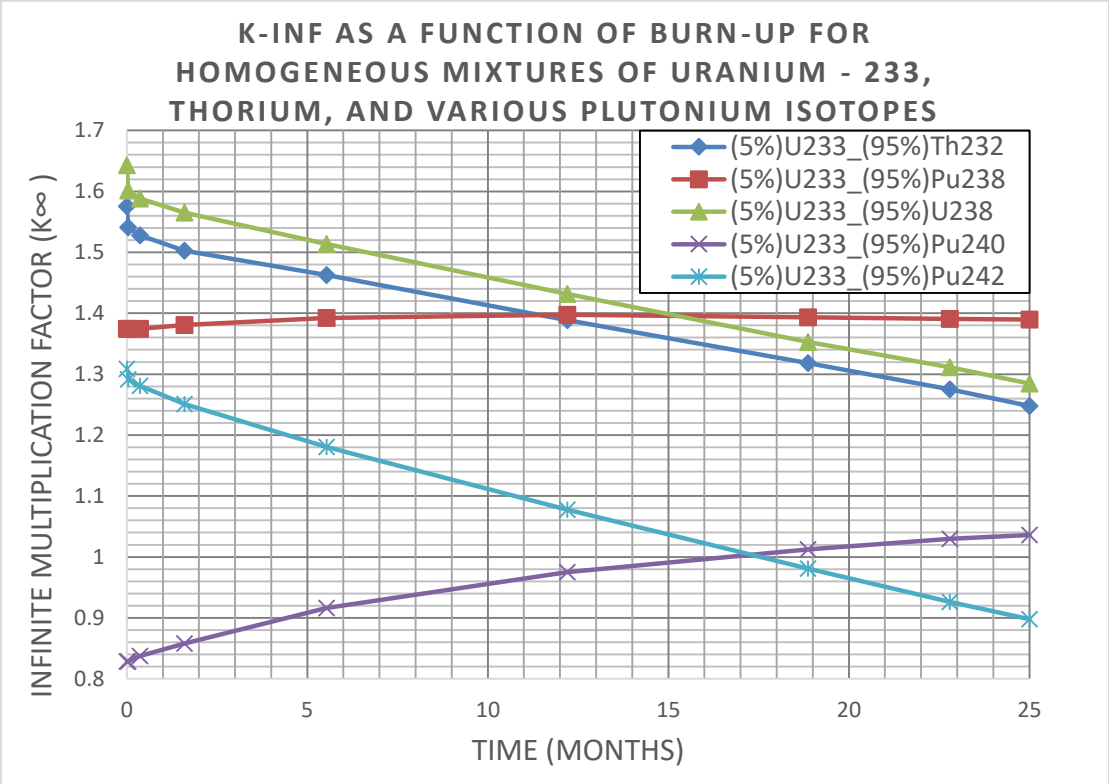

Figure 17: Infinite multiplication factor over time due to burn-up for homogeneous mixtures of 5 a/o ^{233}U and 95% (at.) of selected fertile isotopes

The data presented in Table 6, Table 7, and Table 8 indicate the amount of neutrons that underwent a certain interaction on day zero of the burnup simulations. The data was specifically analysed on day zero, to enable isotope characteristic evaluation before the isotopic composition is changed by burnup and breeding.

The capture data from each of the tested fuel compositions are displayed in Table 6. The acquisitioned data will serve as benchmark to predict the effect of certain isotopic interactions in more complex fuel compositions.

Table 6: Neutron captures in homogeneous mixtures of ^{233}U and other fertile isotopes on day zero of burnup

	Neutron captures					
Isotopic composition	**Moderator (H_2O)**	**Uranium-233**	**Fertile isotope**	**Oxygen (in fuel)**	**Helium**	**Zircaloy-4**
(5%)U233_(95%)Th232	1.8507E+11	4.3236E+11	1.3907E+12	9.1274E+09	0.0000E+00	2.9906E+10
(5%)U233_(95%)U238	1.7471E+11	4.0971E+11	1.2281E+12	8.7753E+09	0.0000E+00	2.8174E+10
(5%)U233_(95%)Pu238	8.1447E+10	2.1196E+11	3.4327E+12	1.3009E+10	0.0000E+00	2.2081E+10
(5%)U233_(95%)Pu240	1.0030E+11	3.0370E+11	7.7585E+12	1.9422E+10	0.0000E+00	3.9178E+10
(5%)U233_(95%)Pu242	1.4633E+11	3.3527E+11	3.0651E+12	1.1411E+10	0.0000E+00	3.0081E+10

Table 7: Total neutron captures for each ^{233}U fuel composition on day zero of burnup

Isotopic composition	Total captures
(5%)U233_(95%)Th232	2.047E+12
(5%)U233_(95%)U238	1.849E+12
(5%)U233_(95%)Pu238	3.761E+12
(5%)U233_(95%)Pu240	8.221E+12
(5%)U233_(95%)Pu242	3.588E+12

Table 8: Fission reactions in homogeneous mixtures of ^{233}U and other fertile isotopes on day zero of burnup

	Fissions	
Isotopic composition	**Uranium-233**	**Fertile isotope**
(5%)U233_(95%)Th232	3.4357E+12	3.8709E+10
(5%)U233_(95%)U238	3.32218E+12	1.52047E+11
(5%)U233_(95%)Pu238	1.4160E+12	2.0000E+12
(5%)U233_(95%)Pu240	1.8263E+12	1.6007E+12
(5%)U233_(95%)Pu242	2.6764E+12	7.8480E+11

5.4.3.1.8 Uranium– 233 fuel composition conclusion

- ^{238}U was the best fertile isotope as it could maintain k_∞ for the longest burn time (Figure 17), and could thus achieve the highest burn-up. k_∞ for ^{232}Th followed the same pattern, but remained somewhat lower throughout. From Table 7 it can be seen that the very low capture rate in ^{238}U, caused by its lower capture cross sections in the thermal energy spectrum as displayed in Figure 13, contributed to this success. The reduced number of neutron captures also resulted in higher abundance of thermal neutrons, which produced more fissions of the fissile ^{233}U, as is indicated in Table 8.
  The logic for the ^{232}Th is similar, except that its neutron capture rate was slightly higher, which resulted in a slightly lower k_∞.

- ^{242}Pu fared much worse, i.e. k_∞ started off on a much lower level and thereafter dropped faster. To lower starting point was be due to the high thermal microscopic radiative capture cross section for ^{242}Pu, which produced the high capture rate in Table 7. The fact that it also dropped faster was probably due to the fact that neutron capture in ^{242}Pu produces ^{243}Am, which is not fissile, as opposed to ^{238}U that produces fissile ^{239}Pu and ^{242}Th that produces fissile ^{233}U.

- ^{238}Pu and ^{240}Pu behaved completely differently in that both started at very low k∞ and then increased with burnup. The very low k∞ for ^{240}Pu was caused by its extremely high radiative capture resonance at 1.05 eV which produced the highest capture rate in Table 7. However, this produced fissile ^{241}Pu at a high rate, which is an excellent fissile fuel. Furthermore, the extremely high capture rate in the ^{238}Pu means that it will be depleted somewhat with burn-up and that its capture rate will thus decrease with burn-up. These two factors explain the sharp increase in k∞ with burn-up.

  The logic for the increase in k∞ for ^{238}Pu is similar, as it also produced the excellent fissile ^{239}Pu fuel at a high rate.

From the infinite neutron multiplication factor (k∞) as a function of burnup, depicted by Figure 17 and the total neutron captures per isotopic composition on day zero of burnup displayed in Table 7, it is evident that ^{232}Th and ^{238}U performed inferior in comparison with the neutron capture capabilities of any of the evaluated plutonium isotopes.

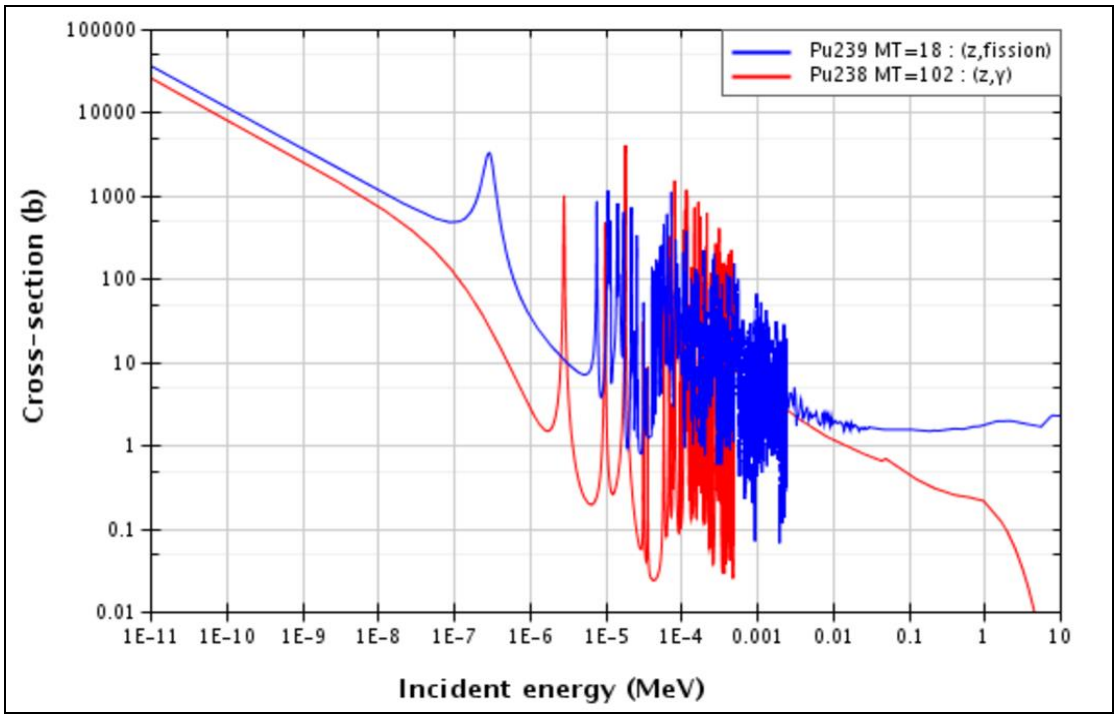

Figure 18: Radiative neutron capture cross section of ^{238}Pu and fission cross section of ^{239}Pu (OECD, 2016)

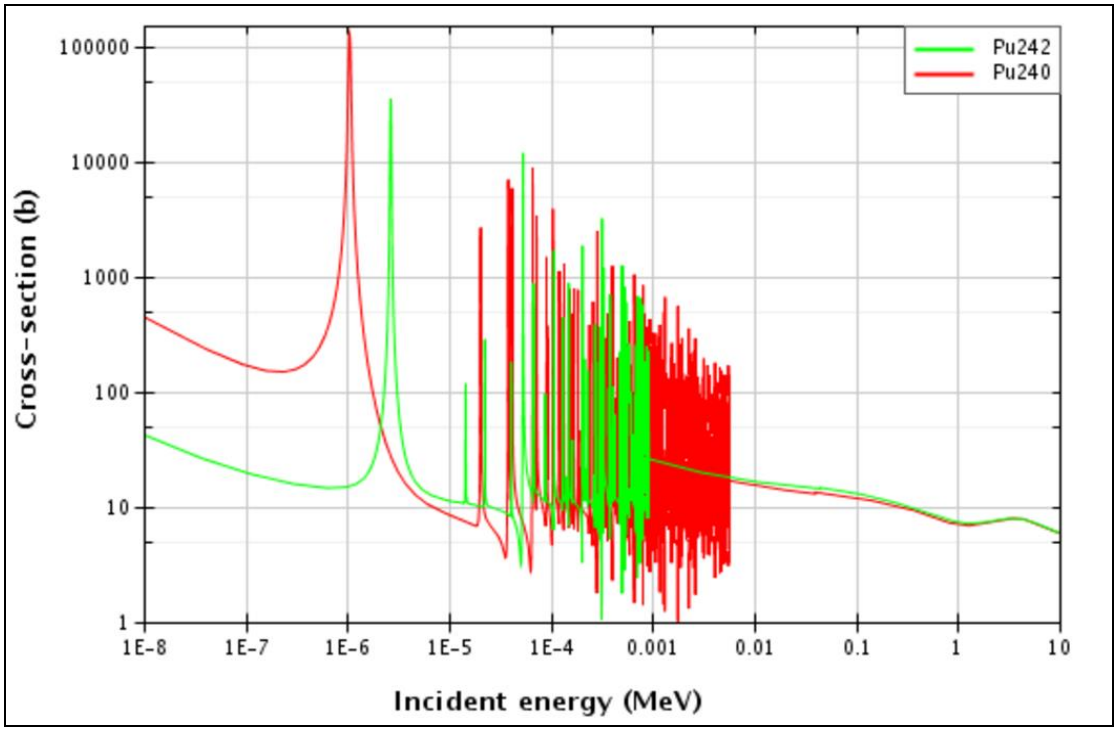

Figure 19: Total capture cross section of ^{240}Pu and ^{242}Pu (OECD, 2016)

The aggressive neutron captures of the ^{240}Pu, and ^{242}Pu fuel compositions, as seen in Table 7 can be contributed to the exceptionally high neutron capture peaks as seen in Figure 19 and provide a clear indication of the neutron energy distribution.

The increase in the infinite neutron multiplication factor (k_∞) over time, in the ^{240}Pu fuel composition can be contributed to the breeding of ^{241}Pu. In the ^{242}Pu fuel compositions, a decrease in the infinite neutron multiplication factor (k_∞) was observed, this can be ascribed to, two factors: the absence of fissile isotope breeding, and the breeding of neutron capture intensive isotopes, like americium (Am).

5.4.3.2 Uranium - 235

The following section depict all relevant data with regard to ^{235}U.

5.4.3.2.1 Characteristics of uranium - 235

Uranium - 235 is the most common fissile material used in currently operational nuclear reactors and has an abundance in natural uranium of 0.7 wt%, with the balance of 99.3 wt% comprised of ^{238}U.

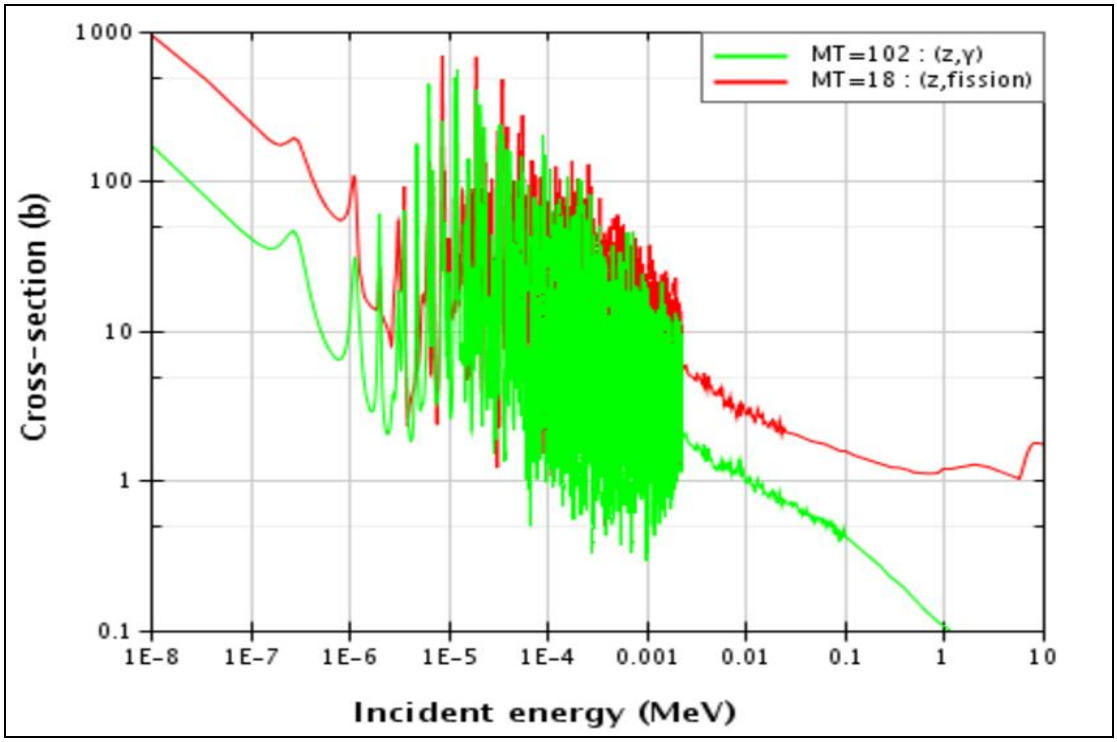

Figure 20: Radiative capture and fission cross section of ^{235}U (OECD, 2016)

From Figure 20 it is evident that the fissile ^{235}U has a higher fission, than radiative capture cross section in the thermal (0.0253 – 0.5 eV), and fast (100 keV – 20 MeV) energy spectrum. The radiative resonance capture peaks, are noticeably higher, on a number of points in the epithermal energy range (0.5 eV – 100 keV).

5.4.3.2.2 Neutron yield per fission neutron for ^{235}U

The fission neutron yield per fission of ^{235}U as seen in Figure 21, can be estimated at 2.44 neutrons per fission neutron, for the thermal energy spectrum, this corresponds with the 2.4355 neutrons per thermal fission neutron for ^{235}U as published by (IAEA, 2007).

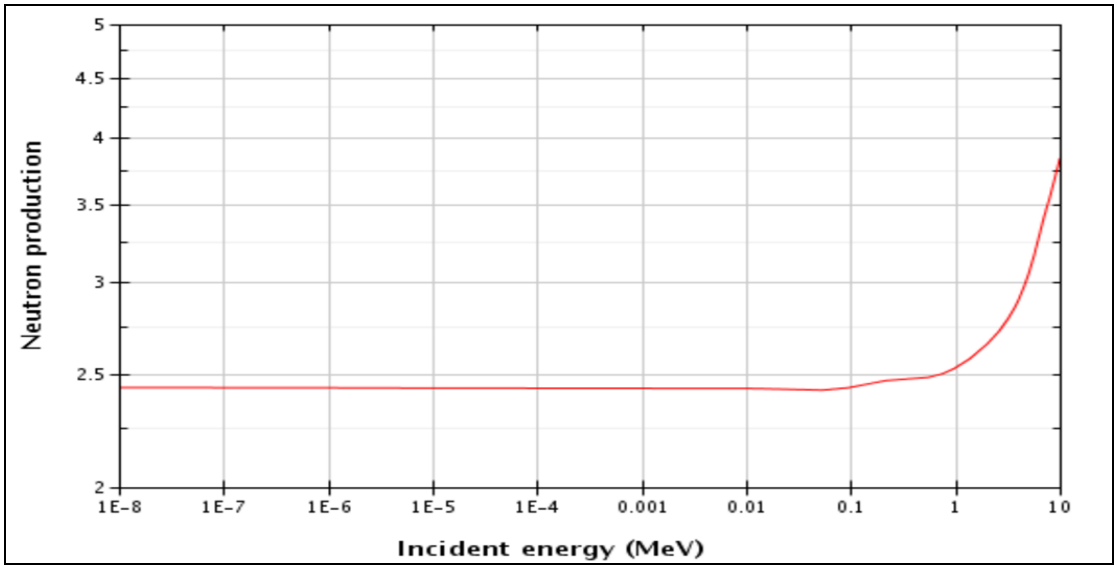

Figure 21: Fission neutrons yield per fission reaction for ^{235}U (OECD, 2016)

5.4.3.2.3 Reactivity coefficients of ^{235}U fuel compositions

Figure 22 and Figure 23 is an amalgamation of the fission and radiative capture cross sections respectively, and depict all the isotopes tested in the above mentioned fuel compositions. By analysing the portrayed data in Figure 22 and Figure 23 predictions can be made of the neutronic and isotopic behaviour of the fuel compositions during accident scenarios.

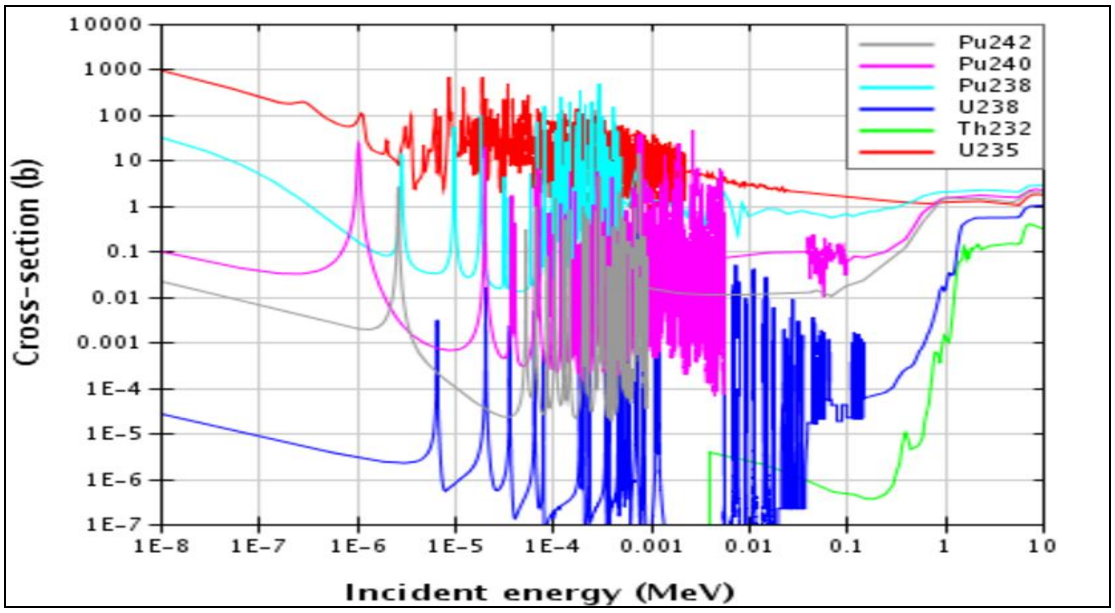

Figure 22: Fission cross sections for all the isotopes tested in the ^{235}U homogeneous fuel mixtures (OECD, 2016)

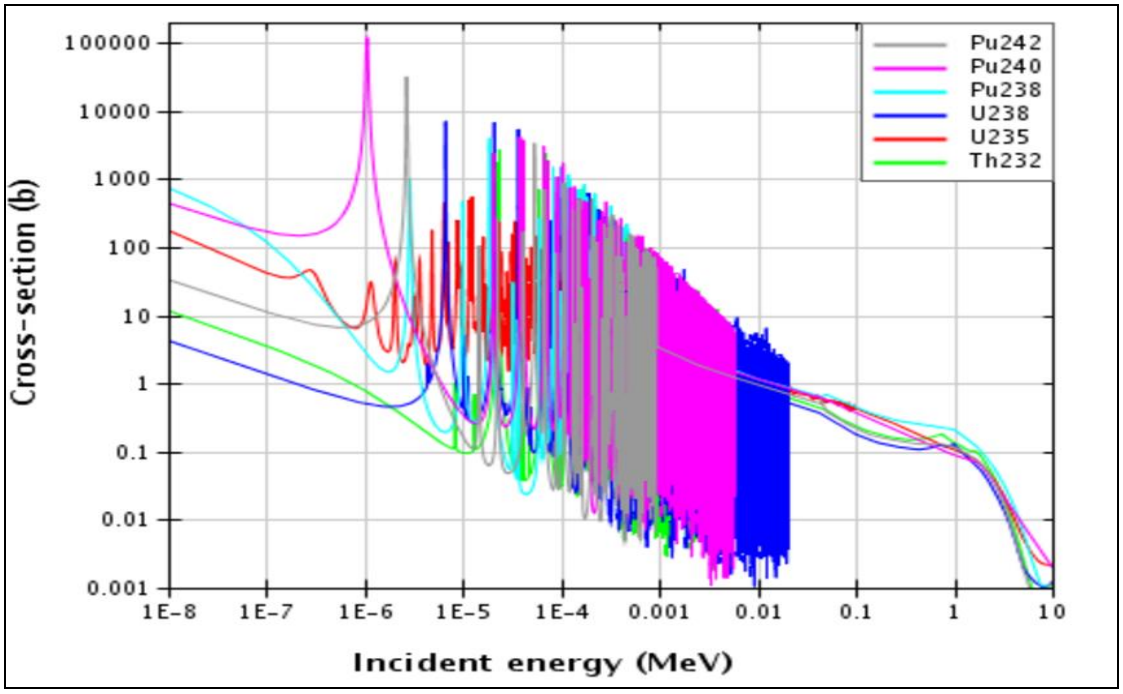

Figure 23: Radiative capture cross section for all the isotopes tested in the ^{235}U homogeneous fuel mixtures (OECD, 2016)

From the fission cross sections portrayed by Figure 22, it is evident that in the thermal energy spectrum ^{235}U has the highest probability of undergoing a fission reaction of all the evaluated isotopes. This ensures utilization of thermal neutrons where intended and provides a level of safety with regard to unsolicited fluctuations in the infinite multiplication factor due to fissioning of unanticipated isotopes.

5.4.3.2.4 Moderator temperature reactivity coefficient

In an accident scenario; for example a temporary loss of coolant loop pressure, where a small to moderate increase in moderator temperature occurs, and consequently a Maxwell neutron distribution in the moderator, peaking towards the epithermal energy spectrum. From Figure 22 it is prominent that a diminished number of fission reactions would occur in the ^{235}U. This can be ascribed to, the decrease in the fission cross section of ^{235}U with the increase in neutron energy. Estimated effects of the aforementioned characteristic of ^{235}U ensures, that even in large concentrations ^{235}U could yield a negative moderator temperate reactivity coefficient, subsequently increasing the inherent safety of any fuel composition containing it. The above mentioned is especially prevalent during a comparison of the fission cross section of ^{233}U and ^{235}U. As mentioned in section 5.4.3.1.4 ^{233}U, will cause a positive moderator

temperature reactivity coefficient. The cross section comparison can be seen in Figure 24.

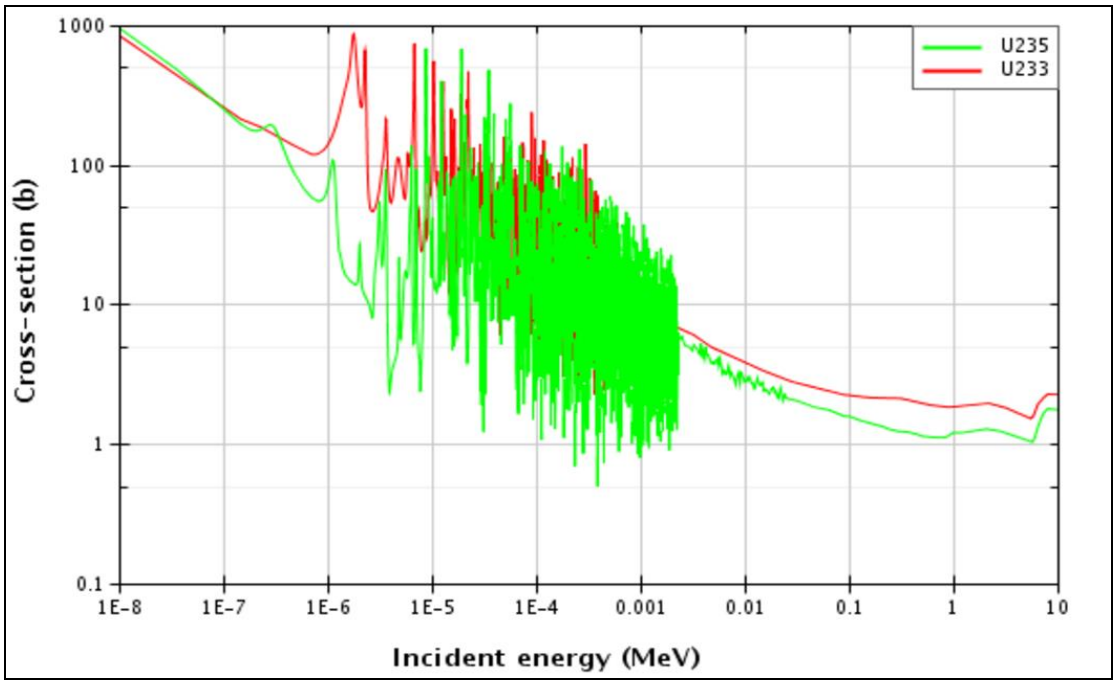

Figure 24: Comparison of the fission cross sections of ^{235}U and ^{233}U (OECD, 2016)

A decrease in the amount of fission reactions of ^{235}U, can be anticipated for shift in the neutron distribution peaking around 0.5 – 8.5 eV. This will provide the reactor with, a reactivity extremely responsive to small changes in moderator temperature.

5.4.3.2.5 Void reactivity coefficient

In the scenario where a void is formed in the reactor, usually caused by moderator boiling (low pressure in primary loop), or insufficient heat removal due to a Loss of Coolant Accident (LOCA). Neutron thermalisation will diminish, due to a lack of moderation by the steam filled void, causing more fast fission in the fissile and fissionable isotopes present in the fuel composition.

Due to relatively low capture cross section of ^{235}U in the epithermal and fast energy spectrum, any increase in neutron energy will automatically result in a decrease of the infinite neutron multiplication factor (k_∞).

As depicted in section 5.4.3.1.5, ^{232}Th and ^{238}U aid in a negative void reactivity coefficient due to their decreased resonance escape probability and lower fast fission

capabilities. Due to the high fast fission cross section of ^{238}Pu, ^{240}Pu, and ^{242}Pu as portrayed by Figure 16, large consecrations of these isotope should be avoided, as it could increase the infinite neutron multiplication factor ($k\infty$), in the absence of efficient neutron thermalisation as seen in Figure 23.

5.4.3.2.6 Fuel temperature reactivity coefficient

In the case of fuel temperature reactivity coefficient, the fast fission cross section of the isotopes should not influence the coefficient. Fuel temperature reactivity coefficients, are determined by the increase or decrease in resonance escape probability of an incident neutron with the increase in fuel temperature.

Fuel compositions comprised of isotopes with the same characteristics, used to mitigate a positive void reactivity coefficient, with the addition of ^{240}Pu can be used to ensure a negative fuel temperature reactivity coefficient. This can be attributed to the distribution of the resonance capture area, severity and density of the resonance capture peaks.

5.4.3.2.7 Computed results of uranium – 235 compositions

The following section contains a discussion of the results acquired during burnup simulations of homogeneous mixtures of 5 a/o ^{235}U and 95 at. % of selected fertile isotopes.

The computed infinite multiplication factor ($k\infty$) for ^{235}U fuel compositions as described in Table 5, are presented in Figure 25. The burnup data with regard to time will provide an indication of the capture, neutron energy spectrum, fission, and breeding capabilities of each homogenous fuel mixture.

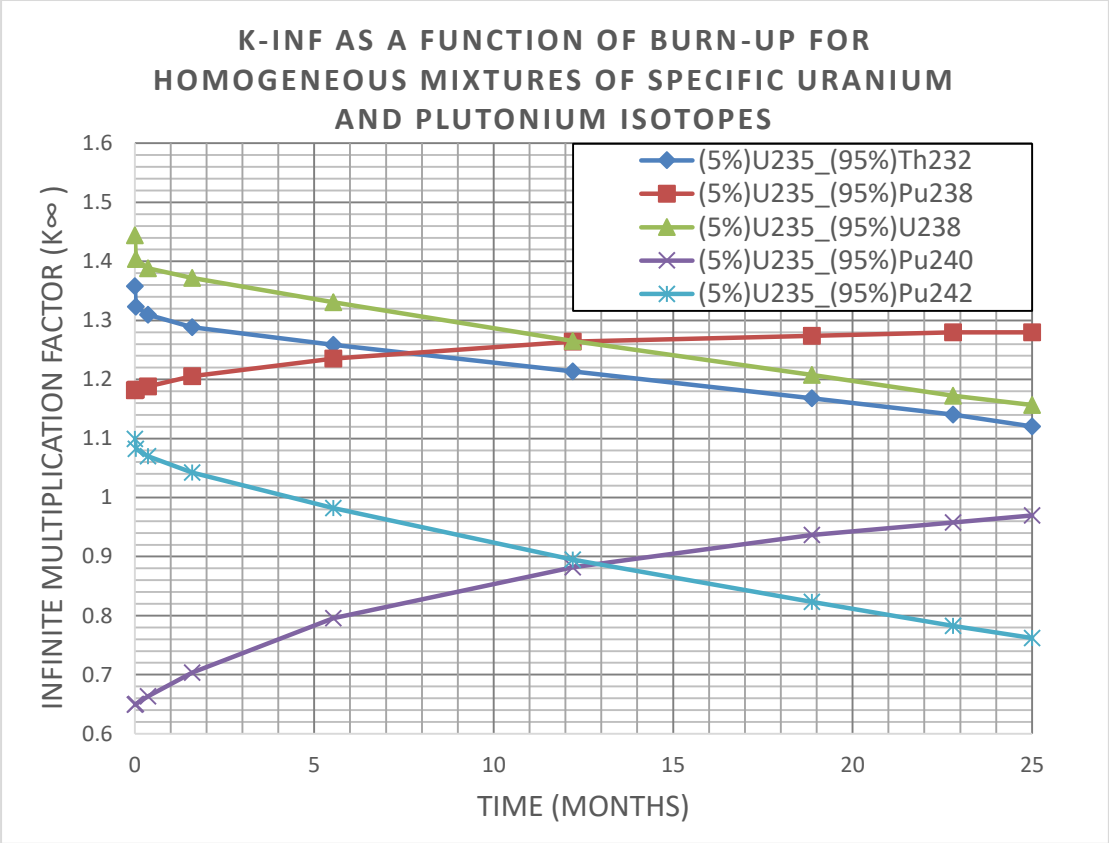

Figure 25: Infinite multiplication factor over time due to burn-up for homogeneous mixtures of ^{235}U and other fertile isotopes

The data presented in Table 9, Table 10, and Table 11, portray the amount of neutrons that underwent a specific interaction on day zero of the burnup simulations. The data was specifically analysed on day zero, to enable uncompromised isotope characteristic evaluation. If an alternative day was chosen, the result would have been compromised due to the presence of bred isotopes.

The capture data from each of the tested fuel compositions are displayed in Table 9. The acquisitioned data will serve as benchmark to predict the effect of certain isotopic interactions in more complex fuel compositions.

Table 9: Neutron captures in homogeneous mixtures of ^{235}U and other fertile isotopes on day zero of burnup

	Neutron captures					
Isotopic composition	**Moderator (H_2O)**	**Uranium-235**	**Fertile isotope**	**Oxygen (in fuel)**	**Helium**	**Zircaloy-4**
(5%)U235_(95%)Th232	2.4172E+11	4.3260E+11	1.6853E+12	9.5795E+09	0.0000E+00	3.5707E+10
(5%)U235_(95%)U238	2.2187E+11	7.5603E+11	1.4197E+12	9.1005E+09	0.0000E+00	3.3028E+10
(5%)U235_(95%)Pu238	1.0886E+11	3.6612E+11	4.5281E+12	1.5156E+10	0.0000E+00	2.2538E+10
(5%)U235_(95%)Pu240	1.3797E+11	6.1936E+11	1.0908E+13	2.5529E+10	0.0000E+00	5.1194E+10
(5%)U235_(95%)Pu242	1.8676E+11	6.8048E+11	3.9317E+12	1.2694E+10	0.0000E+00	3.5539E+10

Table 10: Total neutron captures per ^{235}U fuel composition on day zero of burnup

Isotopic composition	**Total captures**
(5%)U235_(95%)Th232	2.4049E+12
(5%)U235_(95%)U238	2.4397E+12
(5%)U235_(95%)Pu238	5.04548E+12
(5%)U235_(95%)Pu240	1.17417E+13
(5%)U235_(95%)Pu242	4.84717E+12

Table 11: Fission reactions in homogeneous mixtures of ^{235}U and other fertile isotopes on day zero of burnup

	Fissions	
Isotopic composition	**Uranium-235**	**Fertile isotope**
(5%)U235_(95%)Th232	3.4357E+12	4.2223E+10
(5%)U235_(95%)U238	3.3084E+12	1.64729E+11
(5%)U235_(95%)Pu238	1.0226E+12	2.3749E+12
(5%)U235_(95%)Pu240	1.3325E+12	2.0857E+12
(5%)U235_(95%)Pu242	2.5236E+12	9.2234E+11

5.4.3.2.8 Uranium – 235 fuel composition conclusion

As seen in Table 7, from the capture data of the ^{233}U fuel compositions, the same conclusion can be made with regard to the inferior capturing capabilities of the ^{232}Th, and ^{238}U fuel compositions, when compared with that of the plutonium compositions.

The higher infinite neutron multiplication factor ($k\infty$) for the ^{232}Th and ^{238}U fuel compositions, can be contributed to two factors: the first being their inferior capture cross sections in the thermal energy spectrum as displayed in Figure 23, and secondly the higher abundance of thermal neutrons available for fission by the fissile ^{235}U, as indicated in Table 11.

During the burnup of the fuel composition containing ^{238}Pu, the infinite neutron multiplication factor ($k\infty$) varied only slightly. This can be ascribed to the breeding of ^{239}Pu, which has a higher fission cross section than the capture cross section of ^{238}Pu as seen below in Figure 18. The fission reaction of the ^{239}Pu, produces bounteous amounts of neutrons which, either fissions other ^{239}Pu nuclei or breed more ^{239}Pu from the existing ^{238}Pu.

The aggressive neutrons capture of the ^{240}Pu, and ^{242}Pu fuel compositions, as seen in Table 10 can be contributed to the exceptionally high neutron capture peaks as seen in Figure 19, and provide a clear indication of the neutron energy distribution.

The increase in the infinite neutron multiplication factor (k_∞) over time, in the ^{240}Pu fuel composition can be contributed to the breeding of ^{241}Pu. In the ^{242}Pu fuel compositions, a decrease in the infinite neutron multiplication factor (k_∞) was observed, this can be ascribed to, two factors: the absence of fissile isotope breeding, and the breeding of neutron capture intensive isotopes, like americium (Am).

It is evident from the data that ^{233}U, and ^{235}U share the same characteristics and behave almost identical, when homogeneously mixed with the evaluated fertile isotopes. The small variance in the presented data can be contributed to the higher neutron yield per fission neutron of ^{233}U. The amount of neutrons captures in the ^{235}U compositions are significantly higher than that of the ^{233}U fuel compositions. This can be attributed to two factors: the higher capture cross section of ^{235}U in the thermal energy spectrum, or that ^{235}U emits lower energy neutrons as a result of fission.

5.4.3.3 Plutonium – 239

The following section depict all relevant data with regard to ^{239}Pu.

5.4.3.3.1 Characteristics of plutonium – 239

Plutonium – 239 in one of 20 known isotopes of plutonium, none of which are stable isotopes, due to their artificial origin. Some traces of plutonium have been found in nature, but no abundant sources. This can be ascribed to their short half-life, with the longest being that of ^{244}Pu, 80.8 million years

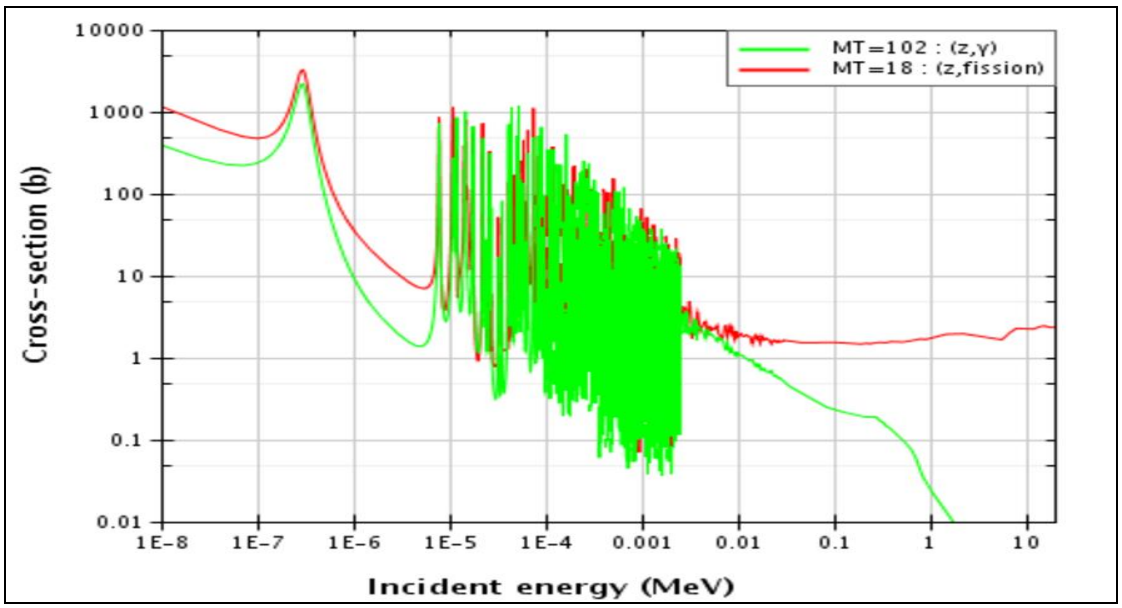

Figure 26: Radiative capture and fission cross section of ^{239}Pu (OECD, 2016)

5.4.3.3.2 Neutron yield per fission neutron for ^{239}Pu

The fission neutron yield per fission of ^{239}Pu as seen in Figure 21, can be estimated at 2.8833 neutrons per fission neutron, for the thermal energy spectrum, this corresponds with the 2.8836 neutrons per thermal fission neutron for ^{239}Pu as published by (IAEA, 2007).

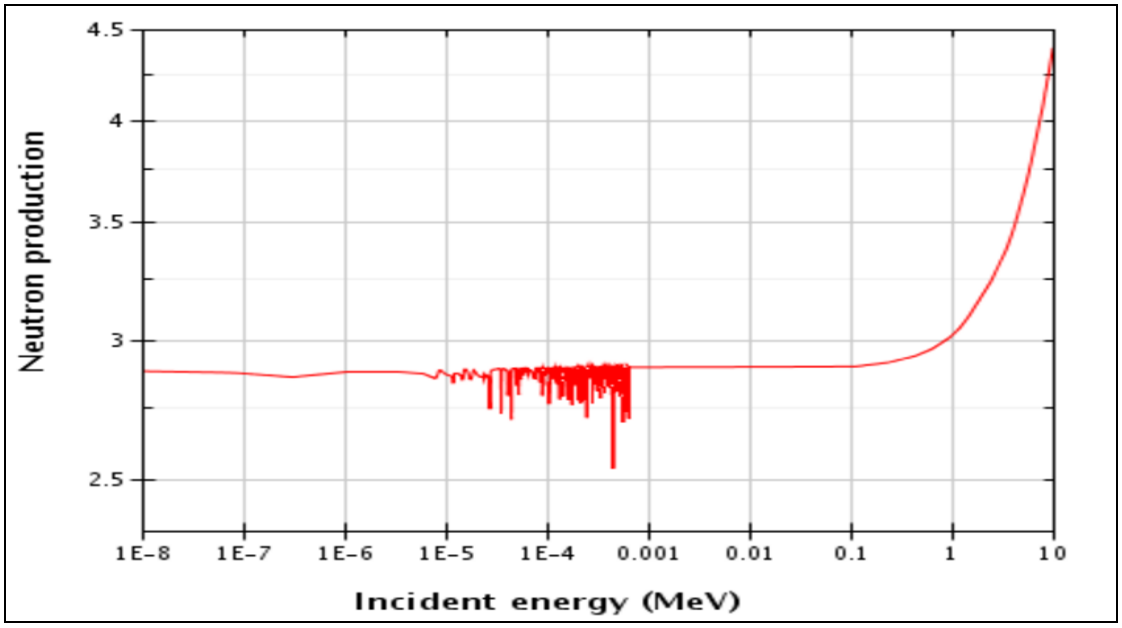

Figure 27: Fission neutrons yield per fission reaction for ^{239}Pu (OECD, 2016)

5.4.3.3.3 Reactivity coefficients of ^{239}Pu fuel compositions

Figure 28 and Figure 29 is an amalgamation of the fission and radiative capture cross sections respectively, and depict all the isotopes tested in the above mentioned fuel compositions. By analysing the portrayed data in Figure 28, and Figure 29 predictions can be made of the neutronic and isotopic behaviour of the fuel compositions during accident scenarios.

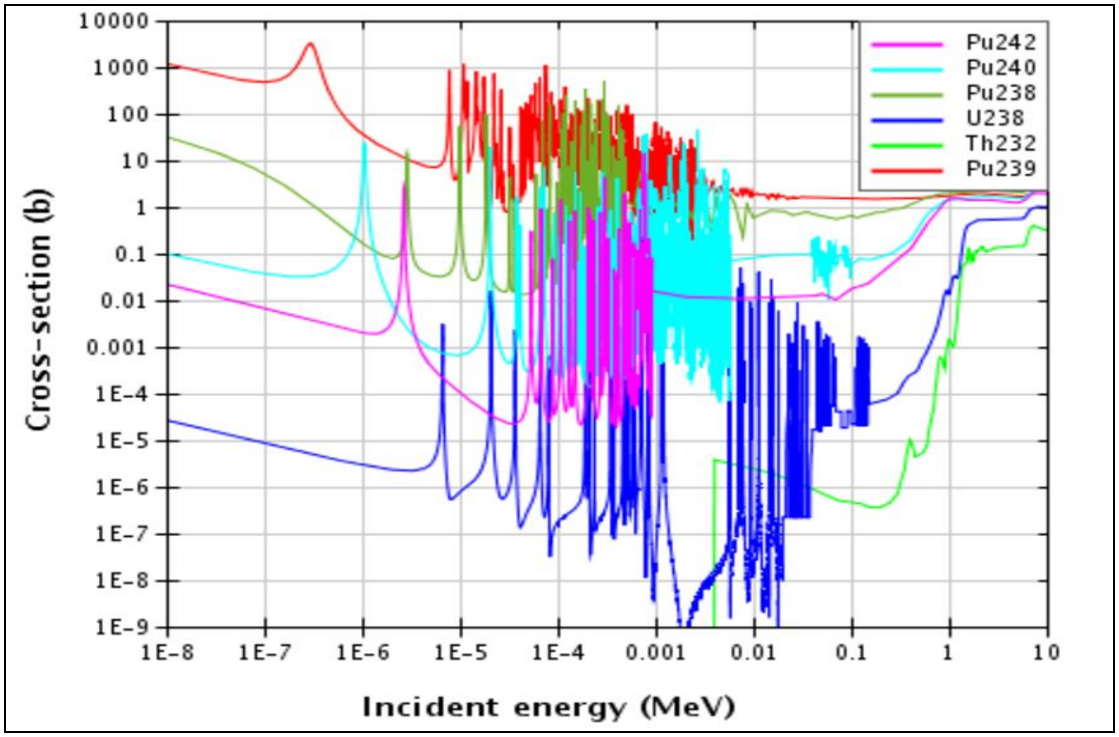

Figure 28: Fission cross sections for all the isotopes tested in the ^{239}Pu homogeneous fuel mixtures (OECD, 2016)

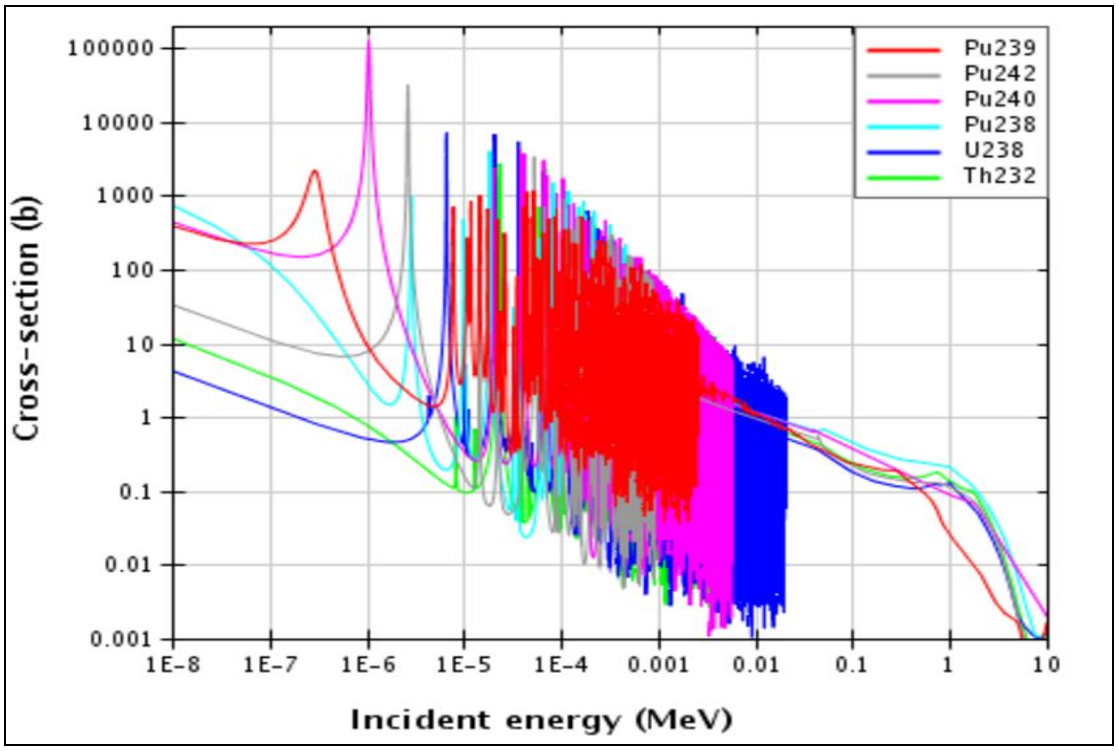

Figure 29: Radiative capture cross section for all the isotopes tested in the ^{239}Pu homogeneous fuel mixtures (OECD, 2016)

From the fission cross sections portrayed by Figure 28, it is evident that in the thermal energy spectrum ^{239}Pu has the highest probability of undergoing a fission reaction of all the evaluated isotopes. This ensures utilisation of thermal neutrons where intended and provides a level of safety with regard to unsolicited fluctuations in the infinite multiplication factor due to fissioning of unanticipated isotopes.

5.4.3.3.4 Moderator temperature reactivity coefficient

In the scenario as described in section 5.4.3.1.4 and 5.4.3.2.4 where a small increase in moderator temperature occurs. From Figure 26 it is projected that a substantial increase in the number, of fission and radiative capture reactions would occur in the ^{239}Pu. This can be attributed to, the fission and radiative capture peak noticeable in the 0.1 – 1 eV energy range of Figure 26. The tendency of ^{239}Pu, to undergo increased fissions with the increase in moderator temperature, compromises the inherent safety characteristic of the fuel, and the isotopes viability as a fuel source in large concentrations. Large concentrations of ^{239}Pu could yield a higher infinite neutron multiplication factor (k_∞), with increased moderator temperature, and subsequently cause a positive moderator temperature reactivity coefficient due to its high fission cross section. It would be difficult to combat the above mentioned tendency, due to absence of fertile isotopes with, neutron capture peaks in the corresponding energy window. The aforementioned is visible in Figure 29.

5.4.3.3.5 Void reactivity coefficient

In the scenario as described in section 5.4.3.1.5, and 5.4.3.2.5 where a void is formed in the reactor. The reduced neutron thermalisation capability of the moderator will result in a significant increases in fast fissions, with ^{238}Pu, ^{239}Pu and ^{240}Pu being the greatest contributors. Large concentrations of any of the aforementioned isotopes, especially in aggregation with one another, could result in an increase in the infinite neutron multiplication factor (k_∞), with the presence of a void or insufficient neutron thermalisation. This could result in a positive void reactivity coefficient.

5.4.3.3.6 Fuel temperature reactivity coefficient

Fuel compositions comprised of isotopes with the same characteristics, used to mitigate a positive void reactivity coefficient as described in section 5.4.3.1.6, with the addition of ^{240}Pu, in small concentrations, can be used to induce a negative fuel temperature reactivity coefficient. This can be attributed to the distribution of the resonance capture area, severity and density of the resonance capture peaks.

5.4.3.3.7 Computed results of plutonium – 239 compositions

The following section contains a discussion of the results acquired during burnup simulations of homogeneous mixtures of 5 a/o ^{239}Pu and 95 at. % of selected fertile isotopes.

The computed infinite multiplication factor (k_∞) for ^{239}Pu fuel compositions, as described in Table 5, are presented in Figure 30. The burnup data with regard to time will provide an indication of the capture, neutron energy spectrum, fission, and breeding capabilities of each homogenous fuel mixture.

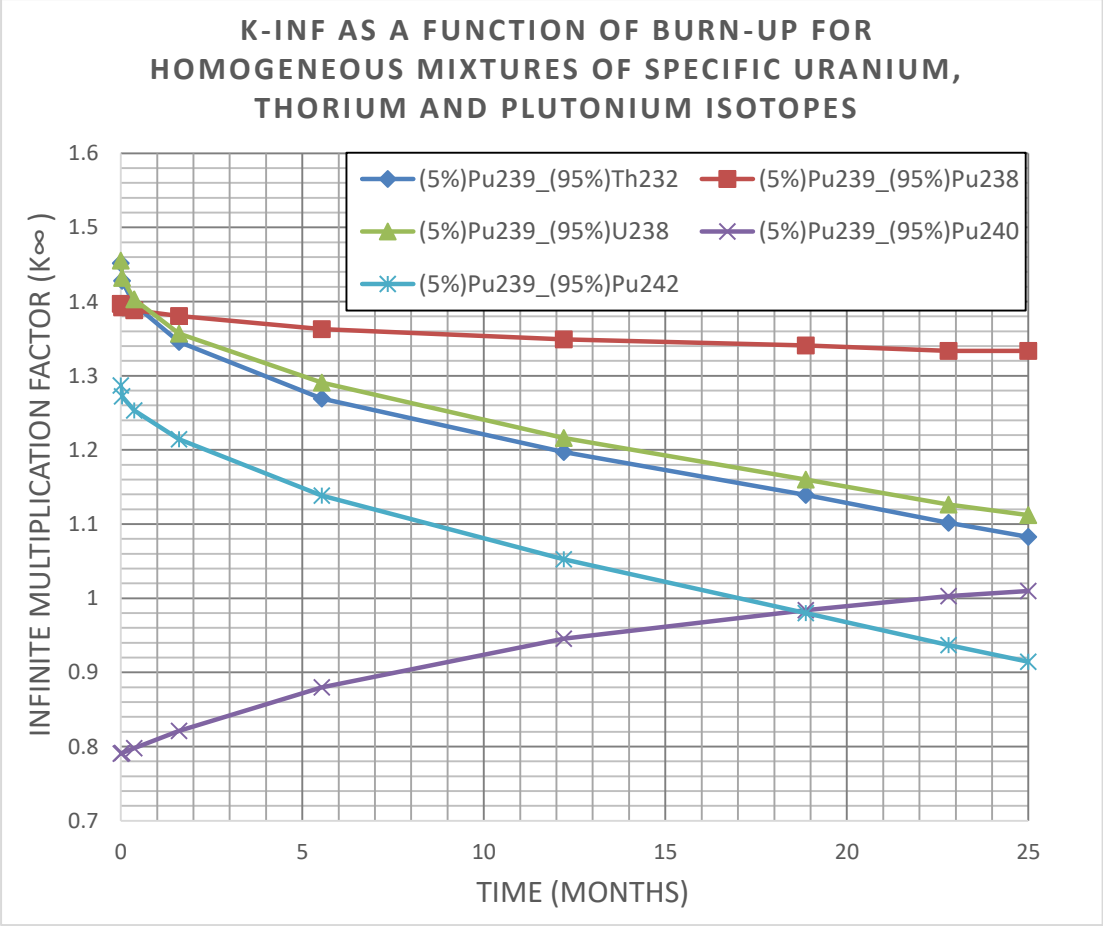

Figure 30: Infinite multiplication factor over time due to burn-up for homogeneous mixtures of ^{239}Pu and other fertile isotopes

The data presented in Table 13, Table 14, and Table 16 portray the amount of neutrons that underwent a specific interaction on day zero of the burnup simulations. The data was specifically analysed on day zero, to enable uncompromised isotope characteristic

evaluation. If an alternative day was chosen, the result would have been compromised due to the presence of bred isotopes.

The capture data from each of the tested fuel compositions are displayed in Table 12. The acquisitioned data will serve as benchmark to predict the effect of certain isotopic interactions in more complex fuel compositions.

Table 12: Neutron captures in homogeneous mixtures of ^{239}Pu and other fertile isotopes on day zero of burnup

	Neutron captures					
Isotopic composition	**Moderator (H_2O)**	**Plutonium-239**	**Fertile isotope**	**Oxygen (in fuel)**	**Helium**	**Zircaloy-4**
(5%)Pu239_(95%)Th232	1.4292E+11	1.7747E+12	1.2920E+12	1.1370E+10	0.0000E+00	3.0553E+10
(5%)Pu239_(95%)U238	1.3261E+11	1.6893E+12	1.3821E+12	1.1788E+10	0.0000E+00	2.9469E+10
(5%)Pu239_(95%)Pu238	8.3309E+10	7.5887E+11	3.0934E+12	1.3414E+10	0.0000E+00	2.2538E+10
(5%)Pu239_(95%)Pu240	1.1510E+11	8.9349E+11	8.4596E+12	2.1906E+10	0.0000E+00	4.3775E+10
(5%)Pu239_(95%)Pu242	1.1426E+11	1.3524E+12	2.8422E+12	1.2985E+10	0.0000E+00	3.0127E+10

Table 13: Total neutron captures per ^{239}Pu fuel composition on day zero of burnup

Isotopic composition	Total captures
(5%)Pu239_(95%)Th232	3.25159E+12
(5%)Pu239_(95%)U238	3.24525E+12
(5%)Pu239_(95%)Pu238	3.97153E+12
(5%)Pu239_(95%)Pu240	9.53387E+12
(5%)Pu239_(95%)Pu242	4.35207E+12

Table 14: Fission reactions in homogeneous mixtures of ^{239}Pu and other fertile isotopes on day zero of burnup

	Fissions	
Isotopic composition	**Plutonium-239**	**Fertile isotope**
(5%)Pu239_(95%)Th232	3.2773E+12	4.6904E+10
(5%)Pu239_(95%)U238	3.1310E+12	1.9281E+11
(5%)Pu239_(95%)Pu238	1.3321E+12	2.0206E+12
(5%)Pu239_(95%)Pu240	1.5753E+12	1.7750E+12
(5%)Pu239_(95%)Pu242	2.4701E+12	8.6622E+11

5.4.3.3.8 Plutonium – 239 fuel composition conclusion

From the data presented in Table 12, it is evident that in the case of the evaluated ^{239}Pu mixtures, contrary to the ^{233}U, and ^{235}U mixtures, the ^{238}U mixture outperformed ^{232}Th, in regard with neutron captures on day zero, subsequently reducing the initial infinite neutron multiplication factor (k_∞) .

The neutron captures in all the fertile materials decreased in comparison with the ^{233}U, and ^{235}U fuel compositions neutron captures per fertile isotope on day zero, as seen in Table 6, and Table 9. This can be contributed to the high fission and capture cross section of ^{239}Pu which absorbed neutrons to the extent that there were less neutrons available for other reactions.

An additional factor to consider, is an upshift in the peak of the energy spectrum of the freshly emitted neutrons due to the release of higher energy fission neutrons by ^{239}Pu. This conclusion is based on the neutron capture data of ^{232}Th and ^{238}U presented in Table 9 and Table 12. A general decrease in fertile isotope captures were noticed in the ^{239}Pu compositions, as described above, but the degree of change varied from the ^{235}U compositions to that of the ^{239}Pu compositions.

As seen in Table 15, the neutron capture in the ^{232}Th, showed a substantial decrease in comparison with the neutron captures of ^{238}U. From Figure 31 it is evident that the abundance of neutrons in the 2.5 – 30 eV energy range increased, subsiquently causing the difference in captures due to the substaintily higher capture cross section of ^{238}U in the aforementioned energy interval.

Table 15 : Comparison of neutron captures in ^{232}Th and ^{238}U fuel compositions with ^{235}U, and ^{239}Pu as fissile isotopes on day zero of burnup

Captures in fertile isotope		
	Fertile isotopes	
Fissile isotopes	Thorium-232	Uranium - 238
Uranium - 235	1.6853E+12	1.4197E+12
Plutonium-239	1.2920E+12	1.3821E+12

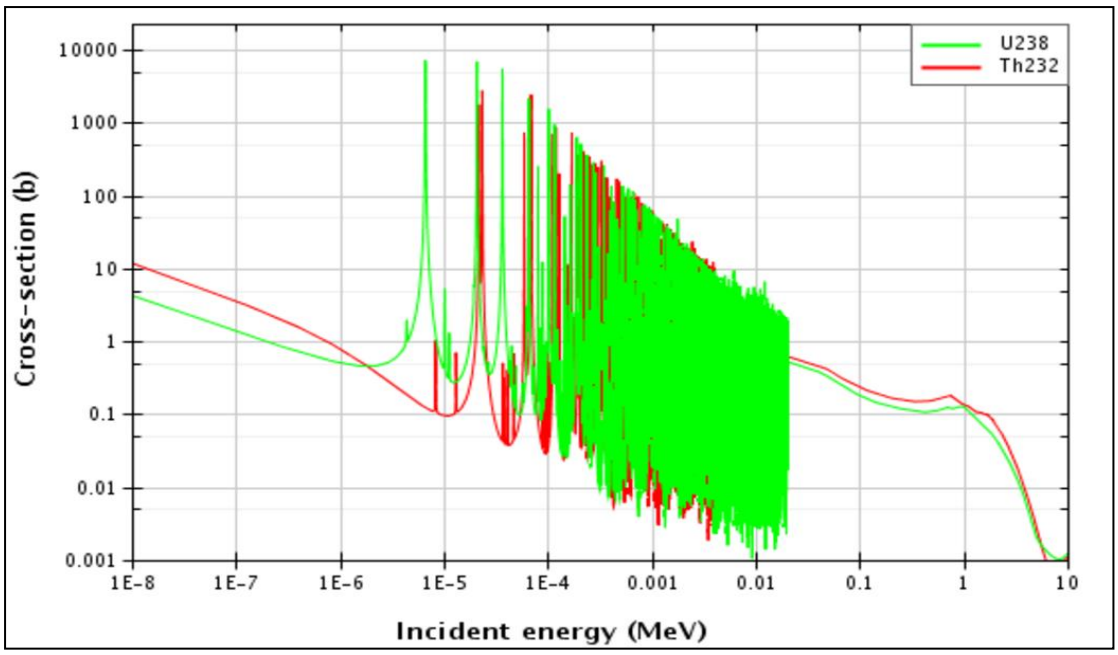

Figure 31: Total capture cross section of ^{232}Th and ^{238}U

5.4.3.4 Plutonium – 241

The following section depict all relevant data with regard to ^{241}Pu.

5.4.3.4.1 Characteristics of plutonium – 241

Plutonium – 241, like all of the plutonium isotopes has no natural abundance and is the result of neutron absorption by ^{238}U in fast and thermal nuclear reactors. It is apparent from Figure 32, that ^{241}Pu has an exceptionally high fission and radiative capture cross section in the thermal energy spectrum, making it an excellent isotope for nuclear fission.

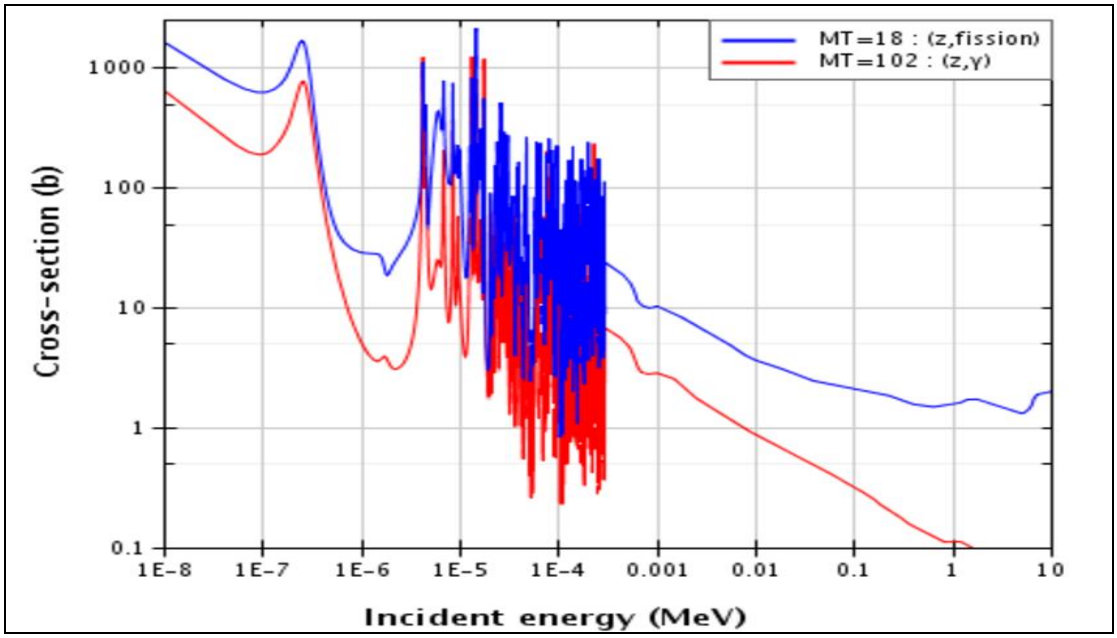

Figure 32: Radiative capture and fission cross section of ^{241}Pu (OECD, 2016)

5.4.3.4.2 Neutron yield per fission neutron for ^{241}Pu

The fission neutron yield per fission of ^{241}Pu as seen in Figure 21, can be estimated at 2.939 neutrons per fission neutron, for the thermal energy spectrum, this corresponds with the 2.9479 neutrons per thermal fission neutron for ^{239}Pu as published by (IAEA, 2007).

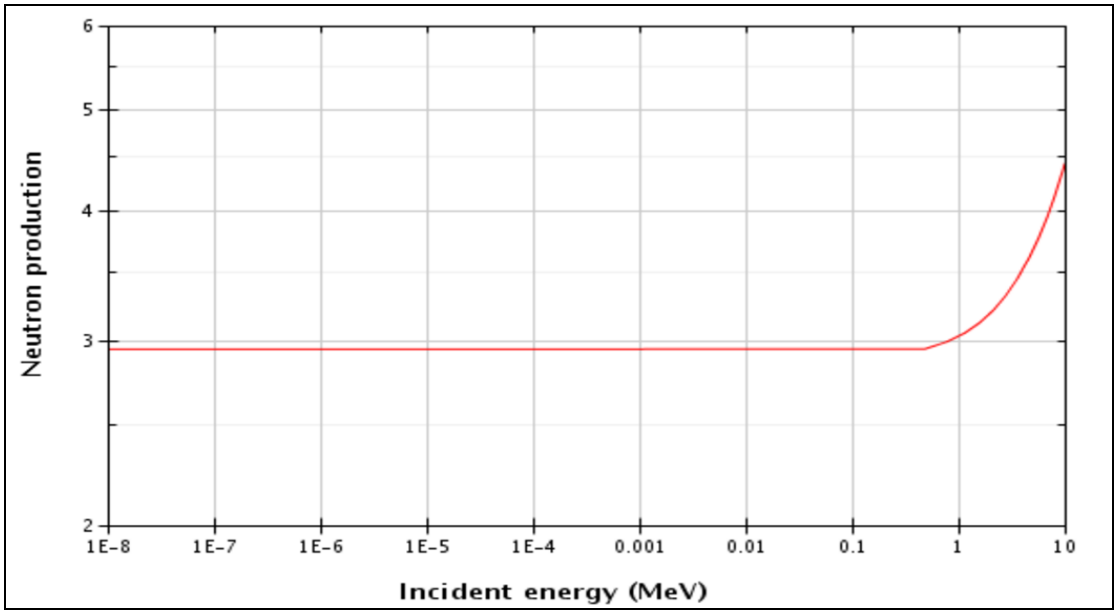

Figure 33: Fission neutrons yield per fission reaction for ^{241}Pu (OECD, 2016)

5.4.3.4.3 Reactivity coefficients of ^{241}Pu fuel compositions

Figure 34 and Figure 35 is an amalgamation of the fission and radiative capture cross sections respectively, and depict all the isotopes tested in the above mentioned fuel compositions.

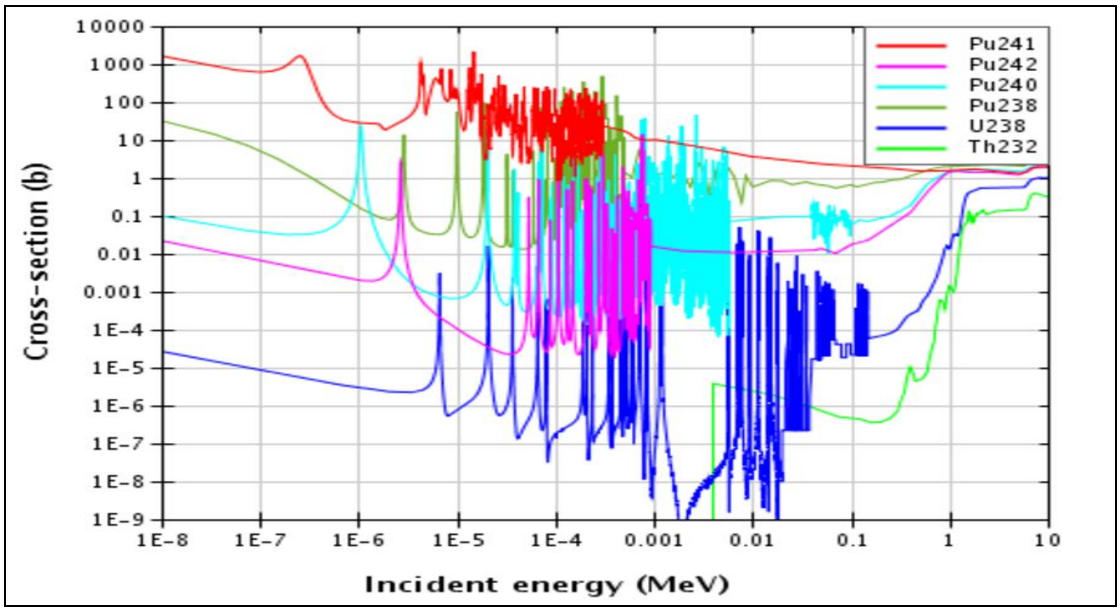

Figure 34: Fission cross sections for all the isotopes tested in the ^{241}Pu homogeneous fuel mixtures (OECD, 2016)

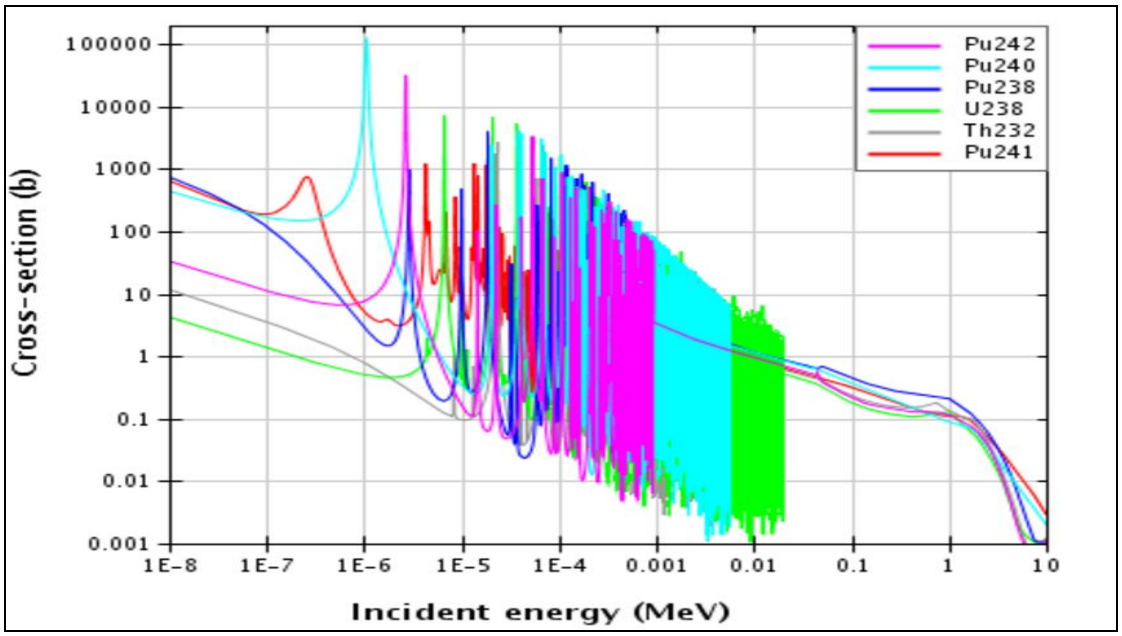

Figure 35: Radiative capture cross section for all the isotopes tested in the ^{241}Pu homogeneous fuel mixtures (OECD, 2016)

From the fission cross sections portrayed by Figure 34, it is evident that in the thermal energy spectrum ^{241}Pu has the highest probability of undergoing a fission reaction of all the evaluated isotopes. This ensures utilization of thermal neutrons where intended and provides a level of safety with regard to unsolicited fluctuations in the infinite multiplication factor due to fissioning of unanticipated isotopes.

5.4.3.4.4 Moderator temperature reactivity coefficient

In the scenario as described in section 5.4.3.3.4 where a small increase in moderator temperature occurs. From Figure 34 and it is predicted that an increase in the number of fission reactions would occur in the ^{241}Pu. This can be attributed to the fission cross section peak at 0.3 eV in Figure 34. The tendency of ^{241}Pu to undergo increased fissions with the increase in moderator temperature, compromises the inherent safety characteristic of the fuel and the isotopes viability as a fuel source in large concentrations. Large concentrations of ^{241}Pu could yield a higher infinite neutron multiplication factor (k_∞), with increased moderator temperature and conceptually cause a positive moderator temperature reactivity coefficient due to its high fission cross section.

5.4.3.4.5 Void reactivity coefficient

In the scenario as described in section 5.4.3.3.5 where a void is formed in the reactor. The reduced neutron thermalisation capability of the moderator could result in a significant increase in fast fissions, with ^{238}Pu, ^{239}Pu and ^{240}Pu being the greatest contributors. Large concentrations of any of the aforementioned isotopes, especially in aggregation with one another could result in an increase in the infinite neutron multiplication factor (k_∞), with the presence of a void or insufficient neutron thermalisation. This consequently could result in a positive void reactivity coefficient.

5.4.3.4.6 Fuel temperature reactivity coefficient

The negative Doppler coefficient of Thorium can be used to combat a positive void reactivity coefficient as described in section 5.4.3.1.6.

5.4.3.4.7 Computed results of plutonium – 241

The following section contains a discussion of the results acquired during burnup simulations of homogeneous mixtures of 5 a/o ^{241}Pu and 95 at. % of selected fertile isotopes.

The computed infinite multiplication factor (k_∞) for ^{241}Pu fuel compositions, as described in Table 5, are presented in Figure 36. The burnup data with regard to time will provide an indication of the capture, neutron energy spectrum, fission, and breeding capabilities of each homogenous fuel mixture.

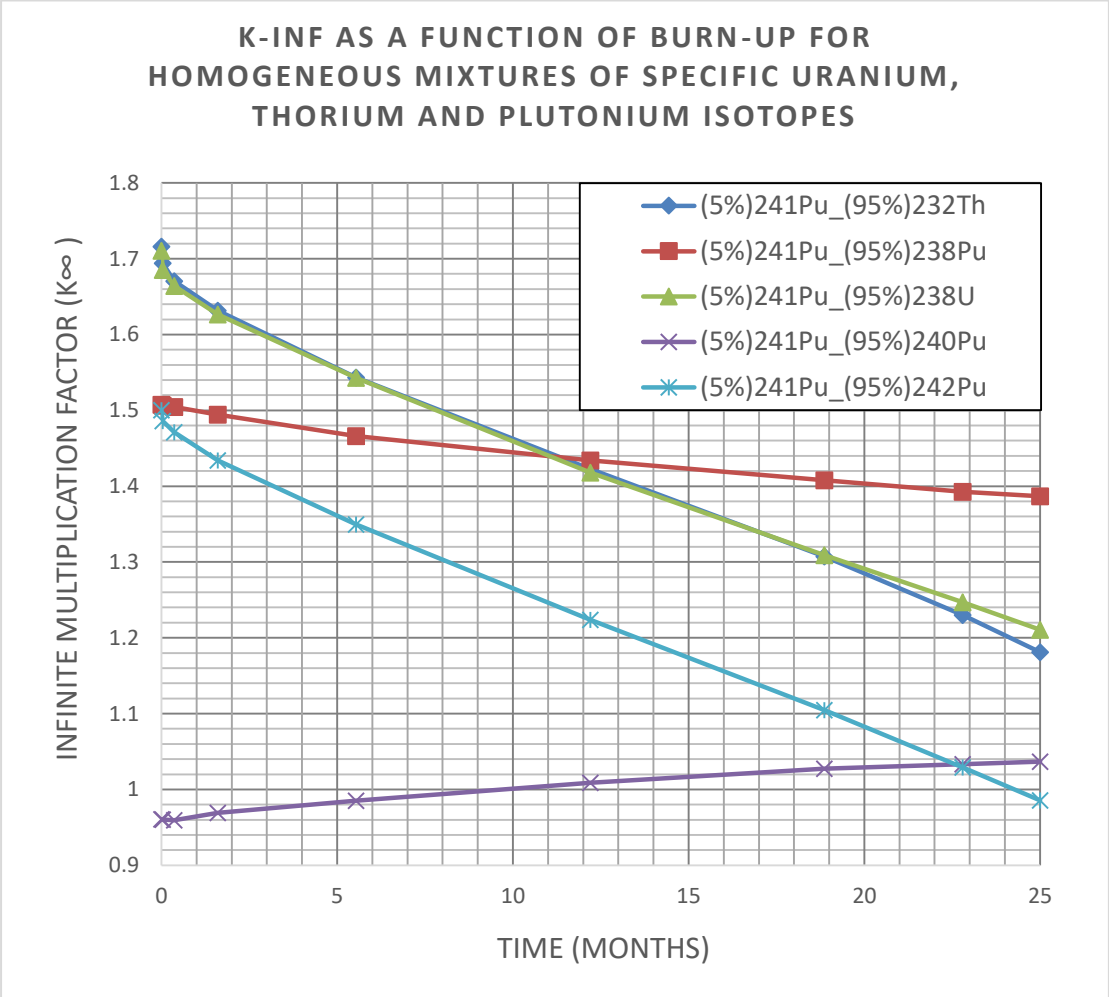

Figure 36: Infinite multiplication factor over time due to burn-up for homogeneous mixtures of ^{241}Pu and other fertile isotopes

The data presented in, Table 16, Table 17, and Table 18 depict the amount of neutrons that underwent a specific interaction on day zero of the burnup simulations. The data was specifically analysed on day zero, to enable uncompromised isotope characteristic evaluation. If an alternative day was chosen, the result would have been compromised due to the presence of bred isotopes.

The capture data from each of the tested fuel compositions are displayed in Table 16. The acquisitioned data will serve as benchmark to predict the effect of certain isotopic interactions in more complex fuel compositions.

Table 16: Neutron captures in homogeneous mixtures of ^{241}Pu and other fertile isotopes on day zero of burnup

	Neutron captures					
Isotopic composition	**Moderator (H_2O)**	**Plutonium-241**	**Fertile isotope**	**Oxygen (in fuel)**	**Helium**	**Zircaloy-4**
(5%)Pu241_(95%)Th232	1.1789E+11	1.1360E+12	1.2920E+12	9.5673E+09	0.0000E+00	2.6190E+10
(5%)Pu241_(95%)U238	1.1217E+11	1.1134E+12	1.1497E+12	9.6577E+09	0.0000E+00	4.3775E+10
(5%)Pu241_(95%)Pu238	7.5078E+10	4.9467E+11	2.8613E+12	1.2073E+10	0.0000E+00	2.1214E+10
(5%)Pu241_(95%)Pu240	8.7244E+10	5.7052E+11	6.5450E+12	1.7667E+10	0.0000E+00	3.5381E+10
(5%)Pu241_(95%)Pu242	9.5076E+10	8.8365E+11	2.3362E+12	1.1049E+10	0.0000E+00	2.5867E+10

Table 17: Total neutron captures per ^{241}Pu fuel composition on day zero of burnup

Isotopic composition	Total captures
(5%)Pu241_(95%)Th232	2.39417E+12
(5%)Pu241_(95%)U238	2.40995E+12
(5%)Pu241_(95%)Pu238	3.46438E+12
(5%)Pu241_(95%)Pu240	7.25577E+12
(5%)Pu241_(95%)Pu242	3.35187E+12

Table 18: Fission reactions in homogeneous mixtures of ^{241}Pu and other fertile isotopes on day zero of burnup

	Fissions	
Isotopic composition	**Plutonium-241**	**Fertile isotope**
(5%)Pu241_(95%)Th232	3.2956E+12	3.8821E+10
(5%)Pu241_(95%)U238	3.17409E+12	1.59111E+11
(5%)Pu241_(95%)Pu238	1.4879E+12	1.8572E+12
(5%)Pu241_(95%)Pu240	1.9080E+12	1.4371E+12
(5%)Pu241_(95%)Pu242	2.6038E+12	7.3265E+11

5.4.3.4.8 Plutonium – 241 fuel composition conclusion

From the data depicted by Table 17, it is evident that similar to the ^{239}Pu compositions, the ^{241}Pu fuel compositions also induced lower neutron captures in the fertile isotopes. This seems to be a characteristic of ^{239}Pu and ^{241}Pu and can be ascribed to their higher fission and radiative capture cross sections in the thermal energy spectrum. The number of neutron captures of ^{241}Pu are lower for all of the fuel compositions than that of ^{239}Pu.

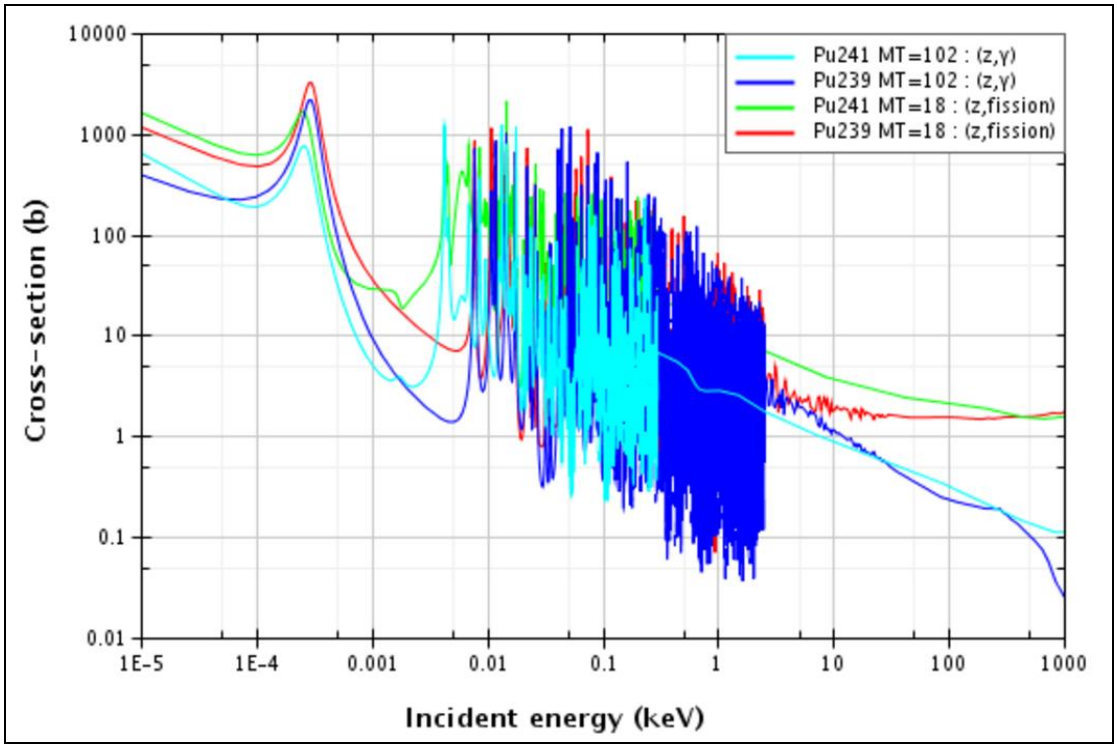

Figure 37: Fission and radiative capture cross sections of ^{239}Pu and ^{241}Pu

5.4.3.5 Breeding rate of fissile isotopes in fuel compositions

The following section depict the breeding rate of selected isotopes. The data was collected from the burnup data.

5.4.3.5.1 Introduction

During burnup, fertile materials capture neutrons and breed an array of new fissile isotopes. The bred isotopes can have significant effects on the, neutronic and isotopic interactions during operation. The aforementioned can increase the infinite neutron multiplication factor, or some of the bred fissionable isotopes serve as neutron capturers, consequently reducing k_∞ and thus the operational lifetime of the fuel.

5.4.3.5.2 Computed results

In the evaluation process of the breeding capabilities of the various isotopes, only the breeding rates of the three fissile isotopes capable of being bred, ^{233}U, ^{239}Pu and ^{241}Pu were analysed. It is important to note that in each of the fuel composition sets, as described in Table 5, one of the fissile isotopes form part of composition used to breed the corresponding isotope. Due to complexity of determining the exact bred quantity of these isotopes, at the different burnup intervals, their data were excluded. The

breeding rate was determined by, evaluating the mass of each isotopes over the 25 month burnup period. Most of the evaluated fissile isotope can be created by various methods of decay or neutron absorption, therefore only the most predominant fissile isotopes breeding chains were evaluated.

5.4.3.5.3 Uranium – 233

Figure 38 depict the breeding rate of ^{233}U from ^{232}Th over a 25 month burnup period, with alternating fissile isotopes. It is evident that a mixture of ^{235}U and ^{232}Th bred ^{233}U the most efficiently, this could be ascribed to the lower fission cross section of ^{235}U, in comparison with the fission cross sections of ^{239}Pu and ^{241}Pu. The inferior fission cross section of ^{235}U resulted in more available neutrons, subsequently more neutron captures in ^{232}Th, and ultimately more ^{233}U.

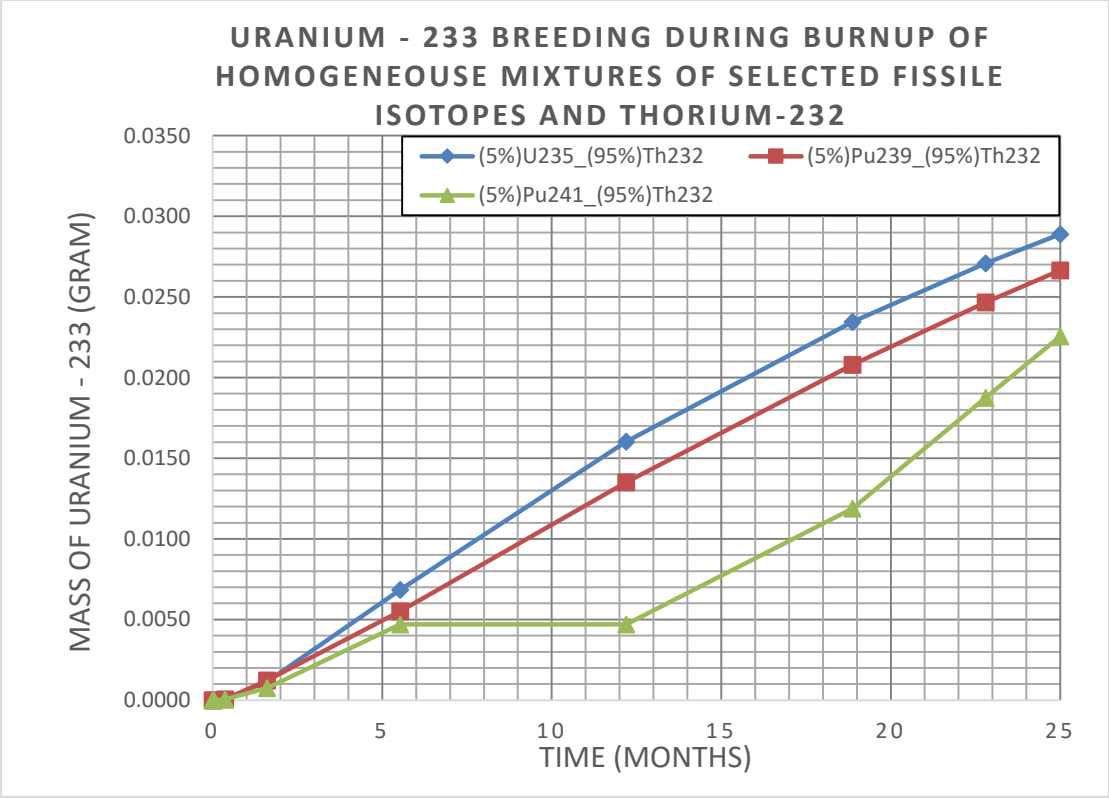

Figure 38: Breeding rate of ^{233}U due to neutron capture by ^{232}Th

It is evident that a mixture of ^{235}U and ^{232}Th produced the highest accumulated mass of ^{233}U. As all the fuel mixtures were by definition operated at the same thermal power output, it can be assumed that the total fission rate in each mixture would have been virtually identical. Therefore different total fission rates can be excluded as a possible

explanation for the different masses of accumulated ^{233}U. However, the following could be possible explanations:

- As ^{235}U has a lower capture to fission rate than ^{239}Pu and ^{241}Pu, for identical fission rates for these three isotopes, ^{235}U would sacrifice the least neutrons to parasitic radiative capture. Therefore ^{235}U would leave the most thermal neutrons unabsorbed, after absorption in ^{235}U for both fission and capture. Since a large fraction of these unabsorbed thermal neutrons will then be captured by ^{232}Th, this would maximise the breeding rate of ^{233}U.

- Alternatively a higher breading rate of ^{233}U with ^{235}U as driver fuel could be explained by better efficiency further down in the transmutation chain: Radiative capture by ^{235}U would produce ^{236}U, which is not a very aggressive neutron capturer. Radiative capture in ^{239}Pu or ^{241}Pu would, on the other hand produce ^{240}Pu and ^{242}PU, which, as we have seen above, are very aggressive neutron capturers. Therefore ^{236}U would leave more neutrons unabsorbed, which could then be captured by ^{232}Th to breed ^{233}U.

- Alternatively it should be noted that the maximum accumulated mass of ^{233}U does not necessarily imply the maximum breading rate thereof. As a substantial fraction of the bred ^{233}U would also have been consumed by both fissioning and capturing of neutrons, a higher accumulated mass of ^{233}U might rather suggest a slower consumption rate of ^{233}U. Since the total fission rate is constant, a lower fission rate for ^{233}U would have to imply a higher fission rate of ^{235}U. However, as ^{235}U has a lower σ_f than both ^{239}Pu and ^{241}Pu, it is not clear why ^{235}U would produce more fissions.

- Lastly, identical fission rates does not imply identical rates or energy spectra of emitted fission neutrons. However, as has been pointed out above, ^{239}Pu and ^{241}Pu emits more neutrons per fission and these have higher energies than for ^{235}U. Therefore it is not clear how these differences could benefit ^{235}U

To conclude, it is not immediately clear why ^{235}U outperformed ^{239}Pu and ^{241}Pu as driver fuels. More research would thus have to be conducted, if this issue were to be resolved.

5.4.3.5.4 Plutonium – 239

Figure 39, and Figure 40 portray the breeding ratio of ^{239}Pu from ^{238}U, and ^{238}Pu respectively, over a 25 month burnup period, with alternating fissile isotopes.

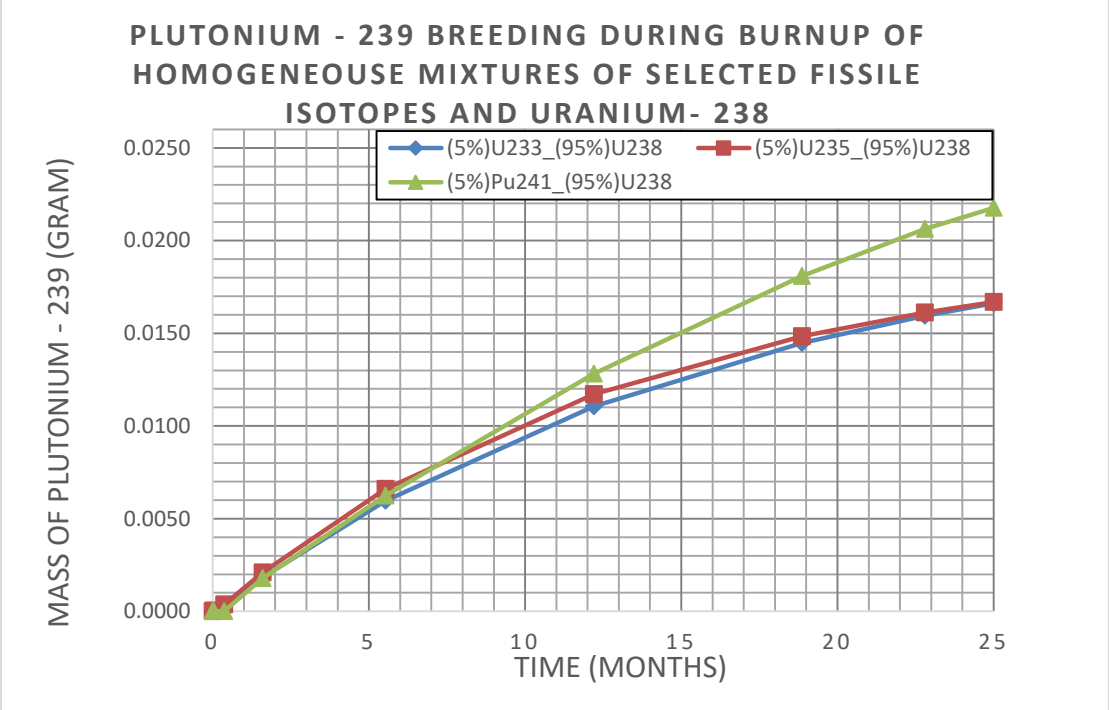

Figure 39: Breeding rate of ^{239}Pu due to neutron capture by ^{238}U

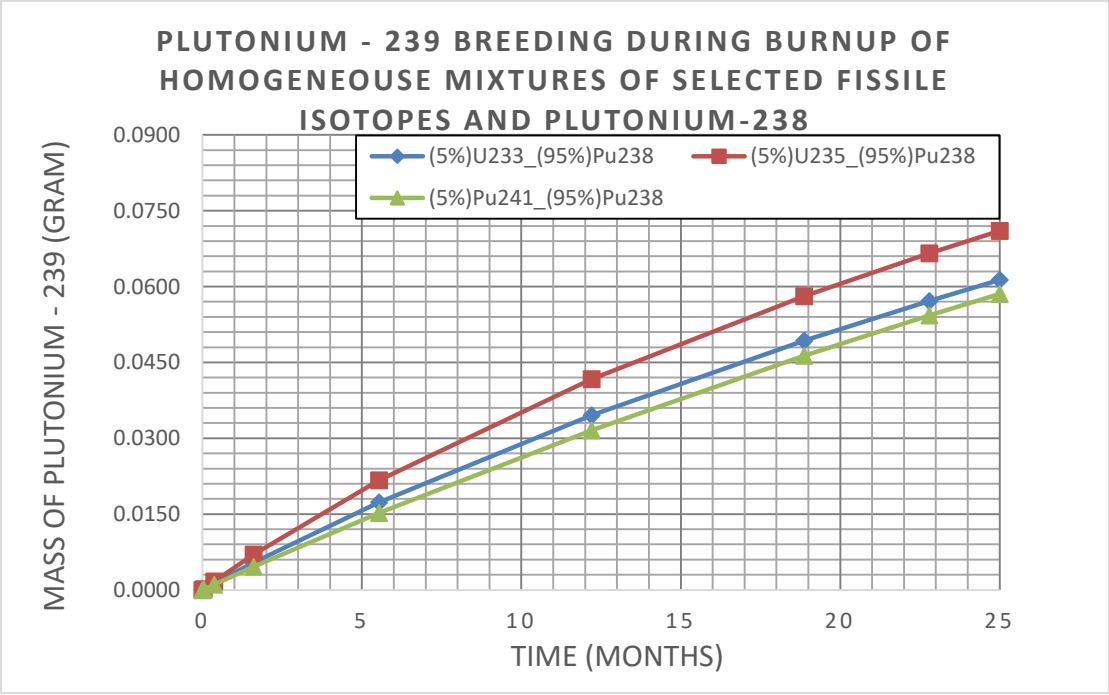

Figure 40: Breeding rate of ^{239}Pu due to neutron capture by ^{238}Pu

It is apparent that ^{238}Pu had the highest ^{239}Pu yield over the 25 month period, this can be attributed to the higher capture cross section of ^{238}Pu, in caparison with the capture cross section of ^{238}U. The breeding rate of the fertile isotopes, also produced interesting results. In the ^{238}U mixtures, ^{241}Pu produced the highest ^{239}Pu yield, where in the ^{238}Pu mixtures ^{235}U had the best ^{239}Pu yield.

This can be ascribed to the fission neutron energies of the two fissile isotopes, as discussed in section 5.4. The higher neutron energy of ^{241}Pu fissions, accompanied by the high capture cross section of ^{238}U, at the start of the epithermal energy spectrum produced the result evident from Figure 39. The lower fission neutron energy of ^{235}U, accompanied by the high capture cross section of ^{238}Pu, in the thermal energy spectrum produced the result evident from Figure 40.

5.4.3.5.5 Plutonium – 241 bred from plutonium - 240

Figure 41 portray the breeding rate of ^{241}Pu from ^{240}Pu, over a 25 month burnup period, with alternating fissile isotopes.

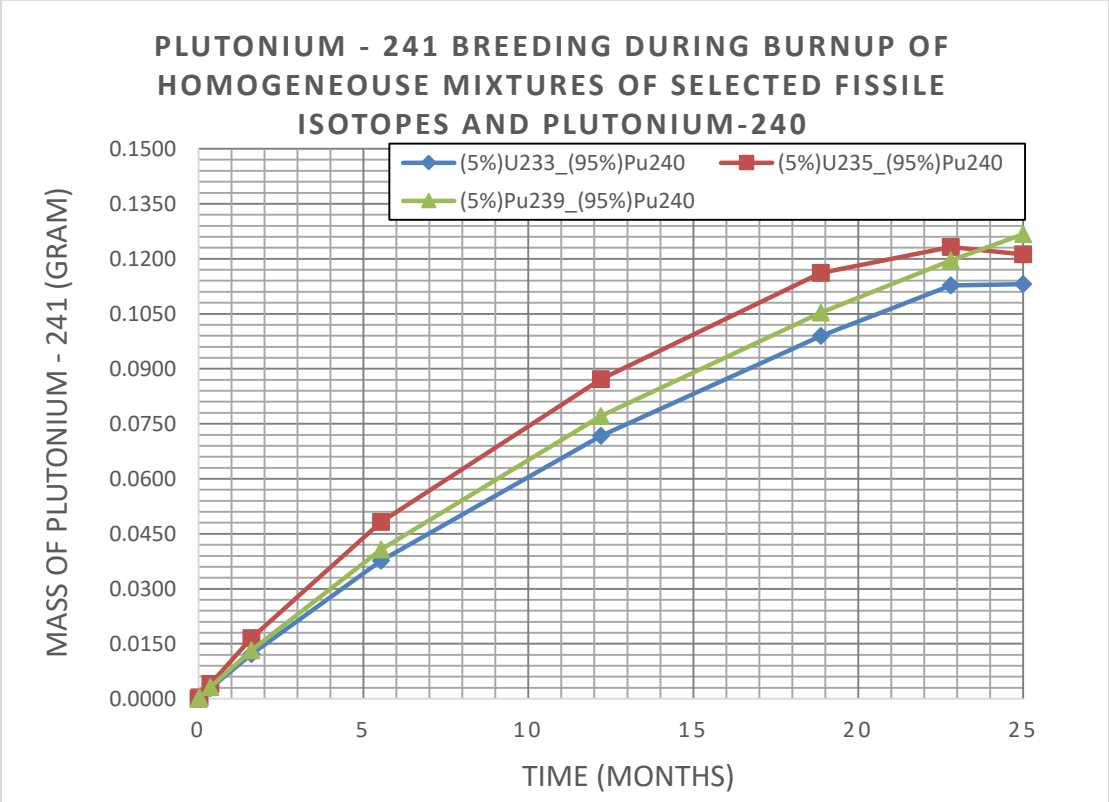

Figure 41: Breeding rate of ^{241}Pu due to neutron capture by ^{238}Pu

From Figure 41 it is evident that due to the high capture cross section of ^{240}Pu in the thermal and epithermal energy spectrum copious amount of ^{241}Pu was bred. The high initial breeding rate from ^{235}U, led to the depletion of ^{240}Pu, as seen from Figure 41. At about 19 months into burnup period, a decrease in production was noticed.

5.4.3.5.6 Conclusion of breeding rates

From the acquired data it is evident that ^{240}Pu, with ^{235}U as fissile driver fuel, is most efficient when it comes to breeding of fissile isotopes, with a yield of almost double that of any other evaluated isotopes.

5.4.4 Conclusion of isotope evaluation

The isotope evaluation process, yielded fundamental knowledge regarding isotope characteristics. The knowledge benchmark, obtained from the neutronic and isotopic interactions during homogeneous amalgamations of the evaluated isotopes may serve a crucial role in the progressive conceptualising of an effective and inherently safe fuel cycle.

5.5 Conceptual fuel compositions for Koeberg PWR

The following section, depict conceptual fuel compositions specifically designed for Koeberg nuclear power plant in South Africa.

5.5.1 Introduction

In this section, a three step approach was implemented to extend the fuel cycle length, of Koeberg nuclear plants 900 MW Pressurized Water-cooled Reactors (PWR).

The current cycle has an effective life cycle length of about 16 months, thereafter the power output has to be reduced, to enable a sustainable fission reaction and continued operation. The infinite neutron multiplication factor (k_∞), of the standard UOX fuel composition with 4.5 a/o ^{235}U at 16 months is equal to 1.205. For the conceptual design, to effectively extend the fuel cycle length at full capacity, the infinite neutron multiplication factor (k_∞) should stay above 1.205 for a time period greater than 16 months.

The first step, was to use the standard UOX fuel composition with 4.5 a/o ^{235}U and isotopically altered it, by the inclusion of selected isotopes to determine if, the standard

fuel composition could be optimised without any geometric changes to the reactor. The second step entailed, a viability analysis of Mixed Oxide fuels (MOX), and the homogenous inclusion thereof, in the standard fuel composition. The third step incorporated a conceptual fuel amalgamation of isotopes, characteristically selected to fulfil the requirements as specified in section 1.4.

The feasibility, and implementability of the proposed fuel design will be evaluated on the following basis:

- Fuel cycle length is defined as the point where a sustainable fission reaction is no longer possible ($k_\infty = 1.205$).
- Infinite neutron multiplication factor (k_∞) at BOL must be, less or equal to, that of the standard UOX fuel composition, subsequently reducing dependency on burnable poisons/absorbers, which could lead to an unacceptable positive moderator temperature coefficient.
- Seek a slower rate of decrease of the infinite neutron multiplication factor (k_∞) over burn-up time.
- Breeding and depreciation rates of predominant isotopes
- Reactivity coefficients
- Neutronic and isotopic interactions during burnup.

5.5.2 Uranium oxide (UOX) concepts

The following section depict the evaluated UOX concepts.

5.5.2.1 Introduction

The standard Koeberg fuel cycle consists of 4.5 a/o ^{235}U and 95.5 at. % ^{238}U. In this section, small changes were made to the isotopic composition, to evaluate whether it is possible to improve the current cycle, on the basis as described in section 5.5.1.

5.5.2.2 Methodology

A systematic approach was used to determine if small alterations in the isotopic composition, could improve the standard Koeberg fuel cycle. The burnup data of the conceptual fuel composition will be evaluated on the following basis:

- infinite neutron multiplication factor (k_∞),
- total number of capture and fission reactions at the Beginning of Life (BOL) and
- fuel compositions ability to breed fissile isotopes (breeding ratio).

5.5.2.2.1 Increased enrichment

The first approach, was to increase the enrichment of the fuel, to the maximum available limit of 5 a/o ^{235}U. The increase in enrichment subsequently increased the fuel cycle length to about 19 months, but as expected increased the infinite neutron multiplication factor (k_∞) at BOL to above the predetermined limit of k_∞ = 1.43316, which is the value at BOL of the standard Koeberg fuel as seen in Figure 42.

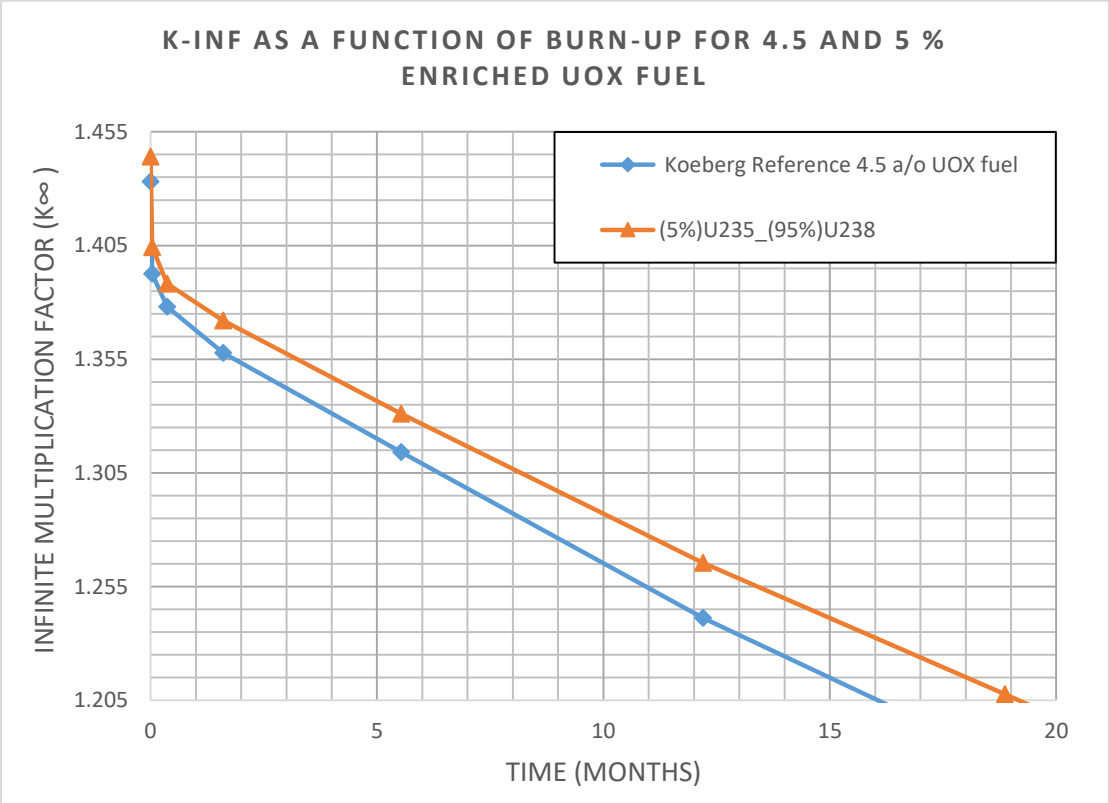

Figure 42: Comparison of the Infinite multiplication factor over time due to burn-up of the standard Koeberg fuel cycle and a 5 a/o ^{235}U and 95% (at.) ^{238}U cycle.

If all other parameters stayed constant, the increased infinite neutron multiplication (k_∞), would cause a higher reactor power output than the reactor and adjacent plant equipment, were designed for. If increased reactivity control is not implemented, the

increased fission reaction rate would consequently yield, more heat which needs to be removed from the pressure vessel.

This higher heat removal rate would entail, higher moderator flow rates (higher capacity pumps), and upgrades to the steam generators and pressurizers. This would be an extremely costly endeavor, and therefore would not suffice as a conceptual solution.

Table 19: Neutron captures in the 4.5% and 5% enriched UOX fuel compositions on day zero of burnup

	Isotopic composition	
Neutron captures	**4.5% U235_95.5% U238**	**5% U235_95.% U238**
Moderator (H_2O)	2.2845E+11	2.2182E+11
Uranium-235	7.4449E+11	7.5603E+11
Fertile isotope	1.4762E+12	1.4197E+12
Oxygen (in fuel)	9.3704E+09	9.1005E+09
Helium	0.00E+00	0.00E+00
Zircaloy-4	3.2863E+10	3.3028E+10

Table 20: Total neutron captures in the 4.5% and 5% enriched UOX fuel compositions on day zero of burnup

Isotopic composition	Total captures
4.5% U235_95.5% U238	2.4914E+12
5% U235_95% U238	2.4397E+12

Due to the 0.5 a/o % ^{238}U increase in the 4.5% enriched UOX fuel composition, as expected a substantial increase in neutron captures were noticed, and explains the decreased infinite neutron multiplication factor (k_∞), in comparison with that of the 5%

enriched UOX fuel composition. The aforementioned is visible in Table 19, and Table 20.

From Figure 43, it is evident that the accumulated ^{239}Pu inventory due to breeding, in the 4.5% and 5% enriched fuel compositions were almost identical for the first 6 months during burnup. It is only after that point that the larger ^{235}U reserve in the 5% enriched fuel composition significantly increased its ^{239}Pu inventory over that of the 4.5% enriched composition. It is quite possible that this is not a case of more breeding for the 5 % case. The more likely explanation is that, as the ^{235}U in the 4.5 % case became depleted, it switched to burning ^{239}Pu and thus started earlier to consume mainly ^{239}Pu than the 5 a/o % case. The above mentioned contributed to the extended fuel cycle length of the 5% enriched fuel composition, as seen in Figure 42.

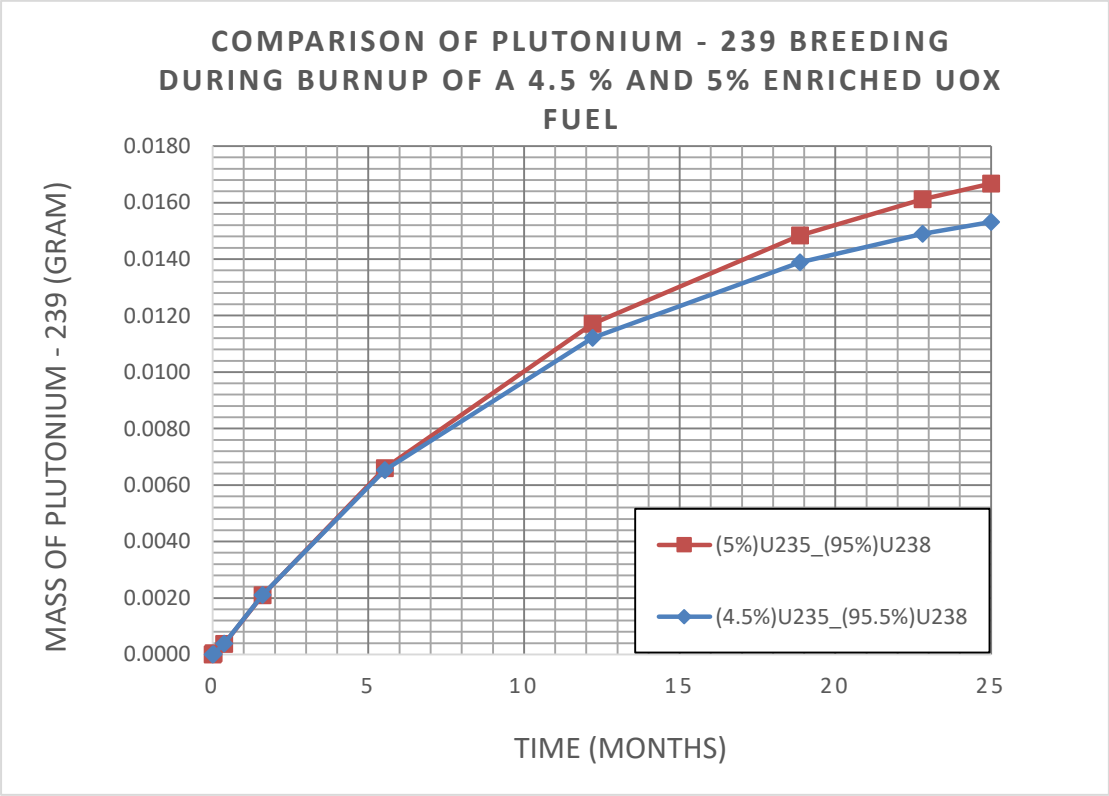

Figure 43: Plutonium – 239 breeding rate in the 4.5% and 5% enriched UOX fuel compositions during burnup

From the ^{235}U depletion data displayed in Figure 44, it appears that the two fuel compositions have the same propensity, with regard to fuel depletion rates. A closer investigation, provided more insight with regard to the neutronic and isotopic interactions of the fuel compositions.

In the 4.5% enriched fuel composition, a decrease in the ^{235}U reserve of 56.79% was observed, compared with a decrease of only 50.96% in the 5% enriched fuel composition. This can be attributed to, the increased ^{239}Pu breeding capabilities of the 5% enriched fuel composition, and therefore effective preservation the ^{235}U reserve.

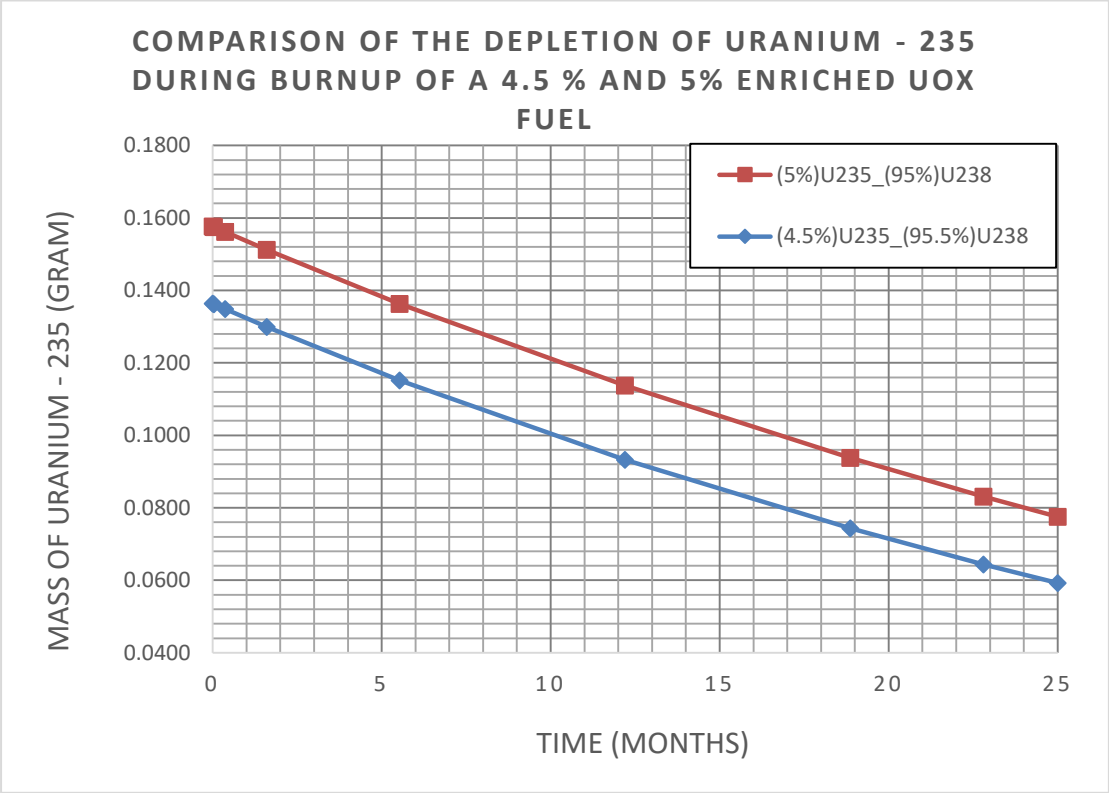

Figure 44: Uranium – 235 depletion rate in the 4.5% and 5% enriched UOX fuel compositions during burnup

The ^{238}U depletion data as presented in Figure 45, also provided an intriguing result. The ^{238}U depleted by, 1.19% and 1.55% in the 4.5% and 5% enriched fuel compositions, respectively. The superior amounts of ^{239}Pu, and ^{235}U in the 5% enriched fuel composition, explains the higher ^{238}U depletion rate, subsequently substantiating the higher breeding capabilities of the 5% enriched fuel composition.

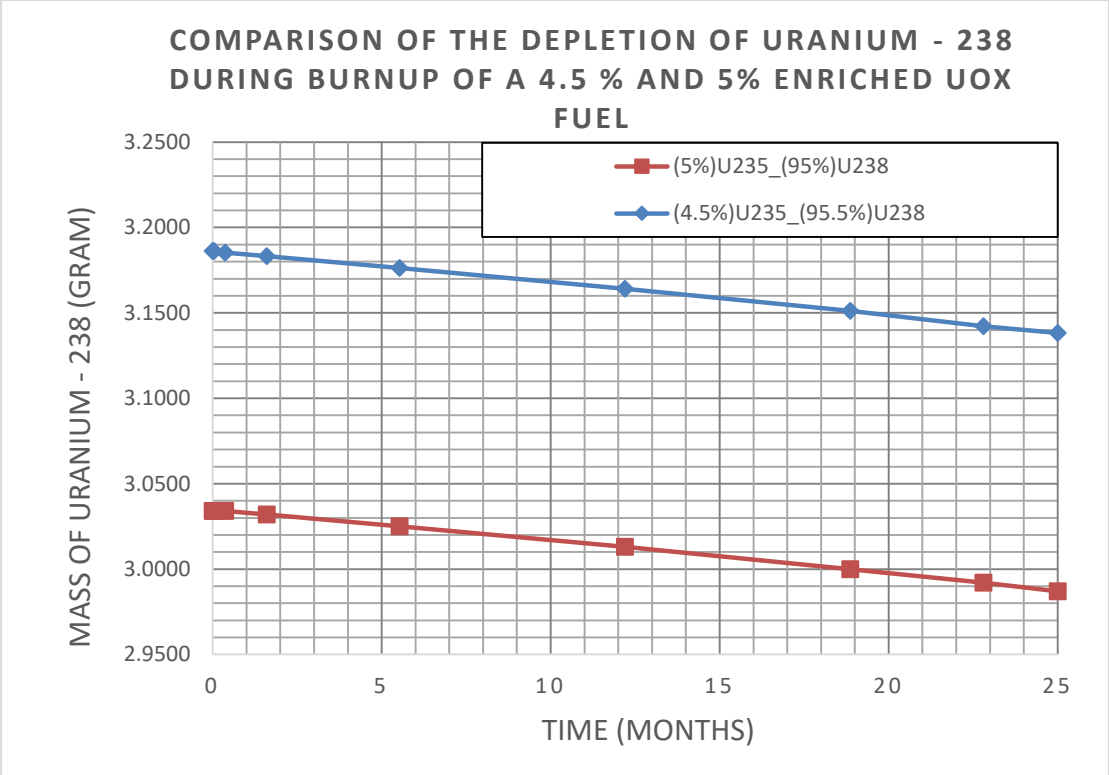

Figure 45: Uranium – 238 depletion rate in the 4.5% and 5% enriched UOX fuel compositions during burnup

5.5.2.2.2 Addition of thorium – 232

The following section, depict the inclusion of thorium-232 in varying concentrations, in a standard UOX fuel compositions comprised of 5% ^{235}U and 95% ^{238}U.

5.5.2.2.2.1 Inclusion of 2% Thorium - 232

In an effort to reduce the initial infinite neutron multiplication (k_∞) at BOL, small amounts of ^{232}Th were iteratively added to the 5 a/o ^{235}U fuel composition as described in section 5.5.1.

Due to the high neutron capture cross section of ^{232}Th in the thermal energy spectrum, only a small percentage of ^{232}Th was required to match the predetermined initial infinite neutron multiplication factor (k_∞) limit, of k_∞ =1.43316.

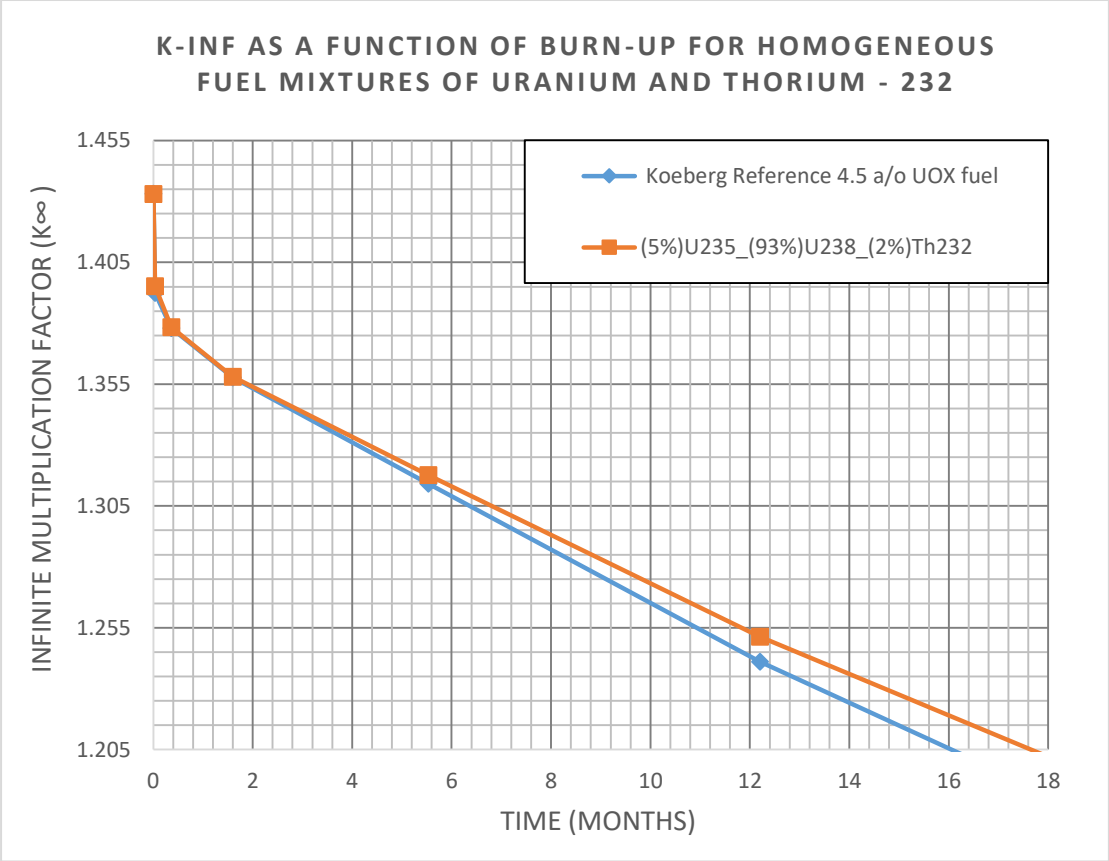

Figure 46: Comparison of the Infinite multiplication factor over time due to burn-up of the standard Koeberg fuel cycle and a conceptual UOX cycle containing traces of thorium.

By manipulating the conceptual fuel composition, to match the upper limit for the infinite multiplication factor (k_∞), a contrivance was established to evaluate the performance of conceptual fuel composition. An inclusion of 2% ^{232}Th, was required to normalize the infinite neutron multiplication factor (k_∞), and delivered a fuel cycle length of 17.6 months, as apparent from Figure 46.

By diluting the 5 a/o ^{235}U fuel composition with thorium, it enabled the breeding of ^{233}U, which as seen in section 5.4.3.1.2 is a good fissile isotope. The addition of ^{232}Th, increased thermalized neutron utilization of the fuel composition at the BOL, where it is required most, and effectively bred fissile material when the depletion of the ^{235}U reserves started to occur.

5.5.2.2.2.2 Thorium -232 substitution in a UOX fuel composition

A feasibility analysis of an alternate fuel composition, where the ^{238}U in the 5 a/o ^{235}U fuel composition was substituted with ^{232}Th was also done. The logic behind this was the larger thermal radiative capture cross section of ^{232}Th, in comparison with the radiative capture cross section of ^{238}U, as seen in Figure 23.

This would conceptually solve two problems; firstly the increased captures would lower the initial infinite neutron multiplication factor (k_∞) and secondly ^{232}Th, breeds ^{233}U over time, which as determined in section 5.4.3.1.2. and 5.4.3.2.2, yields more neutrons per fission neutron than ^{235}U.

From the data displayed in Figure 25 and Figure 47, where an identical composition was tested, it is apparent that the added ^{232}Th, did not deliver the desired result.

The aggressive capture of thermalized neutrons by ^{232}Th radically decreased the infinite neutron multiplication factor (k_∞), to the extent that the cycle could never recover, in spite of the ^{233}U accumulation due to breeding.

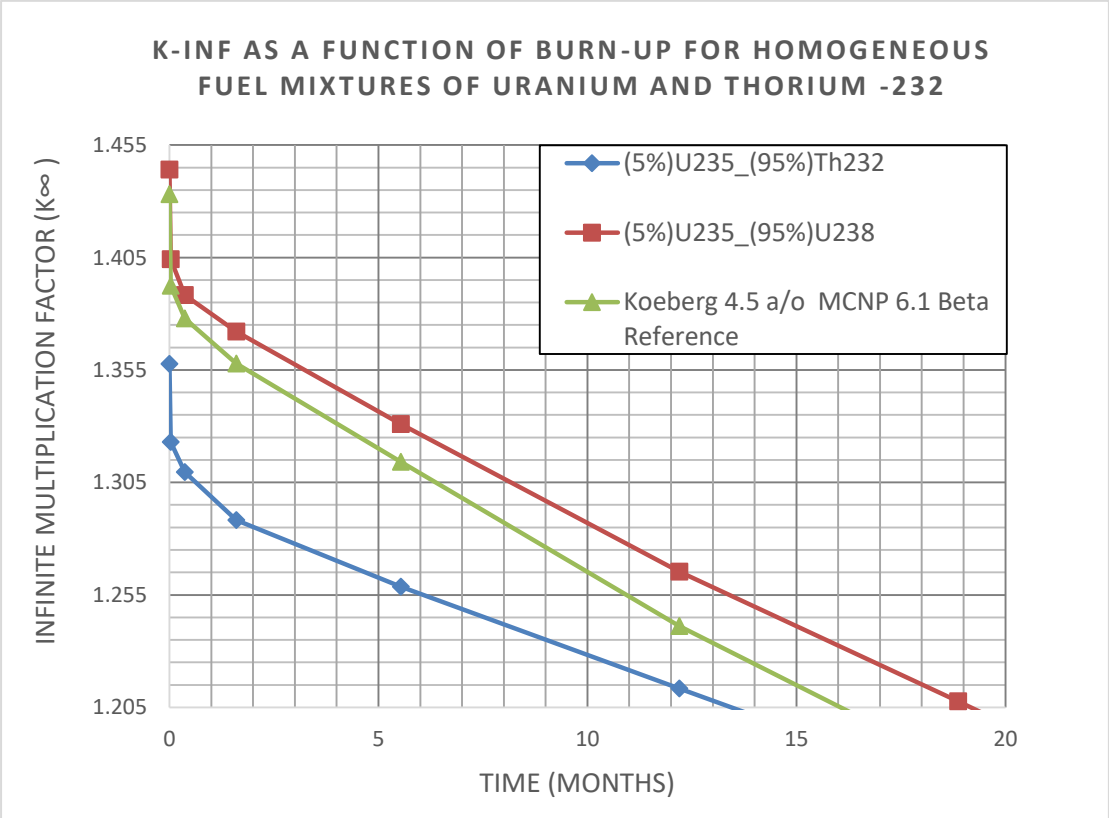

Figure 47: The Infinite multiplication factor over time due to burnup of a standard UOX cycle and a conceptual cycle containing thorium.

5.5.2.2.2.3 Thorium – 232 and UOX composites

Due to the catastrophic failure of, the proposed 5% ^{235}U, and 95% ^{232}Th fuel composition, an alternative was conceptualised, where the fertile isotope composition is comprised of equal parts ^{232}Th, and ^{238}U.

Conceptually this composition, would still decrease, the initial infinite neutron multiplication factor (k_∞), whilst breeding ^{233}U, and ^{239}Pu, subsequently providing an extending fuel cycle length.

The burnup data comparison of the standard 5% enriched UOX fuel, 5% enriched ^{232}Th substitute, and the conceptual fuel composition consisting of: 5% ^{235}U, 47.5% ^{238}U, and 47.5% ^{232}Th are presented in Figure 48.

The equal parts ^{232}Th and ^{238}U fuel composition, delivered a surprising result, in the sense that it delivered a diminutive cycle length, in comparison with the 5% ^{235}U and 95% ^{232}Th fuel composition. The aforementioned can be explained by, attentive analysis of the capture data, as seen in Table 21.

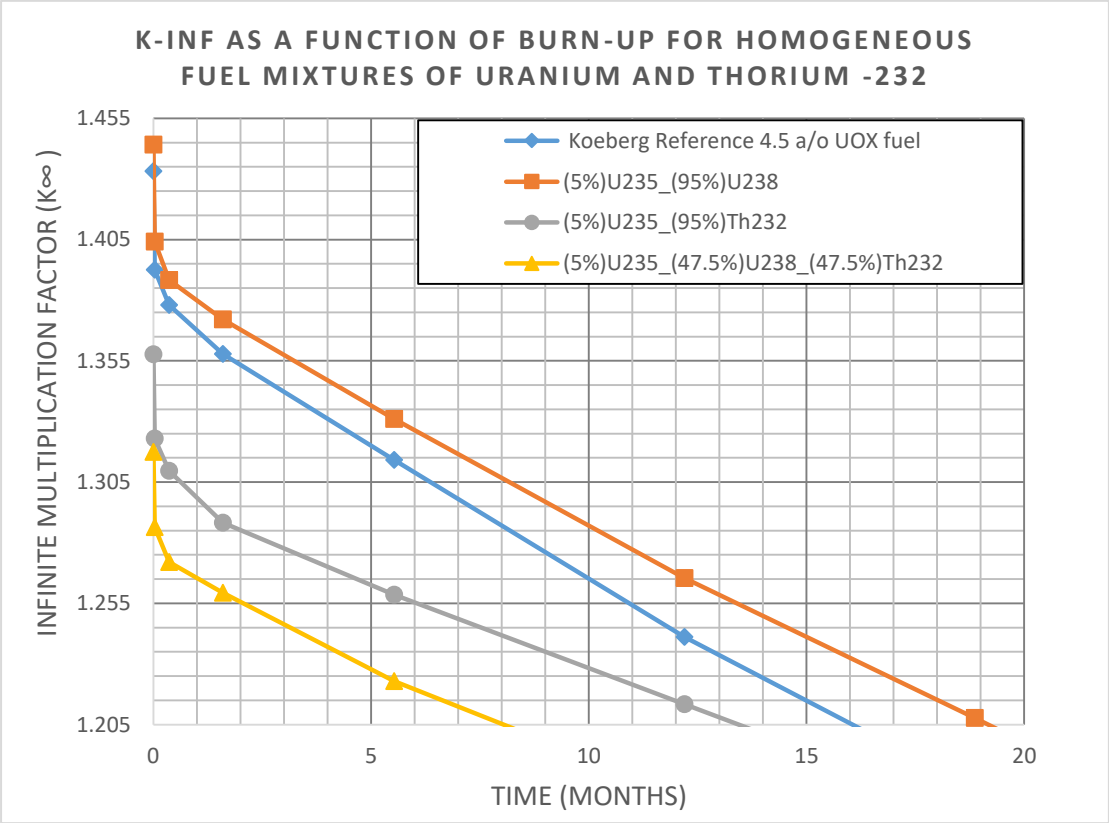

Figure 48: The Infinite multiplication factor over time due to burnup of a standard UOX cycle and a conceptual cycles containing thorium.

To draw an accurate comparison of the various fuel compositions performance, normalization of the data needed to be done.

The 47.5% ^{232}Th, and 47.5% ^{238}U composite, showed an increase in neutron captures (per volume), of 35.66% in the ^{238}U, when compared with the standard 95%^{238}U composite, and 17.54% in the ^{232}Th when compared with the equivalent composition.

The above mentioned, accompanied by the increased neutron captures observed in the oxygen, present in the fuel, adequately explains the radical decrease in the initial infinite neutron multiplication factor (k_∞), and therefore the decreased performance, of the conceptual 47.5% ^{232}Th, and 47.5% ^{238}U fuel composition.

5.5.2.2.2.4 Data analysis

The following section, provides an in-depth analysis of the neutron capture, and fission data obtained during burnup simulations of the various fuel compositions.

Table 21: Neutron captures in homogeneous mixtures of ^{235}U and other fertile isotopes on day zero of burnup

	Isotopic composition		
Neutron captures	**(5%)U235_(95%)Th232**	**(5%)U235_(95%)U238**	**(5%)U235_(47.5%)U238_(47.5%)Th232**
Moderator (H_2O)	2.4172E+11	2.2187E+11	2.3380E+11
Uranium-235	4.3260E+11	7.5603E+11	7.7752E+11
Thorium - 232	1.6853E+12	0.00E+00	9.9044E+11
Uranium - 238	0.00E+00	1.4197E+12	9.6298E+11
Oxygen (in fuel)	9.58E+09	9.1005E+09	1.0213E+10
Helium	0.00E+00	0.00E+00	0.00E+00
Zircaloy-4	3.5707E+10	3.3028E+10	3.4278E+10

The increased captures of the composite fuel composition is also evident in the total captures per fuel composition as indicated in Table 22. The 47.5% ^{232}Th, and 47.5% ^{238}U fuel composition, had 25.13% and 23.34% more captures than the 95% ^{232}Th and 95% ^{238}U fuel compositions respectively.

Table 22: Total neutron captures per ^{235}U fuel composition on day zero

Isotopic composition	Total captures
(5%)U235_(95%)Th232	2.4049E+12
(5%)U235_(95%)U238	2.4397E+12
(5%)U235_(47.5%)U238_(47.5%)Th232	3.0092E+12

The amount of fissions per fertile isotope, exhibited the same propensity, as the total neutron capture data. The 47.5% ^{232}Th, and 47.5% ^{238}U fuel composite, had a fertile isotope fission increase (per volume) of 5.1985%, and 10.8407% in the ^{232}Th, and ^{238}U respectively when compared with the equivalent models.

Table 23: Fission reactions in homogeneous mixtures of ^{235}U and other fertile isotopes on day zero of burnup

	Fissions		
Isotopic composition	**Uranium-235**	**Uranium - 238**	**Thorium - 232**
(5%)U235_(95%)Th232	3.4357E+12	0.0000E+00	4.2223E+10
(5%)U235_(95%)U238	3.3084E+12	1.6473E+11	0.0000E+00
(5%)U235_(47.5%)U238_(47.5%)Th232	3.3675E+12	9.1294E+10	2.2209E+10

5.5.2.2.2.5 Isotopic breeding and depletion rates

In correspondence with the neutron capture data, as seen in Table 21, the breeding rates depicted the same propensity, with regard to the 5% ^{235}U, 47.5% ^{232}Th, and 47.5% ^{238}U, composite. The amalgamation of ^{232}Th, and ^{238}U yielded (per volume), 20.6897% more ^{233}U than the 5% ^{235}U, and 95% ^{232}Th composition, and 12.50% more ^{239}Pu than the 5% ^{235}U, and 95% ^{238}U composition.

The ^{235}U depletion rate, during burnup simulations of the evaluated fuel compositions as seen in Figure 51, correspond well with the breeding rates as described above. The standard 5% ^{235}U, and 95% ^{238}U fuel composition, had the slowest depletion rate, with only 50.960% of the ^{235}U burning away. The 5% ^{235}U, 47.5% ^{232}Th, and 47.5% ^{238}U, composite delivered the second best result with a total ^{235}U loss of 51.29%, and finally the 5% ^{235}U, and 95% ^{232}Th composition had a total ^{235}U depletion of 58.81%.

The conversion of fertile isotopes into fissile isotopes are displayed in Table 24, and Table 25.

Table 24: Mass conversion of fertile to fissile isotopes per unit volume

	Isotopes			
Isotopic composition	**Thorium-232 Depletion [g]**	**Uranium -233 Bred [g]**	**Uranium – 238 Depletion [g]**	**Plutonium -239 Bred [g]**
(5%)U235_(95%)Th232	0.0500	0.0289	0.0000	0.0000
(5%)U235_(95%)U238	0.0000	0.0000	0.0473	0.0168
(5%)U235_(47.5%)U238_(47.5%)Th232	0.0562	0.0353	0.0640	0.0211

It is important to note that Table 25 displays, the conversion efficiency [%], from fertile to fissile isotopes, of the various evaluated fuel compositions, this differs from net fissile isotope yield [g], as displayed in Figure 49, and Figure 50.

Table 25: Conversion percentage

	Breeding efficiency [%]	
Isotopic composition	**Uranium-233**	**Plutonium -239**
(5%)U235_(95%)Th232	57.80	0
(5%)U235_(95%)U238	0	35.52
(5%)U235_(47.5%)U238_(47.5%)Th232	62.81	32.96

The generated data suggests that, ^{232}Th has a greater conversion efficiency than ^{238}U. The above mentioned, was determined on the basis of, total fertile content at the BOL,

and total fissile yield at the End of Life (EOL). It is important to note that, this can vary during operation, due to the breeding chain lengths (half-life dependent), of the evaluated isotopes, and instantaneous fission after birth.

The average time-lapse before ^{233}U is bred from ^{232}Th is 26.95 days, and ^{239}Pu from ^{238}U 2.35 days (NP.net, 2016). The aforementioned, is a possible explanation for the low conversion efficiency of ^{238}U, the ^{239}Pu is bred much faster than ^{233}U, and therefore burned away much quicker, resulting in the illusion of a smaller yield percentage.

It is important to note that the data as displayed in Figure 52, where normalized to ensure that an accurate comparison could be made.

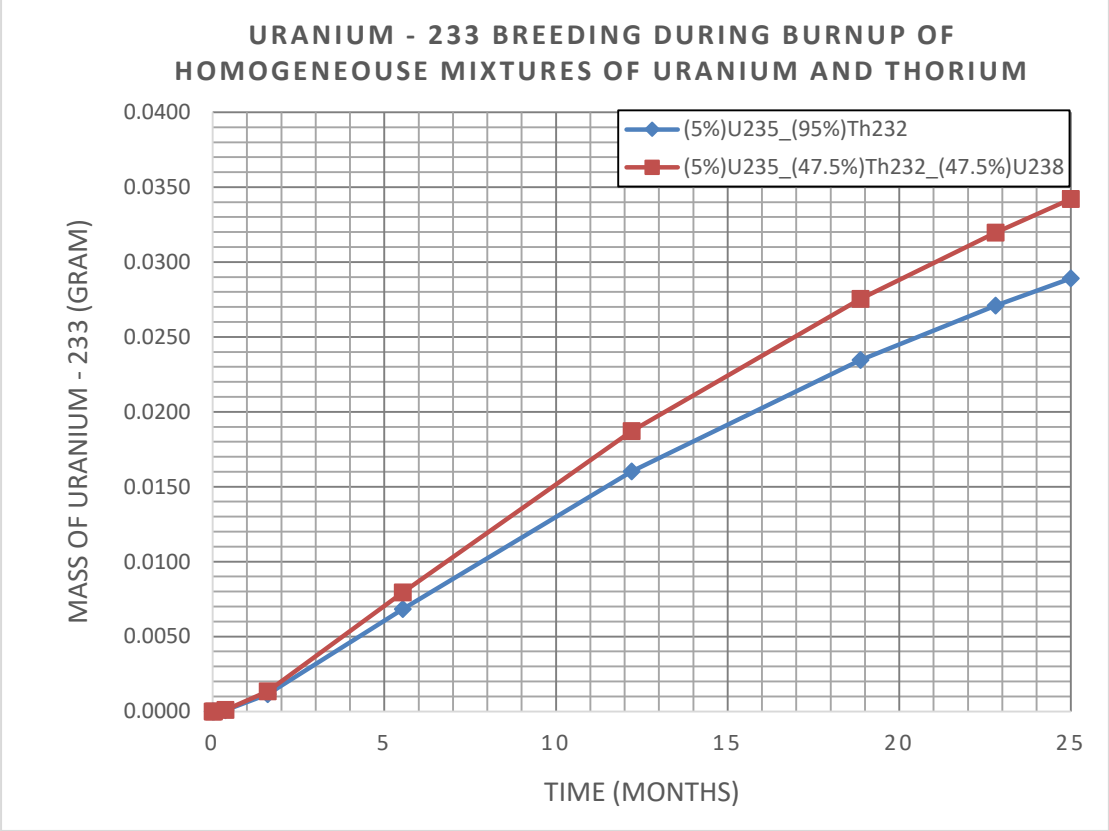

Figure 49: Uranium – 233 breeding rate during burnup of selected ^{232}Th and UOX fuel compositions

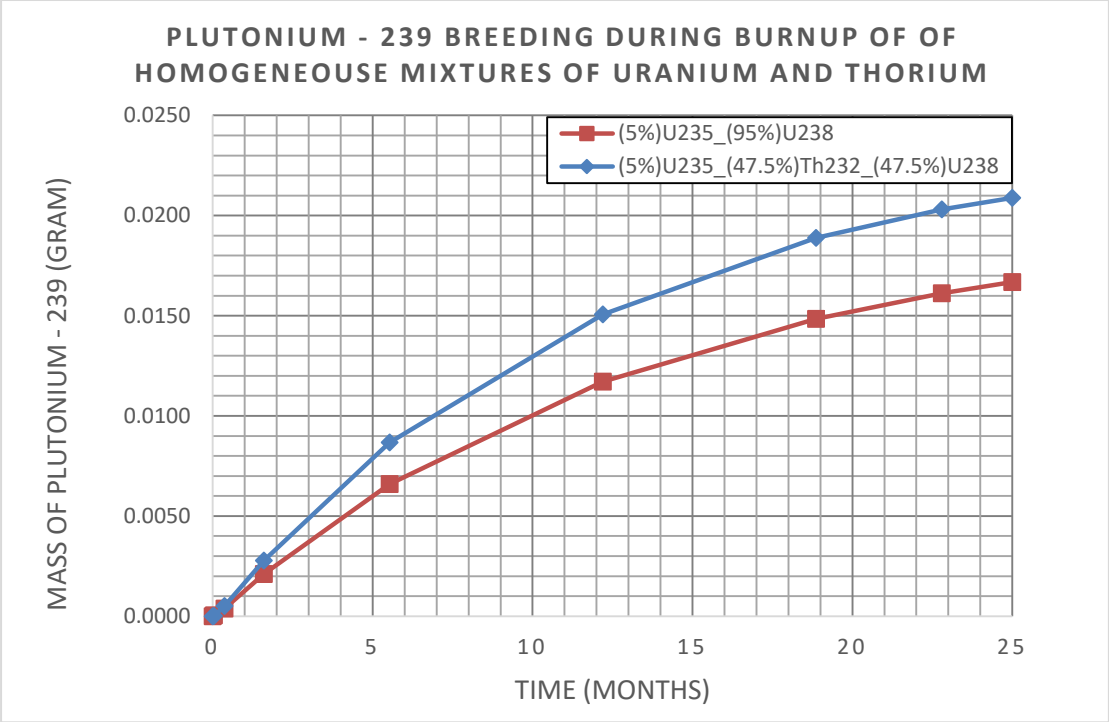

Figure 50: Plutonium – 239 breeding rate during burnup of selected ^{232}Th and UOX fuel compositions

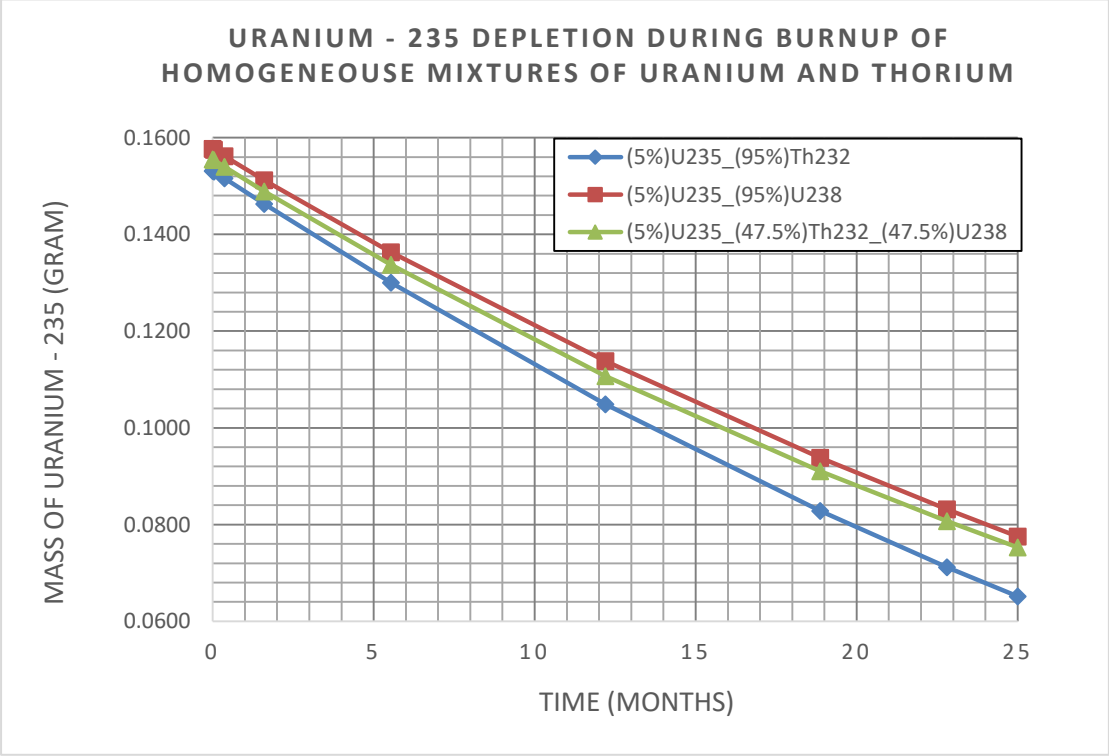

Figure 51: Uranium – 235 depletion rate during burnup of selected ^{232}Th and UOX fuel compositions

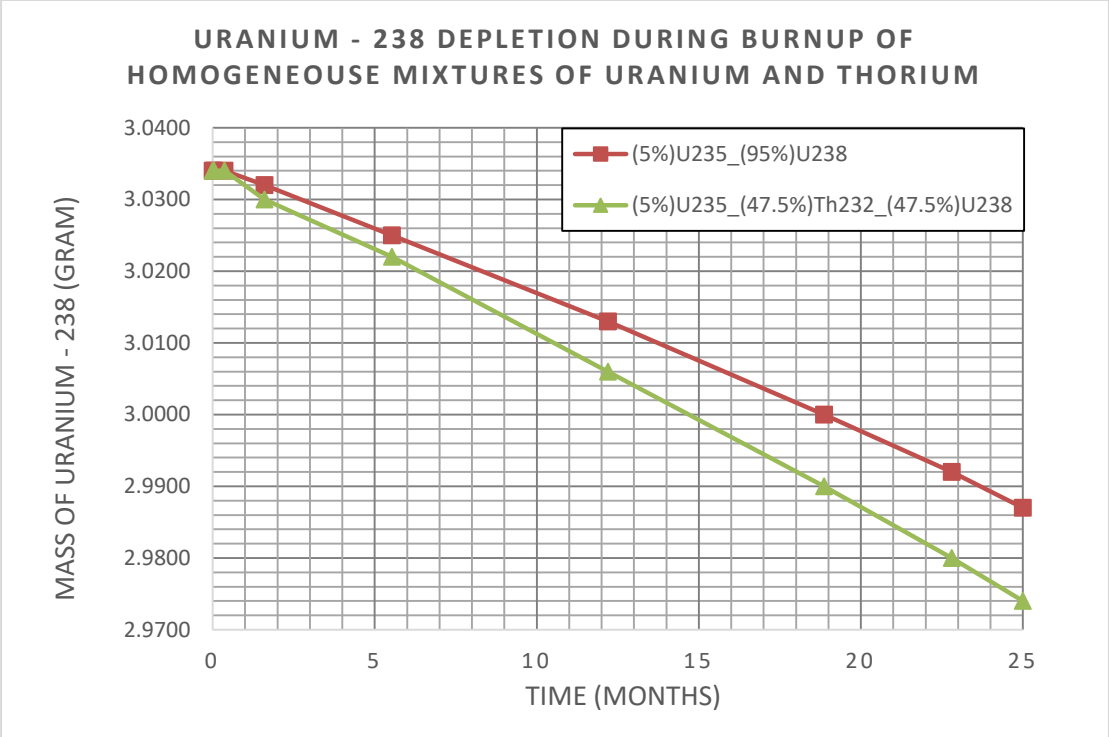

Figure 52: Uranium – 238 depletion rate during burnup of selected ^{232}Th and UOX fuel compositions

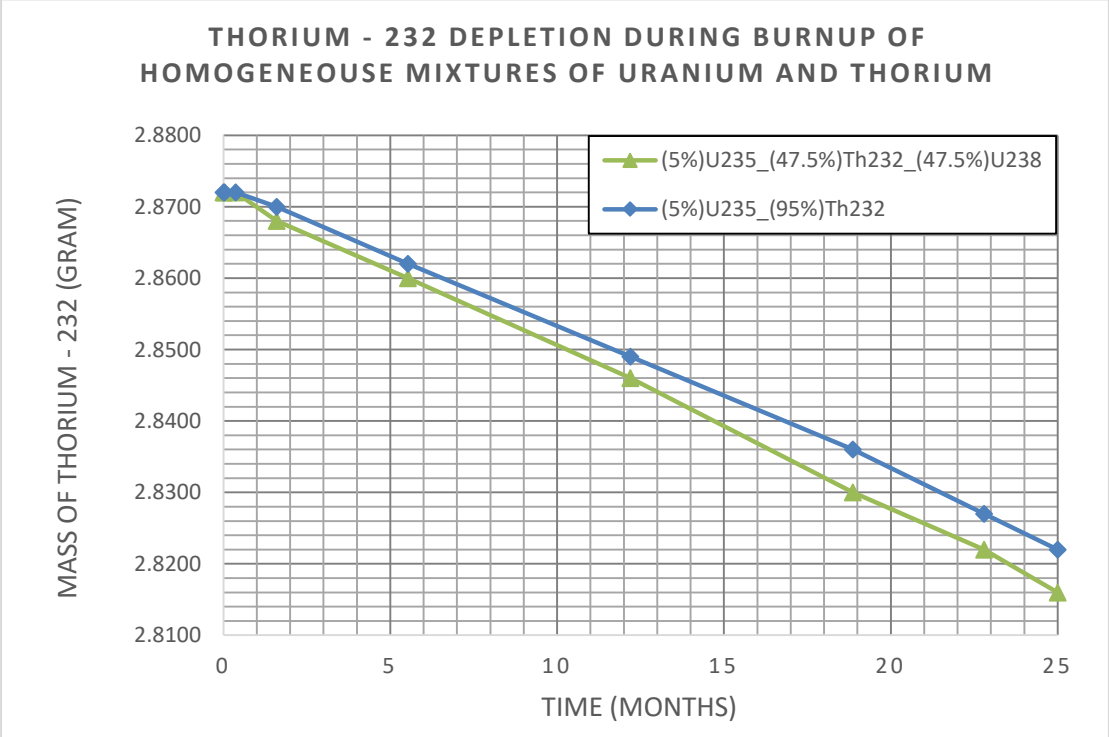

Figure 53: Thorium – 232 depletion rate during burnup of selected ^{232}Th and UOX fuel compositions

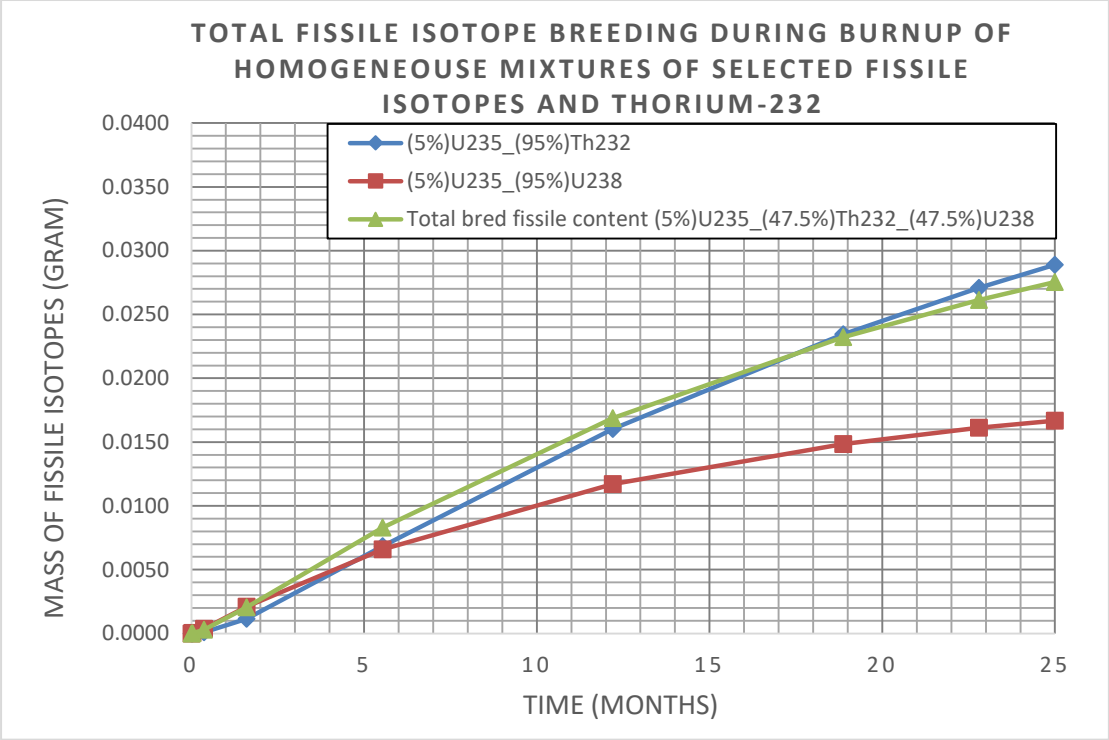

Figure 54: Total fissile isotope breeding rate during burnup of selected ^{232}Th and UOX fuel compositions

5.5.2.2.3 Addition of natural boron

Natural boron, has varying natural isotopic composition of between 18.9 – 20.4 % ^{10}B and 79.6 - 81.1 % ^{11}B (CIAAW, 2010). The boron is then enriched to 100% ^{10}B, and due to its high solubility, it is the added to the moderator of Pressurized Water-cooled Reactors (PWRs). It is used to reduce the initial spike, in the infinite neutron multiplication factor (k_∞), during fresh fuel start-ups, and during accident scenarios, the core can be flooded with borated water, to reduce the neutron populations.

The borated water is then later circulated through an adjacent refinery plant, where the boron is extracted. It is noteworthy to mention that the extracted boron will contain large quantities of ^{11}B and ^{7}Li, due to neutron capture reactions, the boron will then have to be enriched again with ^{10}B. This is a very costly procedure, and served as the basis for testing the concept of adding boron to the fuel composition.

The ^{10}B with its high neutron capture cross section, will capture ample amounts of neutrons, effectively reducing the initial infinite neutron multiplication factor (k_∞), at the BOL. Due to the reduced neutron capture cross section of ^{11}B in comparison with ^{10}B,

natural boron was selected for the concept evaluation. The aforementioned is also used to prevent prolonged effects, on the neutron economy of the fuel.

As in the benchmark test, done in section 5.5.2.2.2, the aim was to lower the initial infinite neutron multiplication factor (k_∞), by homogeneously adding natural boron with an isotopic composition of 18.9 % ^{10}B, and 81.1% ^{11}B to the isotopic composition of the 5 a/o ^{235}U model. The amount of boron required to match the infinite neutron multiplication factor (k_∞) limit, k_∞ =1.43316, was determined iteratively.

The final isotopic composition of the conceptual fuel mixture, in atomic fraction percentage (at. %), consists of: 5 % ^{235}U, 94.9395 % ^{238}U, and 0.0605 % B. The behaviour of the infinite neutron multiplication factor over time due to burnup is presented in Figure 55.

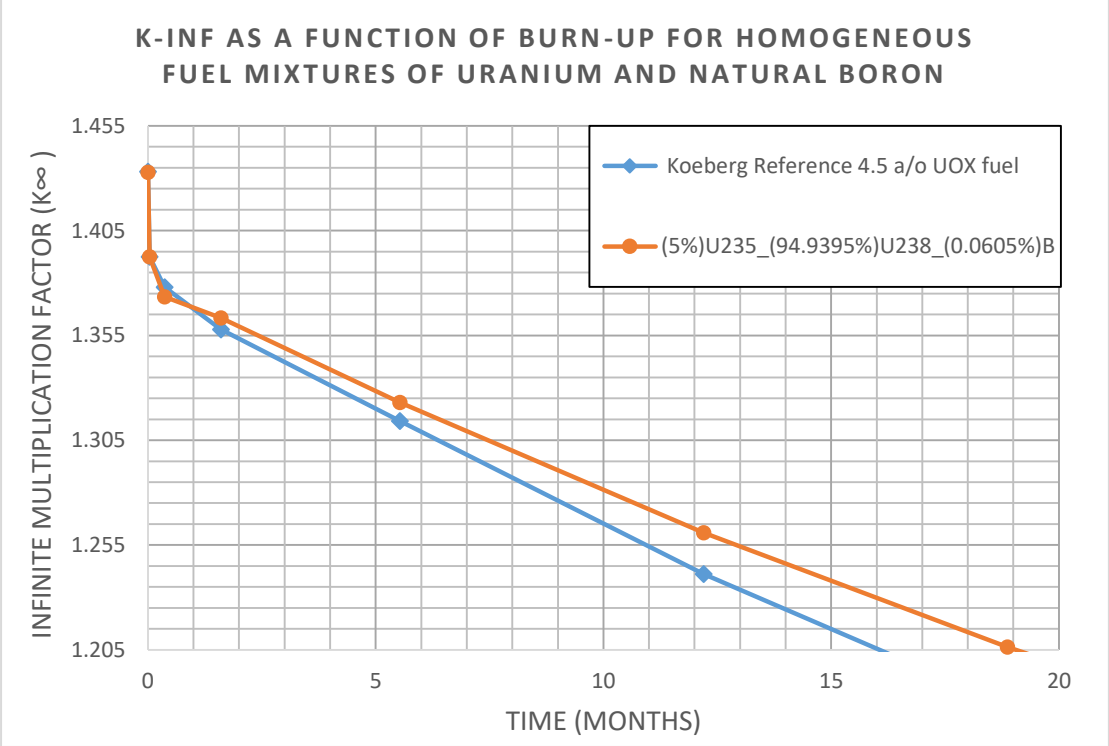

Figure 55: Comparison of the Infinite multiplication factor over time due to burn-up of the standard Koeberg fuel cycle and a conceptual UOX cycle containing traces of natural boron.

As evident from the data portrayed by Figure 55, the homogeneous inclusion of small quantities of natural boron, successfully decrease the infinite neutron multiplication factor (k_∞), to the desired limit of k_∞ =1.43316, and effectively extended the fuel cycle length to 19 months. The above mentioned result, can be contributed to the excessive

capture of thermalized neutrons at the BOL, by the natural boron. The ^{10}B, quickly becomes satiated ^{11}B, and subsequently dramatically decreases the neutron captures, therefore preserving the ^{235}U reserve at the BOL.

Figure 56 shows, the effect of the homogeneous 0.0605 % natural boron inclusion, on the infinite neutron multiplication factor (k_∞). It is evident that the boron, only significantly influenced the fuel cycle for the first few months, during burnup.

After that point, most of the boron had become saturated ^{11}B and underwent alpha – decay to form ^{7}Li. The depletion rate of ^{10}B as seen in Figure 57, indicates that after 5 months, about 50% of the ^{10}B concentration has disappeared.

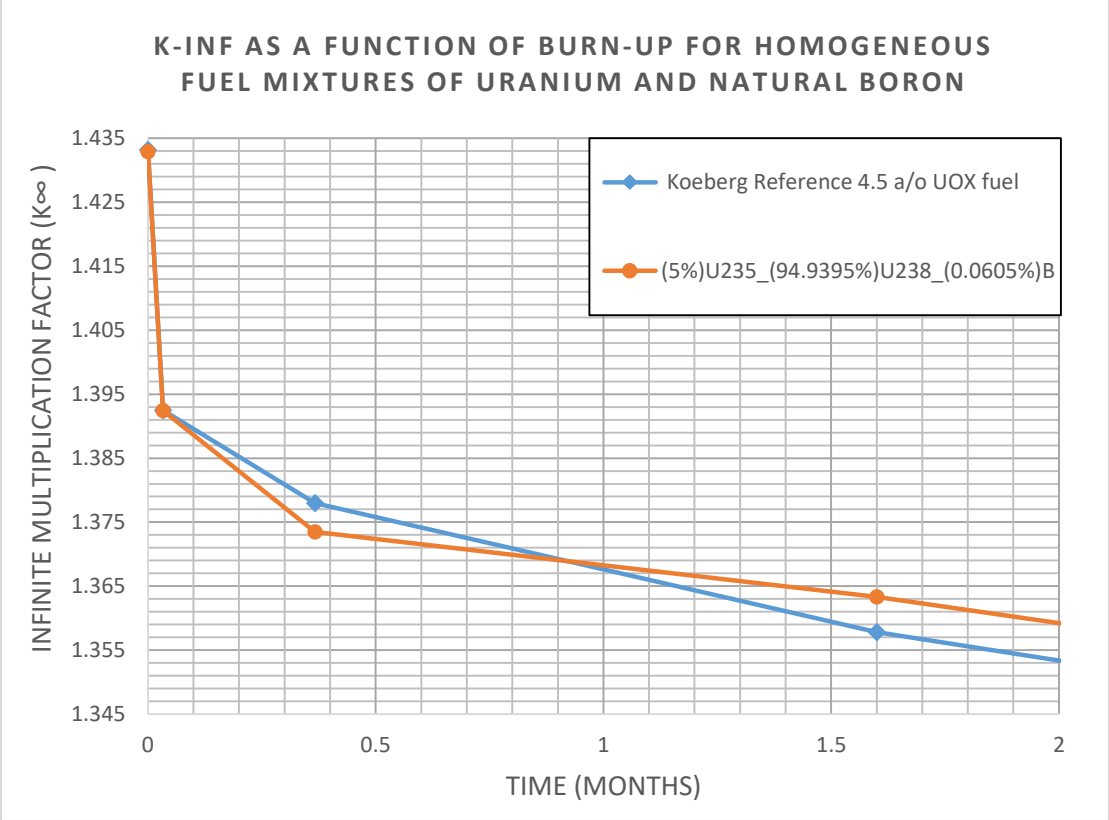

Figure 56: Comparison of the Infinite multiplication factor over the first two months due to burn-up of the standard Koeberg fuel cycle and a conceptual UOX cycle containing traces of natural boron.

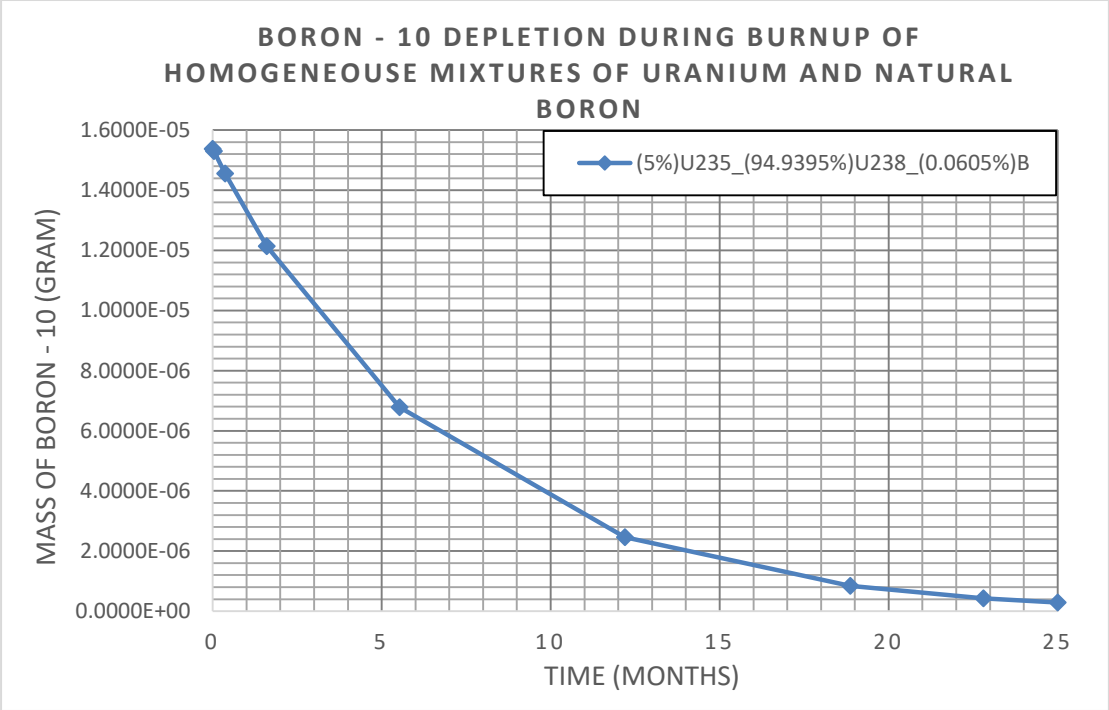

Figure 57: Boron – 10 depletion during burnup of a UOX fuel composition containing traces of natural boron.

For the rest of the burnup period, the fuel composition functions as if, it were boron free, by reaching the same fuel cycle length as the 5 a/o ^{235}U fuel composition, as discussed in section 5.5.2. The increased amount of ^{235}U during the later stages of burnup, provides the necessary fission neutrons, to increase the infinite neutron multiplication factor (k_∞), above the bottom limit of $k_\infty = 1.205$, and evidently extending the fuel cycle length. If a substantial amount of boron is added to the fuel composition, it could reduce the reactors dependency on neutron poisons/absorbers in the moderator.

5.5.2.3 Section results

Figure 58, displays a compilation of the computed data from the evaluated fuel compositions, and will serve as a further feasibility analysis, of the proposed fuel compositions, with regard to the constraints specified in section 5.5.1.

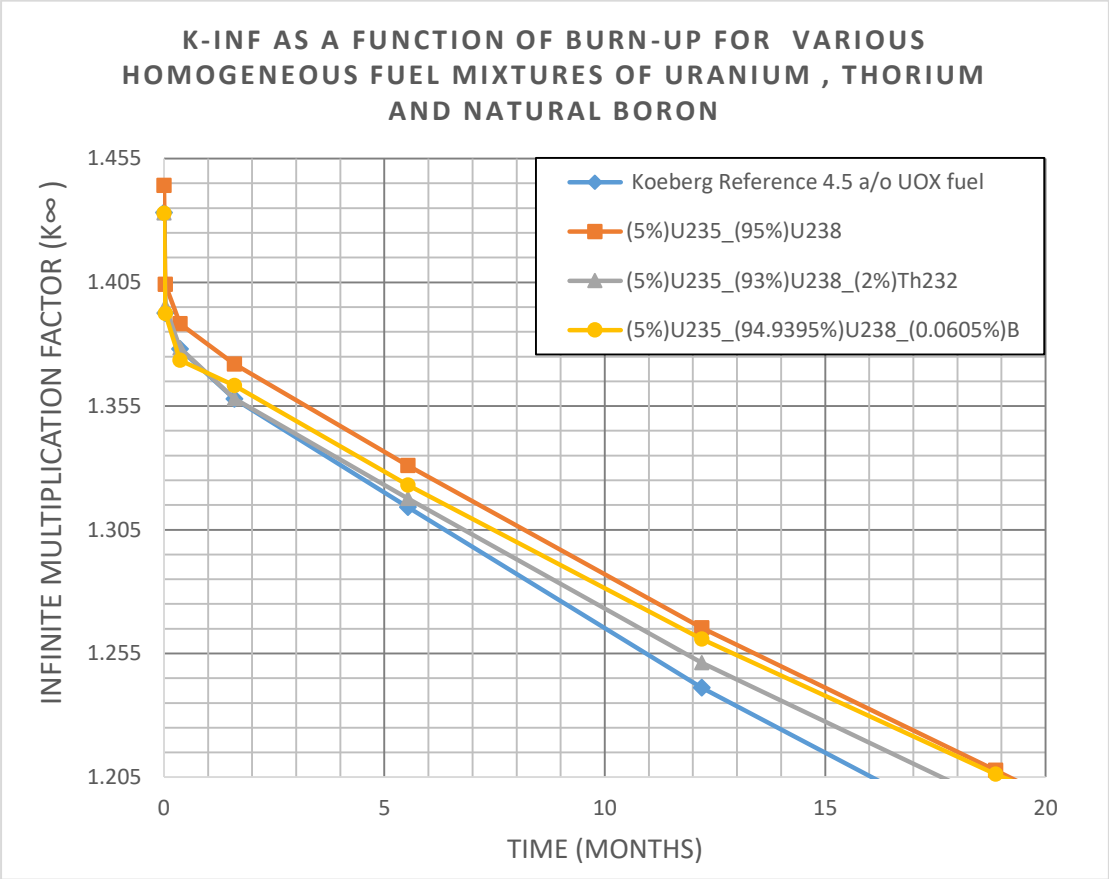

Figure 58: Comparison of the Infinite multiplication factor over time due to burnup of various mixtures of uranium, thorium and natural boron

All of the fuel compositions displayed in Figure 58, successfully increases the fuel cycle length, to varying extents, without any geometric alterations to the fuel pellet or reactor. A comparison of the isotopic neutron captures are displayed in

The only fuel composition that violated one of the prerequisites of feasibility, is the 5% ^{235}U and 95% ^{238}U fuel composition. The fuel composition did extend the fuel cycle dramatically, but unfortunately increased the infinite neutron multiplication factor (k_∞) at BOL above the predetermined limit of $k_\infty = 1.43316$.

Table 26: Neutron captures in homogeneous mixtures of ^{235}U, and selected fertile isotopes and neutron poisons on day zero of burnup

	Isotopic composition			
Neutron captures	**4.5% U235 _95.5% U238**	**5% U235 _95% U238**	**5% U235 _93% U238 _2%Th232**	**5% U235 _94.9395% U238 _0.0605% B**
Moderator (H_2O)	2.2845E+11	2.2182E+11	2.29E+11	2.30E+11
Uranium-235	7.4449E+11	7.5603E+11	7.78E+11	7.55E+11
Fertile isotope	1.4762E+12	1.4197E+12	1.95E+12	1.46E+12
Oxygen (in fuel)	9.3704E+09	9.1005E+09	1.02E+10	9.26E+09
Boron	0.00E+00	0.00E+00	0.00E+00	2.64E+10
Helium	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Zircaloy-4	3.2863E+10	3.3028E+10	3.3054E+10	3.3087E+10

From Table 26, and Table 27 it is apparent, that the only isotope that significantly influences the amount of neutron captures is ^{232}Th. The addition of natural boron did increase the neutron captures, mostly in the fertile material, but only in comparison with its original composition of 5% ^{235}U, and 95% ^{238}U.

Table 27: Total neutron captures per ^{235}U fuel composition on day zero

Isotopic composition	Total captures
4.5% U235_95.5% U238	2.4914E+12
5% U235_95% U238	2.4397E+12
5% U235_93% U238_2%Th232	2.9671E+12
5% U235_94.9395% U238_0.0605%B	2.4814E+12

Table 28: Fission reactions in homogeneous mixtures of ^{235}U, selected fertile isotopes and neutron poisons on day zero of burnup

	Fissions	
Isotopic composition	**Uranium-235**	**Fertile isotopes**
4.5% U235_95.5% U238	3.3142E+12	1.6764E+11
5% U235_95% U238	3.3158E+12	1.6473E+11
5% U235_93% U238_2%Th232	3.3078E+12	1.6462E+11
5% U235_94.9395% U238_0.0605%B	3.3135E+12	1.6514E+11

One of the main consideration points, when determining the feasibility of a conceptual fuel composition, is the breeding rate, depletion rate, and conversion efficiency of the proposed composition. Higher breeding, and slower depletion rates will lead to an extended operational lifetime of the fuel composition.

As seen in Figure 59, all of the proposed compositions produced, higher fissile isotope yields than the standard 4.5% ^{235}U, and 95.5% ^{238}U fuel composition. Prominence should be placed, on the performance of the 5% ^{235}U, 94.9395% ^{238}U, and 0.0605% B fuel composition in this regard. The aforementioned successfully extended the fuel cycle length, to the same extent than the 5% ^{235}U, and 95% ^{238}U fuel composition, without compromising the breeding, and depletion rates of the fuel. The above mentioned is visible from the data presented in Figure 59, Figure 60, and Figure 61.

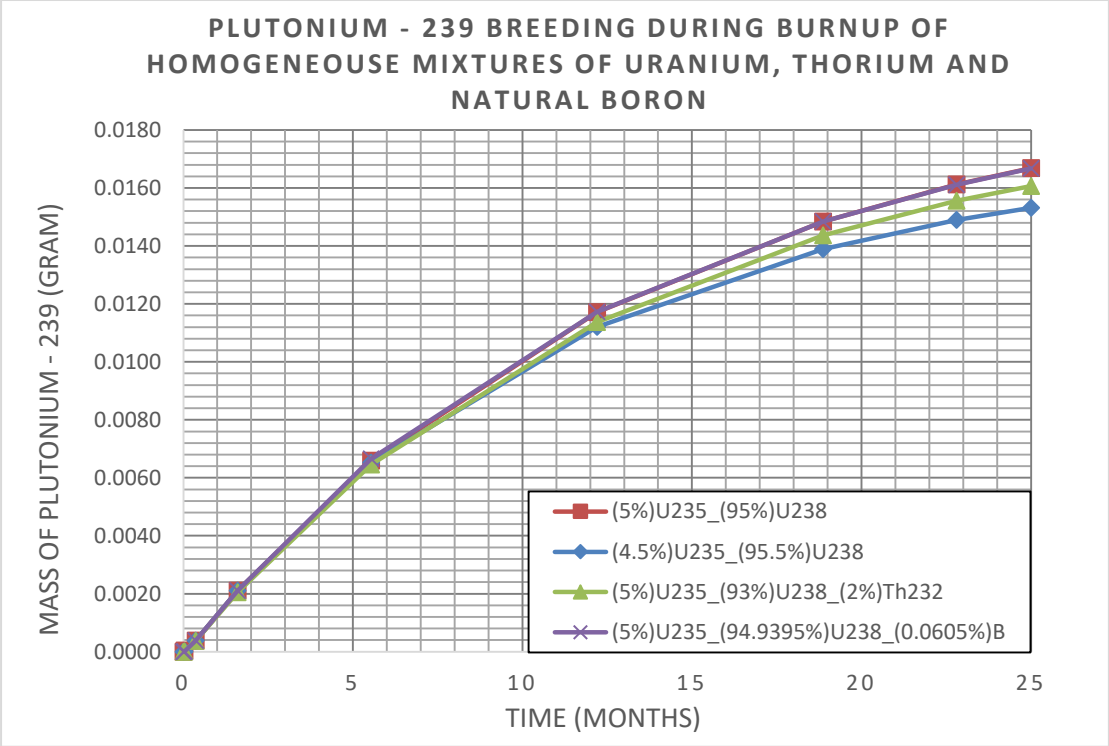

Figure 59: Comparison of plutonium - 239 breeding rate during burnup of homogeneous mixtures of uranium, thorium and natural boron

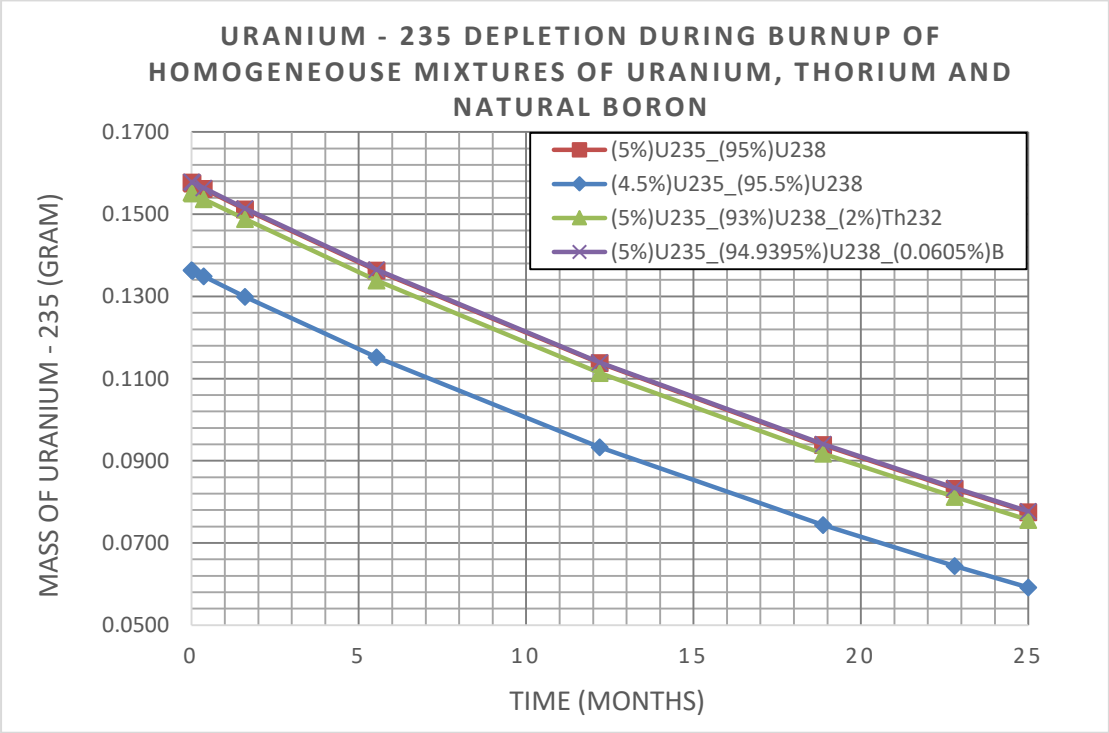

Figure 60: Comparison of uranium - 235 depletion rate during burnup of homogeneous mixtures of uranium, thorium and natural boron

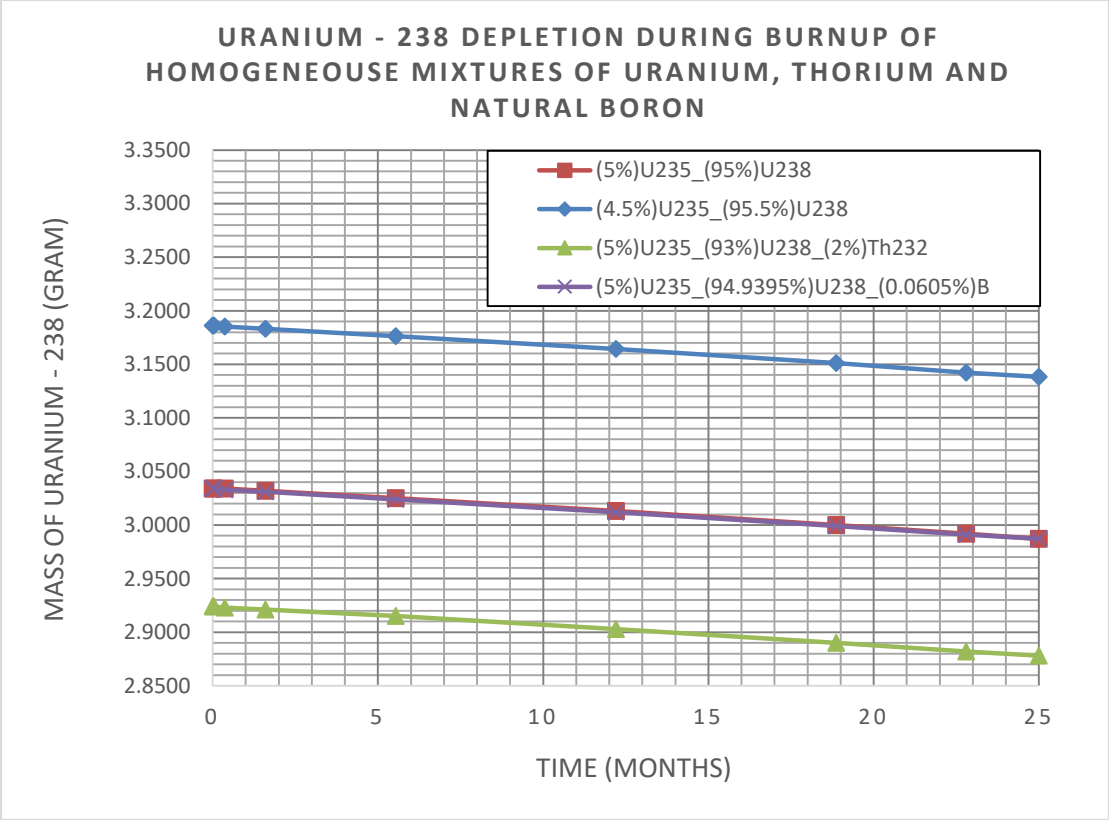

Figure 61: Comparison of uranium - 238 depletion rate during burnup of homogeneous mixtures of uranium, thorium and natural boron

5.5.2.4 Conclusion

From the analysed data, it was determined that all of the proposed fuel compositions would, to varying extents, prolong the fuel cycle length of Koeberg nuclear power plants 900 MW, Pressurized Water-cooled Reactor (PWR). The two isotopic inclusion based conceptual compositions, delivered the best result, with regard to the, feasibility prerequisites as described in section 5.5.1.

The 2% ^{232}Th, and the natural boron fuel composites successfully increased the fuel cycle length, to 17.6 and 19.2 months, respectively. Neither increased the infinite neutron multiplication factor (k_∞), nor negatively influenced, the breeding and depletion rates of the fuel.

One other consideration point, is the reactivity coefficients of the fuel. The addition of ^{232}Th, will benefit the void reactivity coefficient, moderator, and fuel temperature reactivity coefficients, due to the addition of its high resonance capture cross section in the epithermal energy spectrum. Uranium -238, is one of the largest contributors, to

the negative reactivity coefficient, of the standard 4.5% ^{235}U, and 95.5% ^{238}U fuel composition. The natural boron inclusion, will have a reduced amount of ^{238}U, which could negatively influence, the various temperature reactivity coefficients. Although not present in the proposed fuel composition, it could become problematic, with more invasive additions of natural boron.

5.5.3 Mixed oxide (MOX) fuel concepts

The following section, serves as a feasibility analysis, of Mixed Oxide fuels (MOX), as a substitute for Uranium Oxide fuels (UOX).

5.5.3.1 Introduction

In this section, a feasibility analysis was done on the implementability of MOX fuel, and a MOX - UOX amalgamations, as a substitute for the standard UOX fuel composition, currently implemented in Koeberg nuclear power plant.

MOX fuel fabrication, has been taking place since the early 1950's, by facilities in USA, Belgium, France, Germany, Japan and the Russian federation (IAEA, 2003). Standard MOX fuel, is comprised of a combination of PWR reactor-grade plutonium (RPu), and depleted uranium (DU). Generally MOX fuel assemblies, are combined with standard UOX fuel assemblies, in licenced MOX fuel Reactors, and occupy a total core assembly percentage of 30%, and in some cases up to 50% (WNA, 2011). MOX fuel compositions usually consist of, 8 - 10% RPu and 90 - 92 % DU.

The MOX fuel composition evaluated in this document comprises of 8% RPu, and 92% DU. The isotopic composition, of the RPu used in this section is comprised of, 2.763% ^{238}Pu, 53.755% ^{239}Pu, 23.615% ^{240}Pu, 13.108% ^{241}Pu, and 6.758% ^{242}Pu as specified by (Serfontein, 2011), as the isotopic composition of PWR - generated plutonium.

5.5.3.2 Methodology

A systematic approach was used, to determine if substitution of the standard Koeberg fuel composition, with MOX fuel, or a composite of MOX, and UOX fuel, could improve the current fuel cycle length, without violating the feasibility prerequisites, as described in section 5.5.1. The burnup data, of the conceptual fuel composition will be evaluated on the following basis; infinite neutron multiplication factor (k_∞), total number of capture and fission reactions at BOL, and the fuel compositions ability to breed fissile isotopes (breeding ratio).

5.5.3.3 Conceptual MOX fuel composites

The following section depict, the data obtained from burnup analysis, of various MOX fuel compositions.

5.5.3.3.1 100% MOX fuel compositions

The first point of departure, was to test the feasibility of a fuel composition, consisting of 100% MOX fuel. To clarify, a 100% MOX fuel composition consists of 8% RPu, and 92% DU.

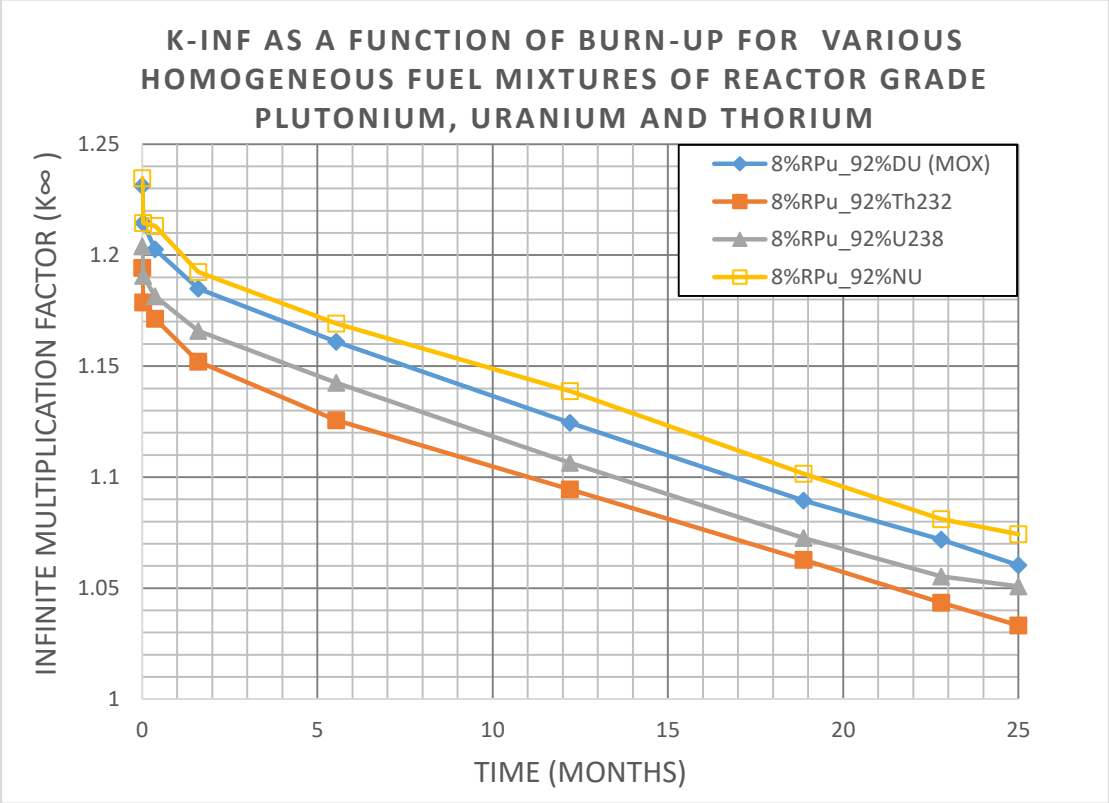

Figure 62: Comparison of the Infinite multiplication factor over time due to burnup of 100% MOX fuel, and other fertile substitutions.

The minimum infinite neutron multiplication factor (k_∞), as described in section 5.5.2.1, required to ensure a sustainable fission reaction chain, is $k_\infty = 1.43316$. From Figure 62, it is evident that, as a sole fuel source, 100% MOX fuel would not be a suitable substitute, for the standard 4.5% ^{235}U, and 95.5% ^{238}U fuel composition.

This can be attributed to, the inferior behaviour of the initial infinite neutron multiplication factor (k_∞) over time, due to burnup. The bottom limit for the infinite

neutron multiplication factor (k_∞) is reached approximately 20 days into the burnup simulation.

The feasibility of the predominant fertile isotopes, as substitutes, for depleted uranium were also evaluated. From Figure 62, it is apparent that only natural uranium (NU), showed a slight improvement in performance, when compared with the current isotopic composition, of standard MOX fuel, this can be attributed to the 0.4% increase in ^{235}U.

Table 29: Neutron captures in 100% MOX fuel, and selected fertile isotope composites on day zero of burnup.

	Isotopic composition			
Neutron captures	**8% RPu _92% DU**	**8% RPu _92% NU**	**8% RPu _92% Th232**	**8% RPu _92% U238**
Moderator (H_2O)	1.1248E+11	1.2226E+11	1.3033E+11	1.2166E+11
Oxygen (in fuel)	1.2626E+10	1.3348E+10	1.3618E+10	1.4063E+10
Uranium - 235	2.7171E+10	6.1349E+10	0.0000E+00	0.0000E+00
Thorium - 232	0.0000E+00	0.0000E+00	1.3925E+12	0.0000E+00
Uranium - 238	1.4436E+12	1.4558E+12	0.0000E+00	1.5188E+12
Plutonium - 238	3.5021E+10	3.3219E+10	3.6309E+10	3.5911E+10
Plutonium - 239	1.2879E+12	1.2390E+12	1.3667E+12	1.3078E+12
Plutonium - 240	1.1209E+12	1.1061E+12	1.2401E+12	1.1475E+12
Plutonium - 241	2.3536E+11	2.2461E+11	2.5369E+11	2.3997E+11
Plutonium - 242	1.5195E+11	1.5478E+11	1.7526E+11	1.6673E+11
Helium	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
Zircaloy-4	3.3157E+10	3.2021E+10	0.0000E+00	1.4027E+11

The performance of the conceptual fuel compositions, can be ascribed to the excessive neutron captures by the various plutonium isotopes, as presented in Table 29, and

Table 30. The neutron capture cross sections of, ^{238}Pu, ^{240}Pu, and ^{242}Pu are superior in the thermal energy spectrum, in comparison with the capture cross section of, ^{232}Th, and ^{238}U, as evident from Figure 23.

Table 30: Total neutron captures in 100% MOX fuel, and selected fertile isotope composites on day zero of burnup.

Isotopic composition	Total captures
8% RPu_92% DU	4.4603E+12
8% RPu_92% NU	4.4424E+12
8% RPu_92% Th232	4.7528E+12
8% RPu_92% U238	4.6928E+12

As seen in Table 31, excessive amounts of fissions take place in the fertile isotopes, this can be ascribed to the higher neutron yield, of the fissile plutonium isotopes, and the shifted neutron energy distribution, as described in section 5.4.3.3.8, and 5.4.3.4.8.

Table 31: Fission reactions in 100% MOX fuel, and selected fertile isotope composites on day zero of burnup.

	Fissions	
Isotopic composition	**Fissile isotopes**	**Fertile isotopes**
8% RPu_92% DU	3.1165E+12	2.4221E+11
8% RPu_92% NU	3.0995E+12	2.4291E+11
8% RPu_92% Th232	3.2394E+12	9.2615E+10
8% RPu_92% U238	3.0778E+12	2.5303E+11

Figure 63, displays a comparison of the 100% MOX fuel composition and the standard Koeberg UOX fuel composition. As indicated earlier in this section, 100% MOX fuel is not a viable substitute for the currently implemented UOX fuel composition.

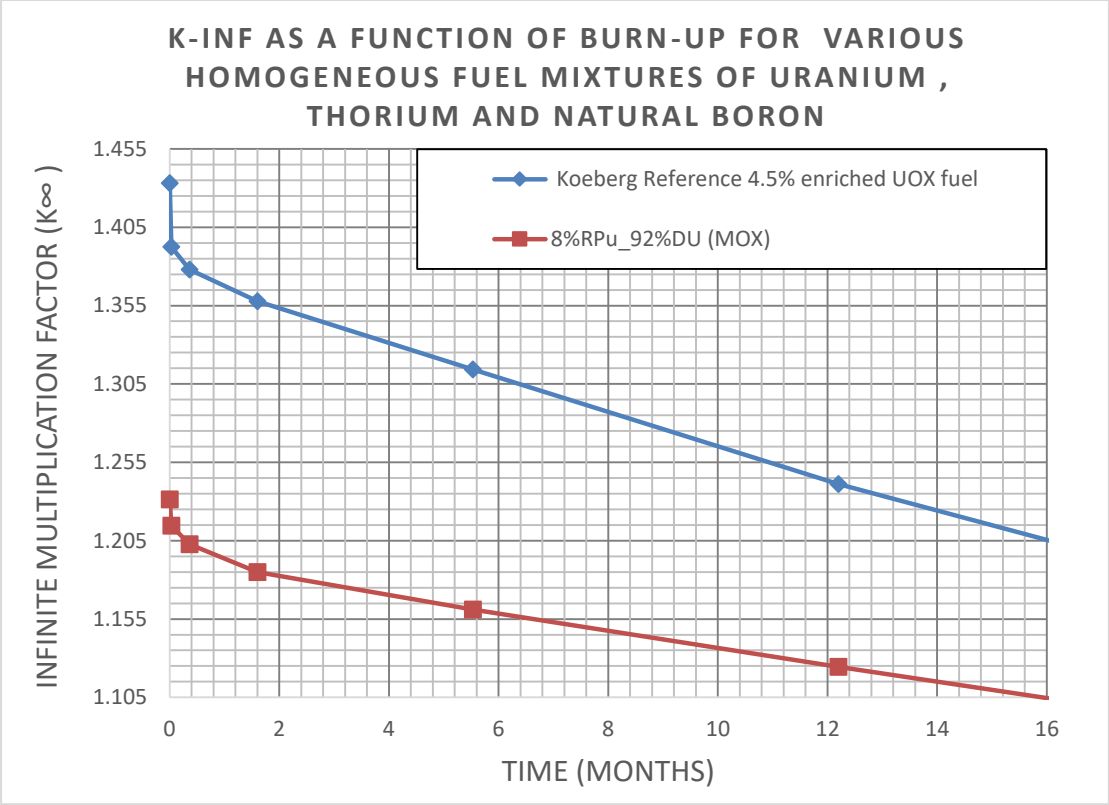

Figure 63: Comparison of the Infinite multiplication factor over time due to burnup of 100% MOX fuel, and the standard Koeberg UOX fuel composition.

The total capture data presented in Table 32, also validate the low initial infinite neutron multiplication factor (k_∞), of the 100% MOX fuel composition. The 100% MOX, captured 79.03% more neutrons than the standard UOX fuel composition on day zero of burnup.

Table 32: Total neutron captures in 100% MOX fuel, compared with the standard Koeberg UOX fuel composition.

Isotopic composition	Total captures
4.5% U235_95.5% U238	2.4914E+12
8% RPu_92% DU (MOX)	4.4603E+12

Table 33: Total fissions in 100% MOX fuel, compared with the standard Koeberg UOX fuel composition.

	Fissions	
Isotopic composition	**Fissile isotopes**	**Fertile isotopes**
4.5% U235_95.5% U238	3.3142E+12	1.6764E+11
8% RPu_92% DU (MOX)	3.1165E+12	2.4221E+11

Currently there are no standard PWRs, designed to operate on UOX fuel, operating on a 100 % MOX fuel loading. These reactors have been conceptualised, but are all based on one very specific principle, minimal neutron losses. Due to the excessive neutron capture, of the plutonium isotopes, neutron economy is a fundamental parameter to consider.

The 100% MOX fuel loadings, are conceptually possible, with excessive moderation, and improved reactivity control systems. To convert a currently implemented reactor, like Koeberg, the addition of “water rods”, or decreased fuel pin radius would be compulsory (Du Toit & Cilliers, 2014). This violates the feasibility prerequisites as described in section 5.5.1, with regard to geometric alterations to the fuel pin, and/or reactor.

Due to the high fission cross sections of ^{239}Pu, and ^{241}Pu, as seen in large Figure 37, it is apparent that large concentrations of these isotopes in a fuel composition, could become problematic, with regard to the various reactivity coefficients. Both of the fissile isotopes of plutonium, will induce an increase in the infinite neutron multiplication factor (k_∞), with an increase in temperature (moderator or fuel), and/or the presence of a void, thus prohibiting implementation thereof in commercial reactors.

5.5.3.3.2 MOX and UOX fuel composites

An alternative design was conceptualised, where instead of 100% MOX fuel, occupying 30 % of the total fuel assemblies in a reactor. A fuel pin composite was designed, with an isotopic composition that mimics, a 30% MOX: 70% UOX relationship, as currently implemented, in MOX fuel licenced reactors. The UOX fuel used for the feasibility analysis, has an isotopic composition, of 5% ^{235}U, and 95% ^{238}U.

From the data presented in Figure 64, it is evident that a 30 MOX%:70% UOX fuel compositions, still placed a phenomenal drag on the infinite neutron multiplication factor (k_∞), to the point where the bottom limit for the infinite neutron multiplication factor (k_∞), was reached about 6 months into the burnup simulation.

An iterative approach was then applied to determine the homogeneous combination of MOX, and UOX fuel, able to sustain a fission reaction for a period greater than 16 months. As indicated in Figure 64, the 10% MOX: 90% UOX fuel composition, outperformed the standard Koeberg UOX fuel composition. The 10% MOX: 90% UOX fuel composition, had an effective isotopic composition of 0.8% RPu, 4.75276% ^{235}U, and 94.6724% ^{238}U.

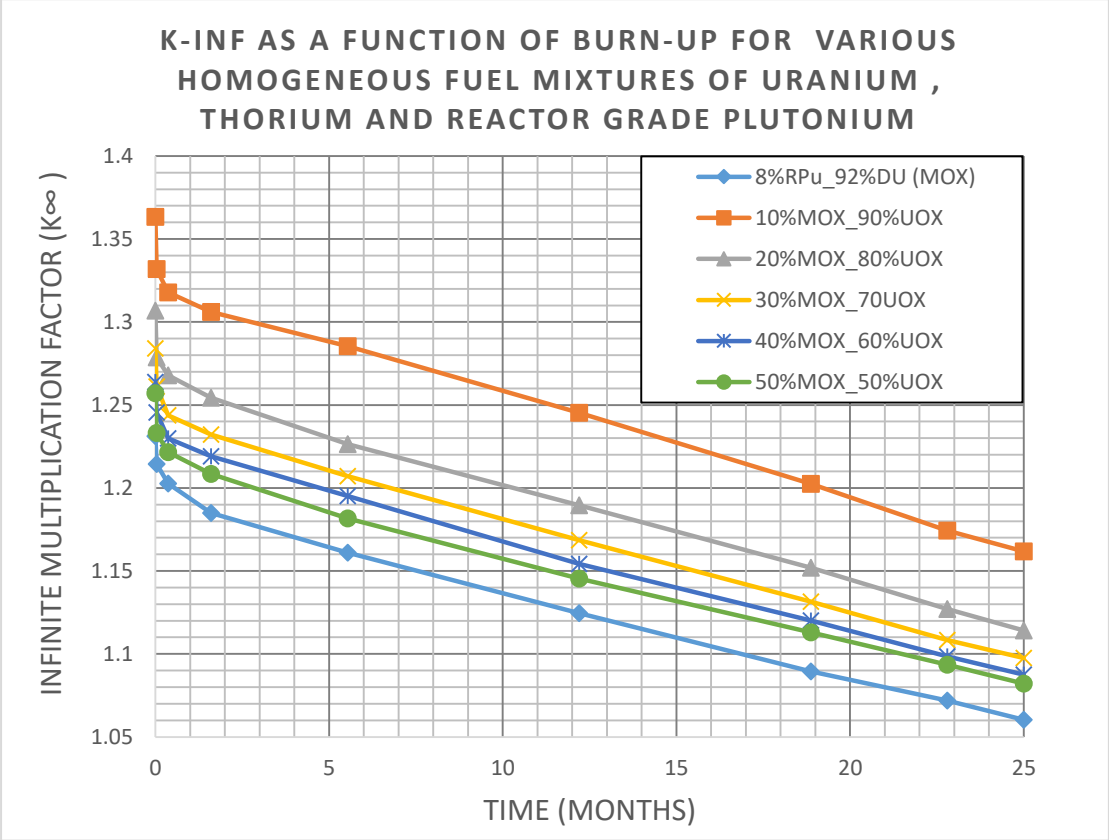

Figure 64: Comparison of the Infinite multiplication factor over time due to burnup of 100% MOX fuel, and various MOX – UOX fuel composites

A comparison of the standard Koeberg UOX fuel composition, and the conceptual 10% MOX: 90% UOX fuel composition are displayed in Figure 65. The conceptual fuel composition, preformed excellently in the sense that, it lowered the initial infinite

neutron multiplication factor (k_∞), and successfully extended the fuel cycle to 18.5 months.

The addition of plutonium isotopes, in trace quantities to the fuel composition, with their high neutron capture cross sections, provided the necessary captures at the BOL, to effectively reduce the initial infinite neutron multiplication factor (k_∞), without compromising the fuel cycle length.

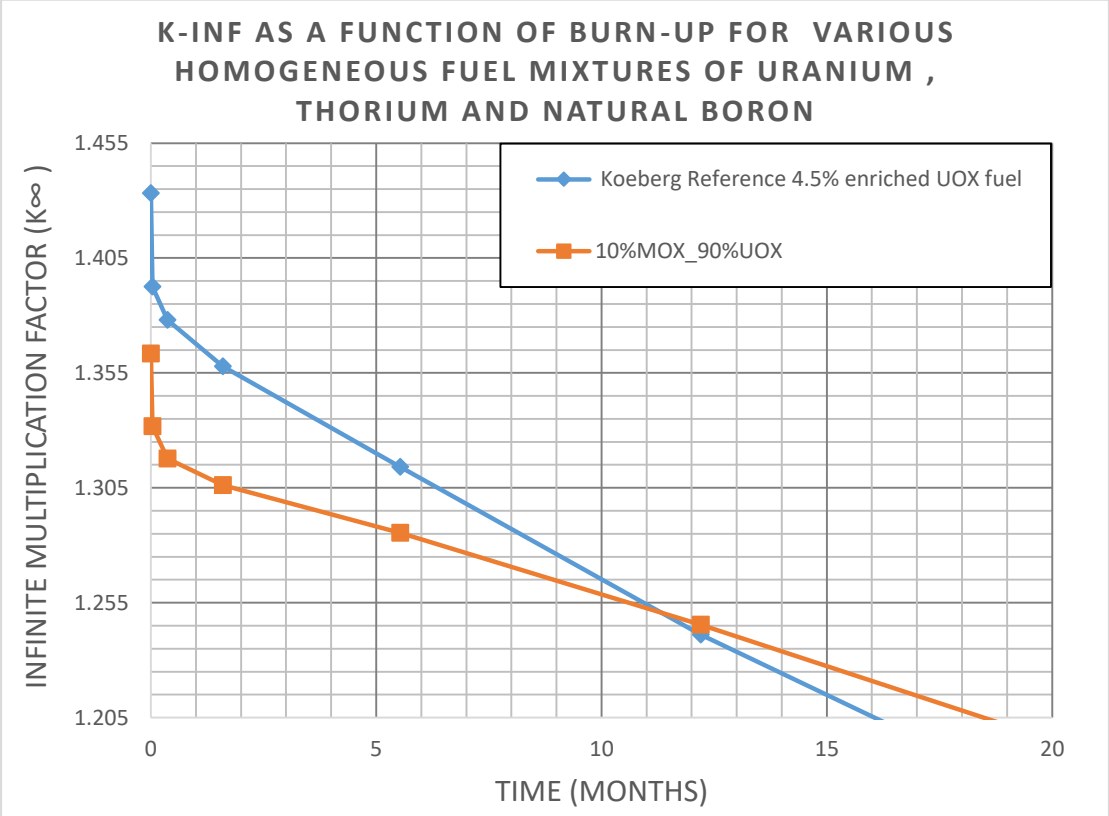

Figure 65: Comparison of the Infinite multiplication factor over time due to burnup of 100% MOX fuel, and various MOX – UOX fuel composites

The small quantities of the plutonium, in the aforementioned fuel composition, will neither require any additional moderation, nor increased reactivity control, to be implementable in Koeberg nuclear power plant.

The 10% MOX: 90% UOX fuel composition, will not negatively influence any of the reactivity coefficients, therefore making it a safe and effective substitute for the currently implemented, UOX fuel composition.

From Table 34, and Table 35 it is evident that the 10% MOX: 90% composite, captured far less neutrons on day zero of burnup than the 100% MOX fuel composition. The data also validates the lower infinite neutron multiplication factor (k_∞) at the BOL, for the 10% MOX: 90% UOX fuel composite, when compared to the standard UOX fuel composition.

Table 34: Neutron captures in 100% MOX fuel, and various MOX – UOX fuel composites on day zero of burnup

	Isotopic composition		
Neutron captures	**4.5% U235 _95.5% U238**	**8% RPu _92% DU**	**10% MOX _90% UOX**
Moderator (H_2O)	2.2845E+11	1.1248E+11	1.7444E+11
Oxygen (in fuel)	9.3704E+09	1.2626E+10	1.4063E+10
Uranium - 235	7.4449E+11	2.7171E+10	6.4319E+11
Uranium - 238	1.4762E+12	1.4436E+12	1.4044E+12
Plutonium - 238	0.00E+00	3.5021E+10	5.5473E+09
Plutonium - 239	0.00E+00	1.2879E+12	3.0856E+11
Plutonium - 240	0.00E+00	1.1209E+12	3.3885E+11
Plutonium - 241	0.00E+00	2.3536E+11	4.8881E+10
Plutonium - 242	0.00E+00	1.5195E+11	2.6059E+10
Helium	0.00E+00	0.0000E+00	0.0000E+00
Zircaloy-4	3.2863E+10	3.3157E+10	3.1728E+10

Table 35: Total neutron captures in 100% MOX fuel, and various MOX – UOX fuel composites on day zero of burnup

Isotopic composition	Total captures
4.5% U235_95.5% U238	2.4914E+12
8% RPu_92% DU (100% MOX)	4.4603E+12
10% MOX_90% UOX	2.9921E+12

Table 36: Total fissions in 100% MOX fuel, and various MOX – UOX fuel composites on day zero of burnup

	Fissions	
Isotopic composition	**Fissile isotopes**	**Fertile isotopes**
4.5% U235_95.5% U238	3.3142E+12	1.6764E+11
8% RPu_92% DU (100% MOX)	3.1165E+12	2.4221E+11
10% MOX_90% UOX	3.2490E+12	1.8333E+11

The addition of reactor grade plutonium, made it difficult to determine the breeding and conversion efficiencies, this is attributed to the presence of all the fissile isotopes normally bred during burnup. The only way to effectively determine the breeding and conversion efficiency is, by evaluating the growth in isotopic mass during burnup. The 10% MOX: 90% UOX composite, produced a 54.3478%, mass increase in ^{239}Pu, and an increase of 70.5882% in ^{241}Pu.

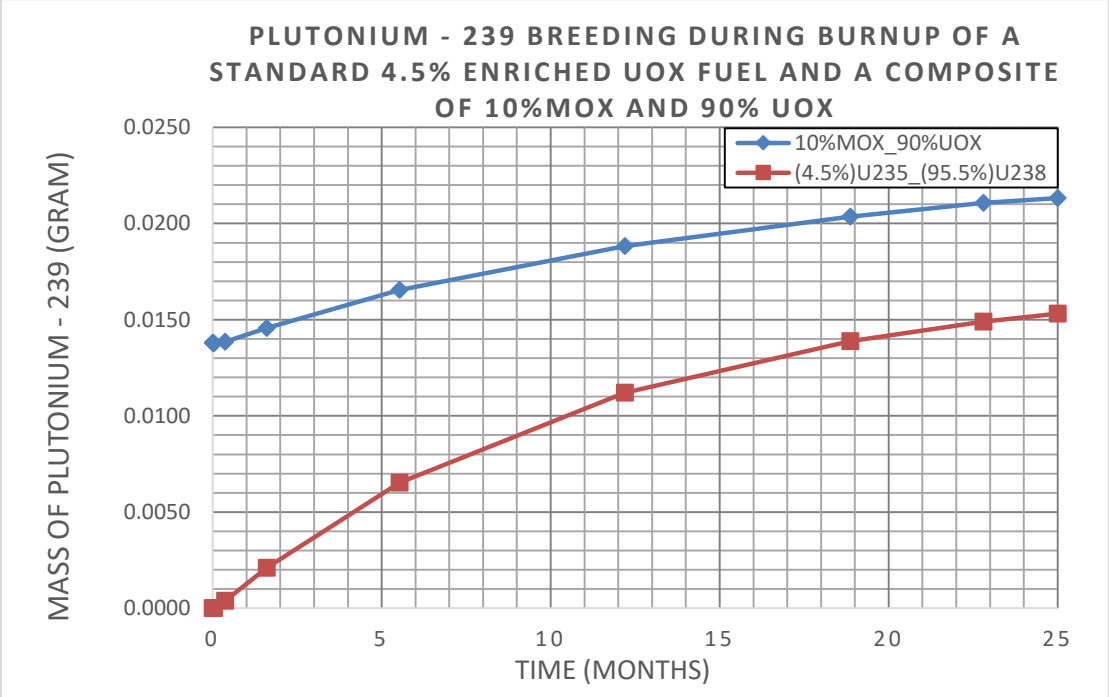

Figure 66: Comparison Of plutonium - 239 breeding rate during burnup of a standard 4.5% enriched UOX fuel and a composite of 10% MOX and 90% UOX

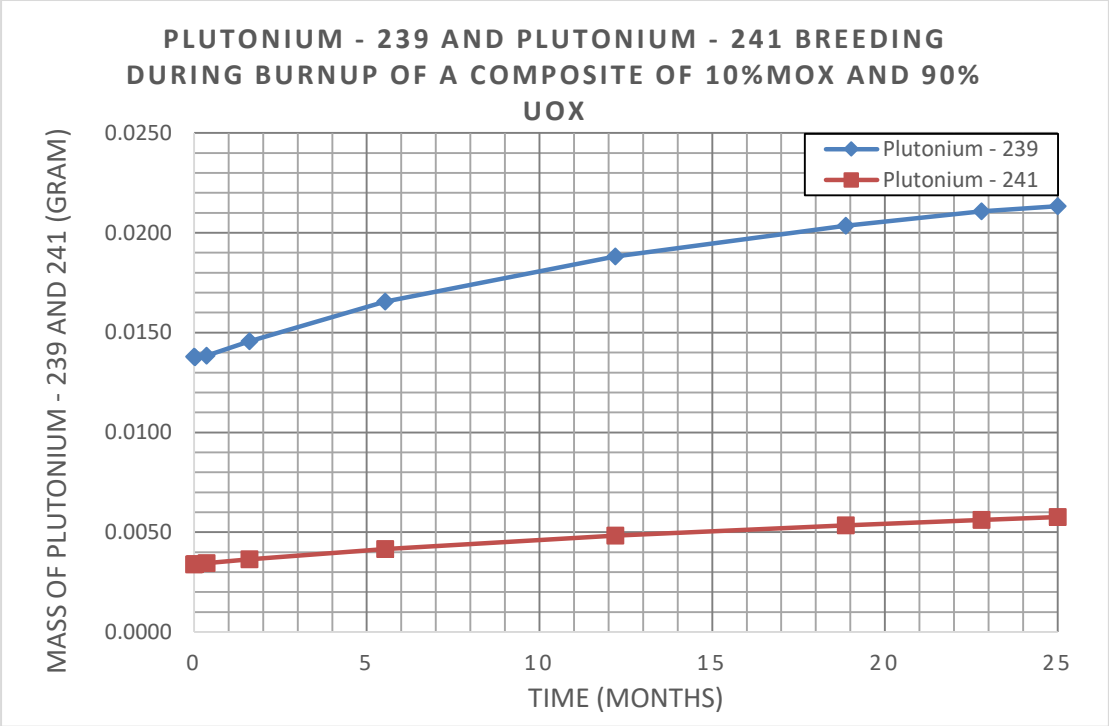

Figure 67: Comparison of plutonium – 239 and 241 breeding rate during burnup of a composite of 10% MOX and 90% UOX

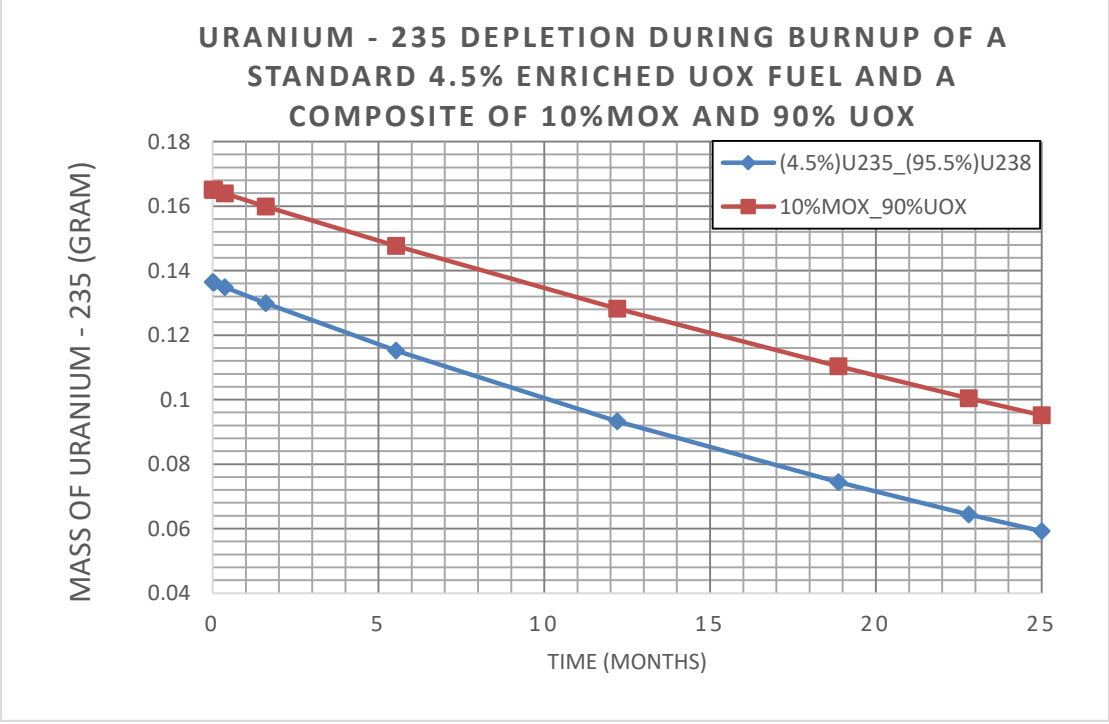

Figure 68: Comparison of uranium – 235 depletion rate during burnup of a standard 4.5% enriched UOX fuel and a composite of 10%mox and 90% UOX

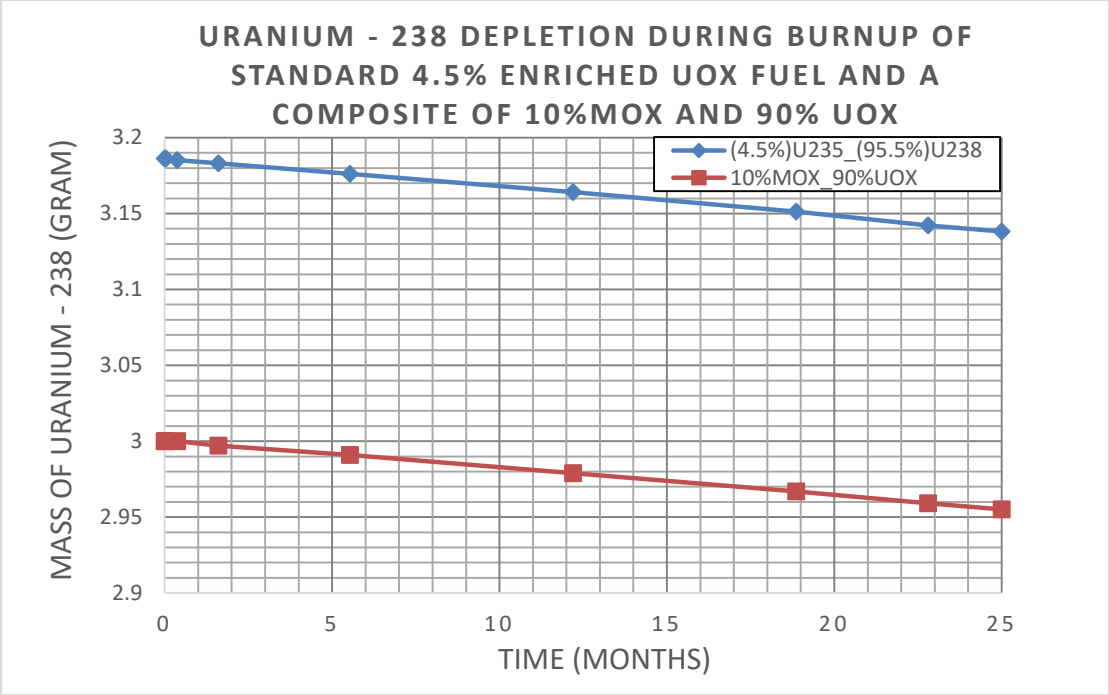

Figure 69: Comparison of uranium – 235 depletion rate during burnup of a standard 4.5% enriched UOX fuel and a composite of 10%mox and 90% UOX

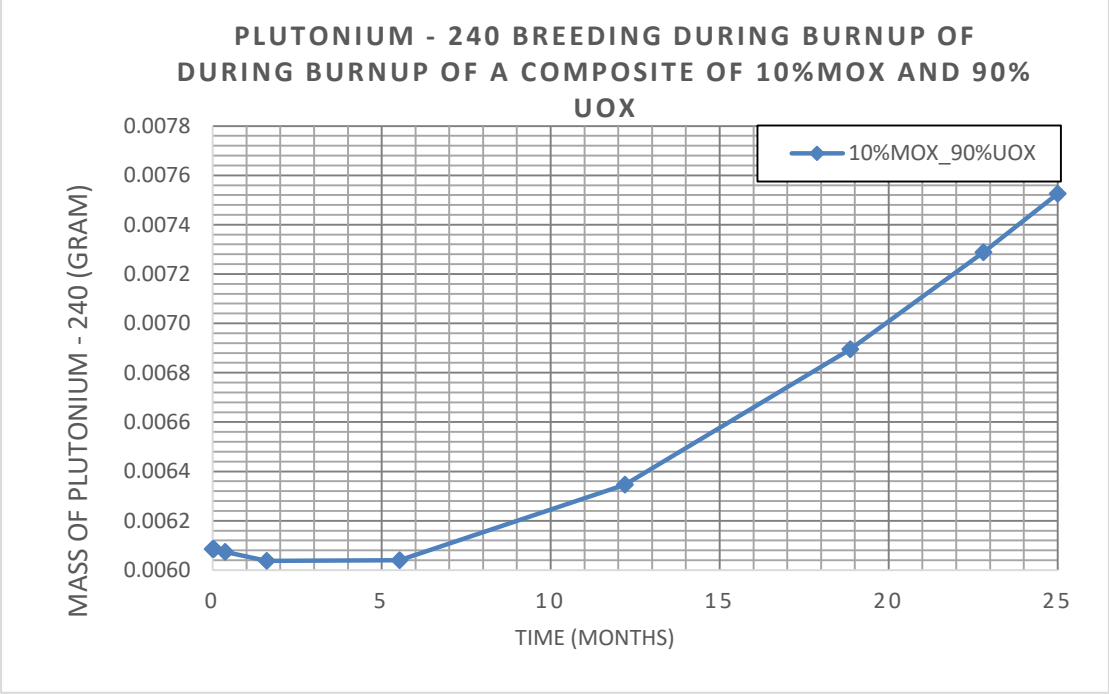

Figure 70: Comparison of uranium – 235 depletion rate during burnup of a standard 4.5% enriched UOX fuel and a composite of 10%mox and 90% UOX

The breeding rate of ^{239}Pu, and ^{240}Pu, as displayed in Figure 66, and Figure 70 respectively, indicate that a large percentage of the ^{239}Pu isotopes, will rather fission than capture neutrons. The small increase in the ^{240}Pu, mass can also be attributed to its, breeding ability of ^{241}Pu.

Some further constraints with regard to plutonium composite fuels, from a heat transfer perspective, plutonium has an exceptionally low thermal conductivity coefficient (6.74 [W/mK]), especially when compared with thorium (54.12 [W/mK]), and uranium (27.5 [W/mK]). The low thermal conductivity coefficient, will result in increased fuel temperatures, due to reduced heat transfer capabilities. Fortunately, the small amounts of plutonium, currently in the 10% MOX: 90% UOX fuel composite will not greatly affect the composites heat transfer capabilities. The fuel composition has a thermal conductivity coefficient of 25.424 [W/mK], which is a 7.5490% decrease from the standard UOX fuel composition, and within the acceptable limit.

If more substantial inclusions of plutonium are implemented, significant functional upgrades will be required, to increase the heat transfer capabilities of the reactor. The extraction of the excess heat will require larger coolant pumps, in the primary and secondary circuit, increased pressurizer capabilities, and the addition of steam generators or upgrades to the current steam generators. The economic gain, will be substantially reduced due to the large expenditures, with regard to upgrades, and will ultimately become an unviable option.

The increased fuel operating temperature, can also become problematic with regard to the fuel, and moderator temperature reactivity coefficient. As evident from Figure 23, excessive captures will take place, and lower the infinite neutron multiplication factor (k_∞), to the point where a sustained fission reaction chain is no longer possible.

5.5.3.3.3 Conceptual plutonium fuel compositions

From the knowledge obtained, during the analysis of the various fuel composition, and the isotopic, and neutronic integration benchmark, obtained from the isotopic comparison analysis, as displayed in section 5.4.3, a few conceptual fuel compositions were created.

The fuel compositions, where created by characteristically selecting isotopes, to ensure the best possible result. The main objective was to utilize the current reactor grade plutonium stockpile, in an effort to decrease environmental impact, and fuel

costs. The feasibility of the fuel compositions will be evaluated on the same basis as mentioned in section 5.5.2.1.

Various homogeneous fuel compositions were analysed, but the composites with the best performance, are amalgamations of fissile plutonium (^{239}Pu and ^{241}Pu), and combinations of ^{238}Pu, and either ^{232}Th, or ^{238}U. The conceptual fuel compositions with the best overall performance are displayed in Figure 71.

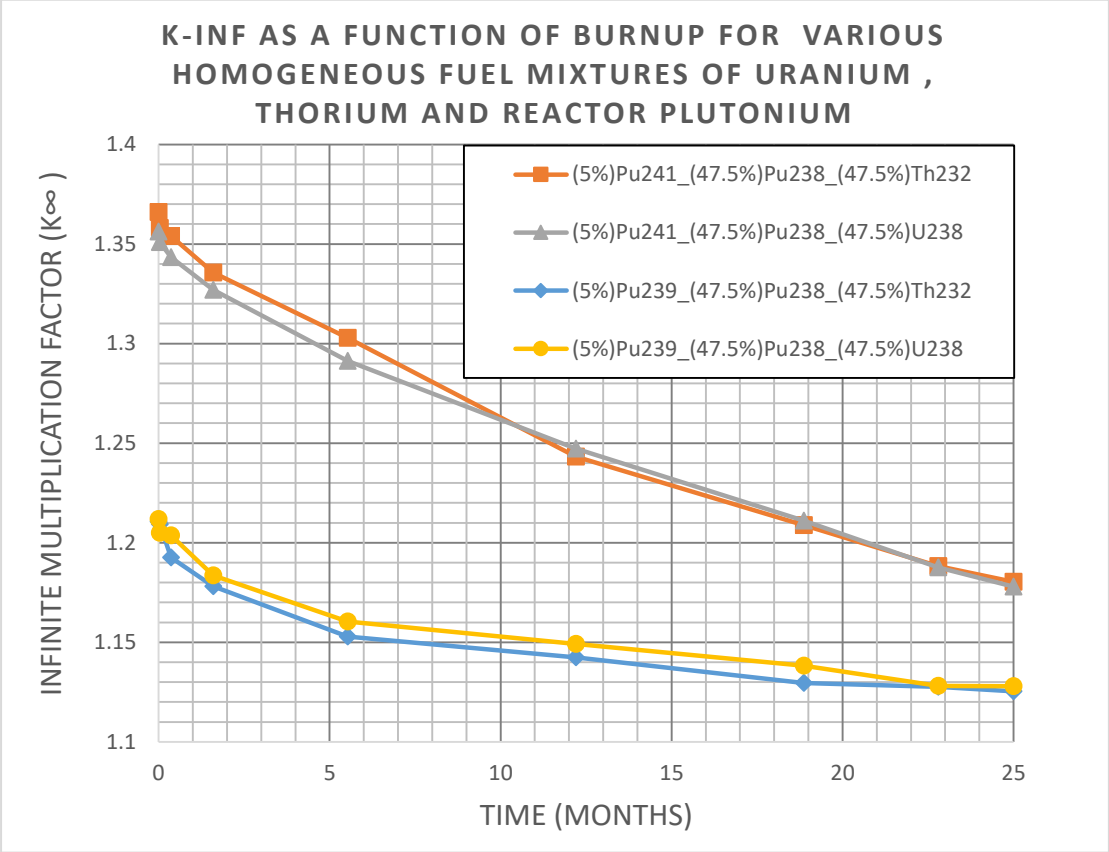

Figure 71: Comparison of the Infinite multiplication factor over time due to burnup of fuel composites containing, uranium, plutonium, and thorium.

It is evident from Figure 71, that the ^{241}Pu, amalgamations performed the best, with regard to fuel cycle length, delivering a sustainable fission reaction for just over 20 months. The inferior performance of the ^{239}Pu amalgamations, can be ascribed to the lower neutron yield per fission neutron, when compared with ^{241}Pu, as seen in section 5.4.3.3.2, and 5.4.3.4.2.

There is a substantial increase in the fuel cycle length, in comparison with that of the standard Koeberg UOX fuel composition as evident from Figure 72, where the two conceptual ^{241}Pu fuel compositions, are compared with the standard Koeberg UOX fuel composition.

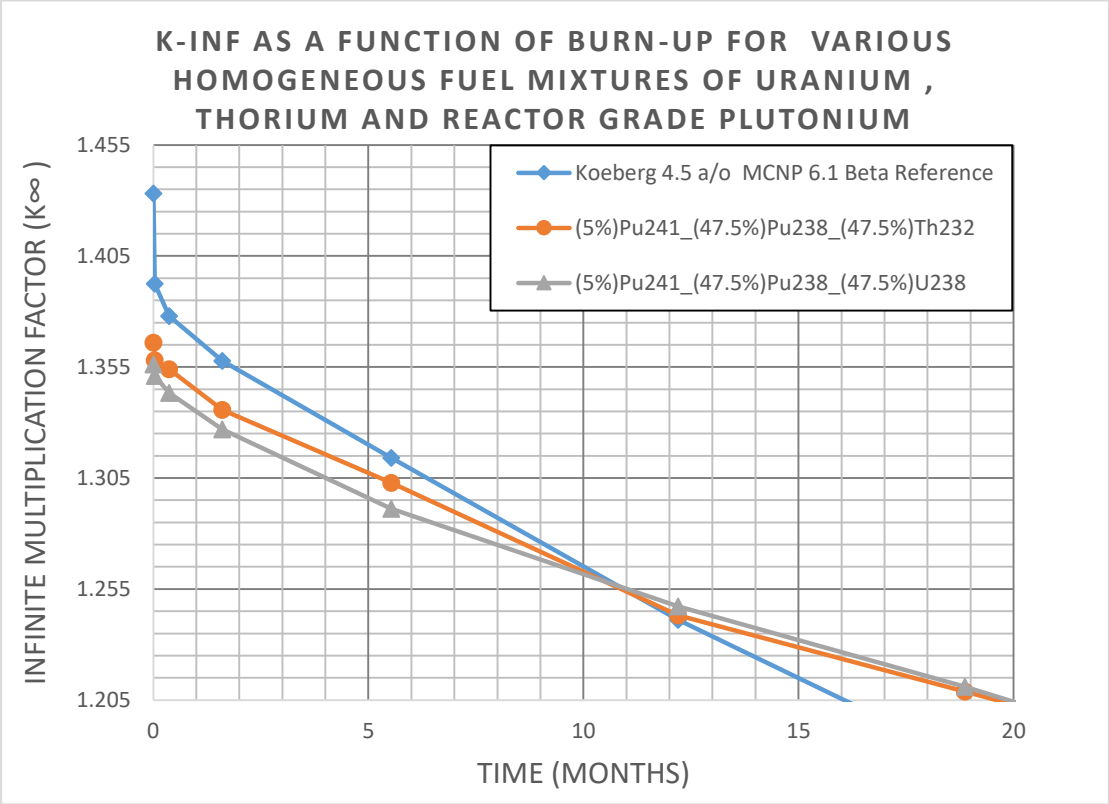

Figure 72: Comparison of the Infinite multiplication factor over time due to burnup of the standard Koeberg UOX fuel composition and a conceptual fuel composition.

The conceptual plutonium composites, significantly reduced the initial infinite neutron multiplication factor (k_∞), whilst prolonging the fuel cycle by 4 months. The 5% ^{241}Pu, 47.5% ^{238}Pu, and 47.5% ^{238}U, fuel composition delivered the optimal result by delivering a lower initial infinite neutron multiplication factor (k_∞), than the 5% ^{241}Pu, 47.5% ^{238}Pu, and 47.5% ^{232}Th fuel composition, and a superior fuel cycle length.

The aforementioned, yet again proves that the neutron energy distribution, for fuels compositions containing plutonium, peaks toward the epithermal energy spectrum, and further more validates the increased moderation required when large concentrations of plutonium are present in the fuel composition. The increased neutron captures, on

day zero of burnup as seen in Table 37, proves that the neutron energy distribution peaks in the 1.5 – 10 eV energy range, as evident from Figure 23.

Table 37: Neutron captures in standard Koeberg UOX fuel, and a conceptual plutonium amalgamations on day zero of burnup.

	Isotopic composition		
Neutron captures	**4.5% U235 _95.5% U238**	**5%Pu241 _47.5%Pu238 _47.5%Th232**	**5%Pu241 _47.5%Pu238 _47.5%U238**
Moderator (H_2O)	2.2845E+11	9.5762E+10	9.3511E+10
Oxygen (in fuel)	9.3704E+09	1.2561E+10	1.3090E+10
Uranium – 235	7.4449E+11	0.00E+00	0.00E+00
Thorium - 232	0.00E+00	6.60198E+11	0.00E+00
Uranium - 238	1.4762E+12	0.00E+00	7.7771E+11
Plutonium - 238	0.00E+00	2.4917E+12	2.4801E+12
Plutonium - 241	0.00E+00	7.3659E+11	4.8881E+10
Helium	0.00E+00	0.0000E+00	0.0000E+00
Zircaloy-4	3.2863E+10	2.6032E+10	2.6032E+10

The aforementioned propensity is also visible in the total neutron captures, on day zero of burnup.

Table 38: Total neutron captures in standard Koeberg UOX fuel, and a conceptual plutonium amalgamations on day zero of burnup.

Isotopic composition	Total captures
4.5% U235_95.5% U238	2.4914E+12
5%Pu241_47.5%Pu238_47.5%Th232	4.0228E+12
5%Pu241_47.5%Pu238_47.5%U238	4.1079E+12

The ^{232}Th composition produced more fissions in the fissile isotope, than the ^{238}U composition. This contradicts the standard behaviour of ^{232}Th, and ^{238}U, in the sense that in a standard thermal neutron energy distribution, the ^{232}Th will capture more neutrons than ^{238}U, resulting in fewer fissions by the fissile material.

Table 39: Total fissions in standard Koeberg UOX fuel, and a conceptual plutonium amalgamations on day zero of burnup.

	Fissions	
Isotopic composition	**Fissile isotopes**	**Fertile isotopes**
4.5% U235_95.5% U238	3.3142E+12	1.6764E+11
5%Pu241_47.5%Pu238_47.5%Th232	2.1748E+12	1.1662E+11
5%Pu241_47.5%Pu238_47.5%U238	2.0849E+12	1.2633E+11

The 5% ^{241}Pu, 47.5% ^{238}Pu, and 47.5% ^{238}U, fuel composition delivered the highest yield, with regard to ^{239}Pu breeding. This is attributed to combination of ^{238}Pu, and ^{238}U, both of the aforementioned are capable of breeding ^{239}Pu. The ^{232}Th composite breeds ^{233}U, which is also a fissile isotope but performs, inferiorly with regard to neutron production per fission neutron, as evident from section 5.4.3.1.2, and 5.4.3.3.2.

The higher neutron yield, enables higher breeding rates, and a decreased depletion rate of ^{241}Pu as evident from Figure 73, and Figure 74, respectively.

From Figure 75, it is apparent that the depletion rates of ^{238}Pu have the same tendency, which is expected, due to the high capture cross section of ^{238}Pu in the thermal energy spectrum. The ^{238}Pu has a higher probability of capturing an incident neutron, than ^{232}Th, and ^{238}U, which explains the uniform depletion rate of ^{238}Pu.

From Figure 76, the depletion rates of ^{232}Th, and ^{238}U also seem to have the same depletion propensity, except for the first few days, where there is a greater depletion in ^{238}U, than ^{232}Th. This due to the shorter breeding chain length of ^{239}Pu, in comparison with ^{233}U, as evident from Figure 77, and Figure 78.

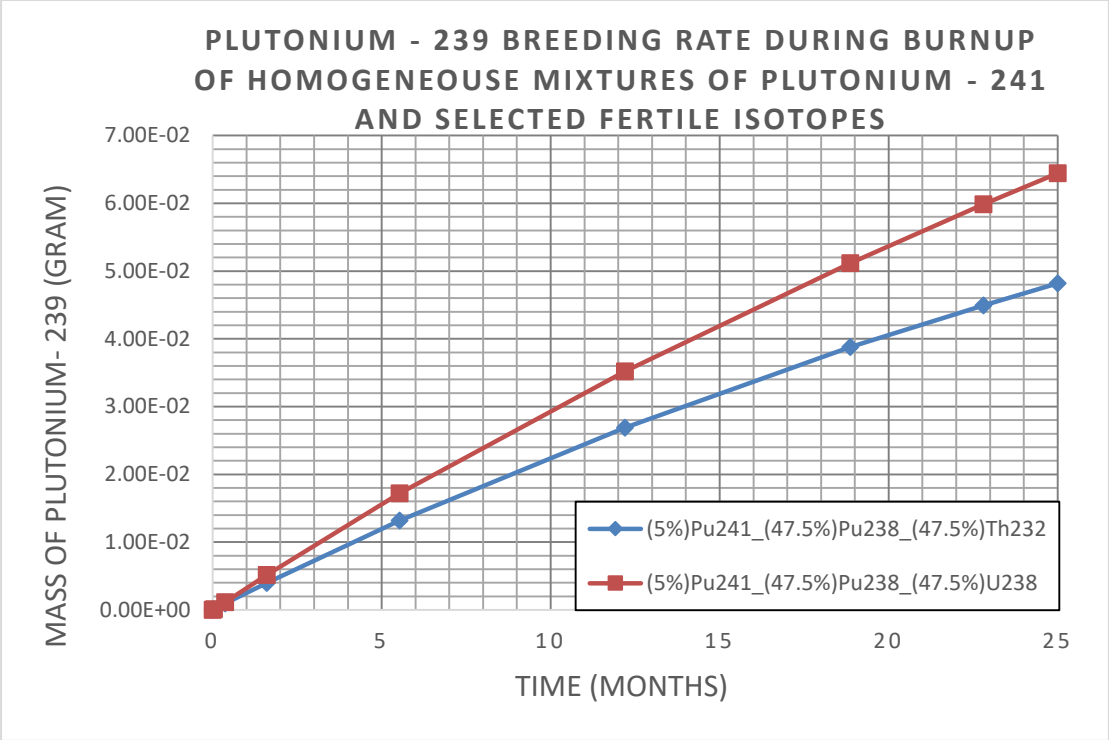

Figure 73: Comparison of ^{239}Pu breeding rate during burnup of homogeneous mixtures of ^{241}Pu and selected fertile isotopes

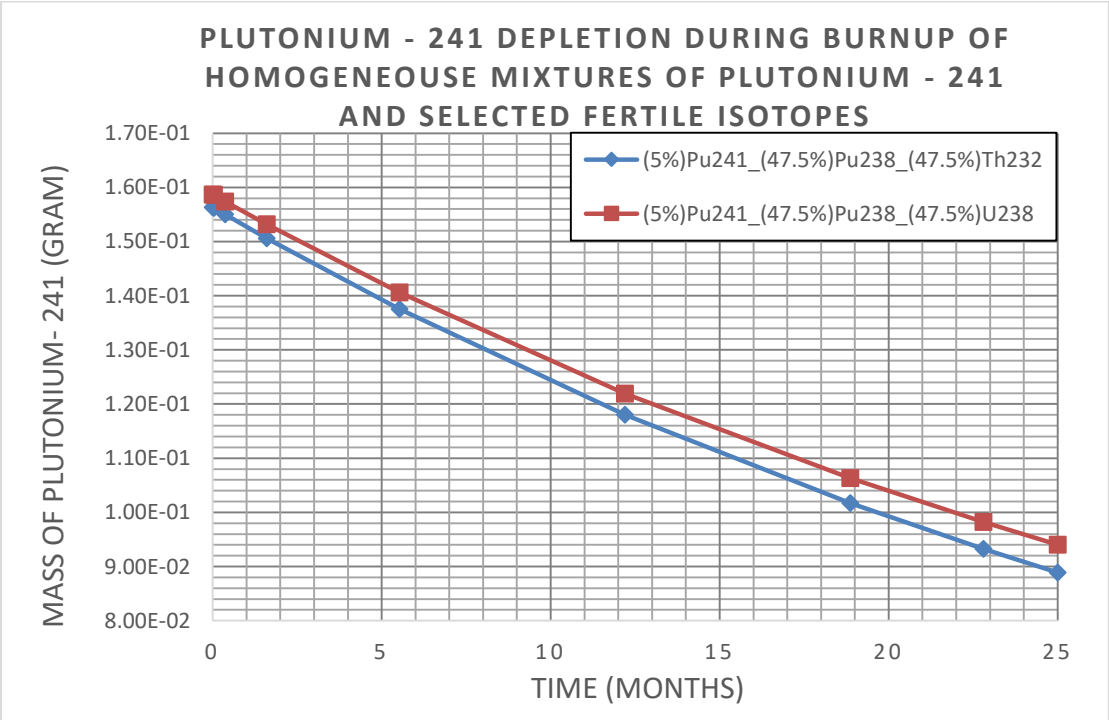

Figure 74: Comparison of ^{241}Pu depletion rate during burnup of homogeneous mixtures of ^{241}Pu and selected fertile isotopes

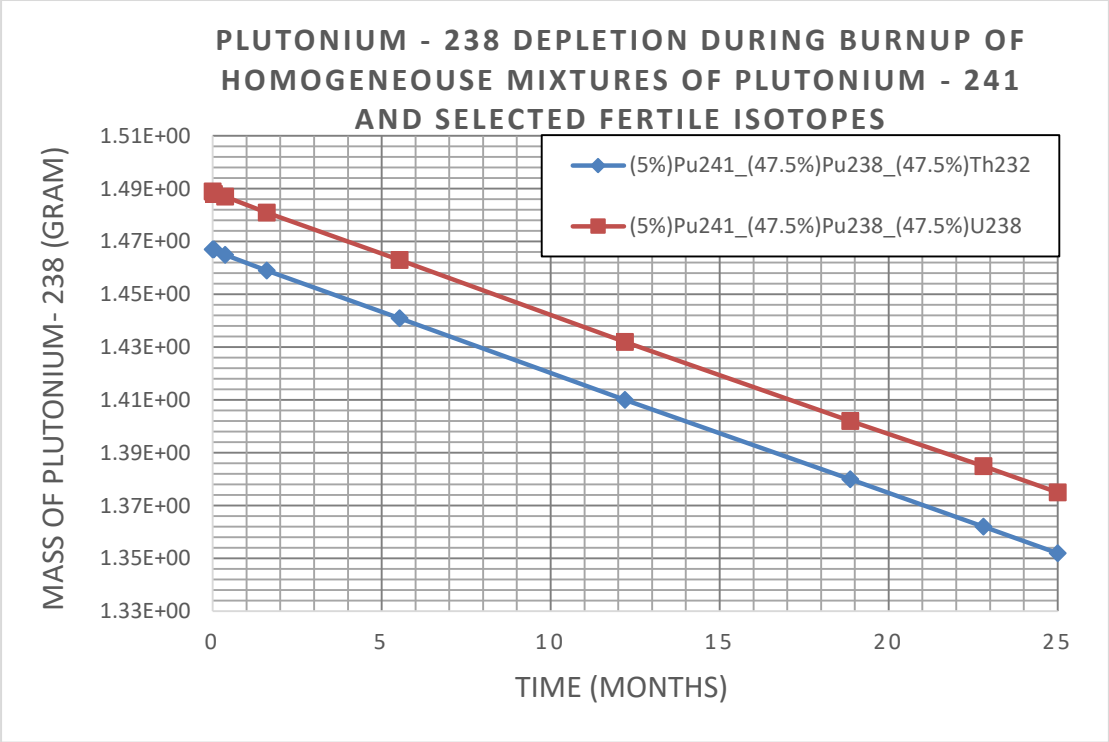

Figure 75: Comparison of ^{238}Pu depletion rate during burnup of homogeneous mixtures of ^{241}Pu and selected fertile isotopes

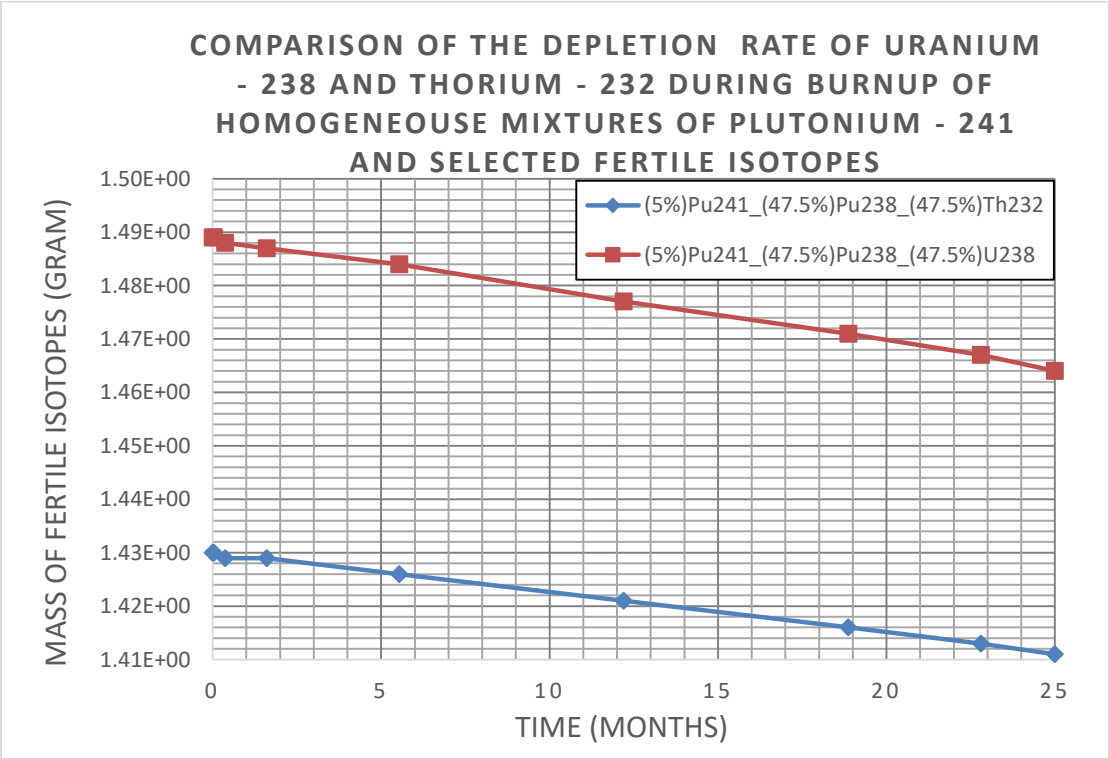

Figure 76: Comparison of ^{232}Th and ^{238}U depletion rate during burnup of homogeneous mixtures of ^{241}Pu and selected fertile isotopes

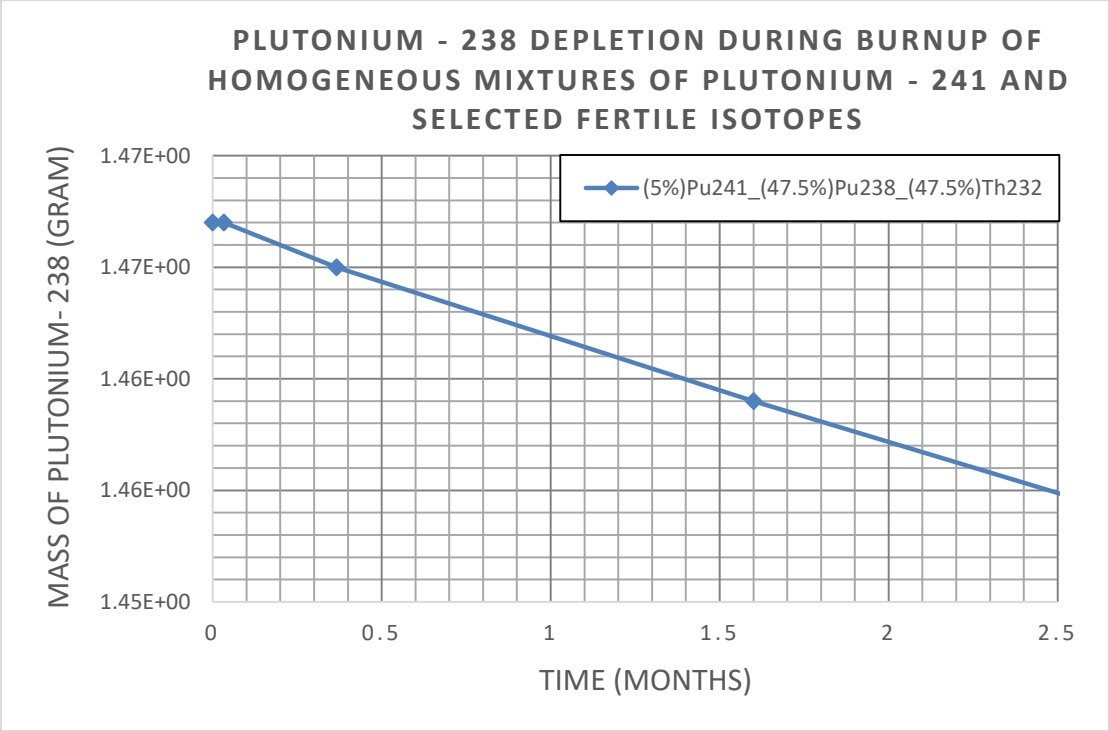

Figure 77: Depletion rate of ^{238}Pu during burnup of homogeneous mixtures of ^{241}Pu and selected fertile isotopes

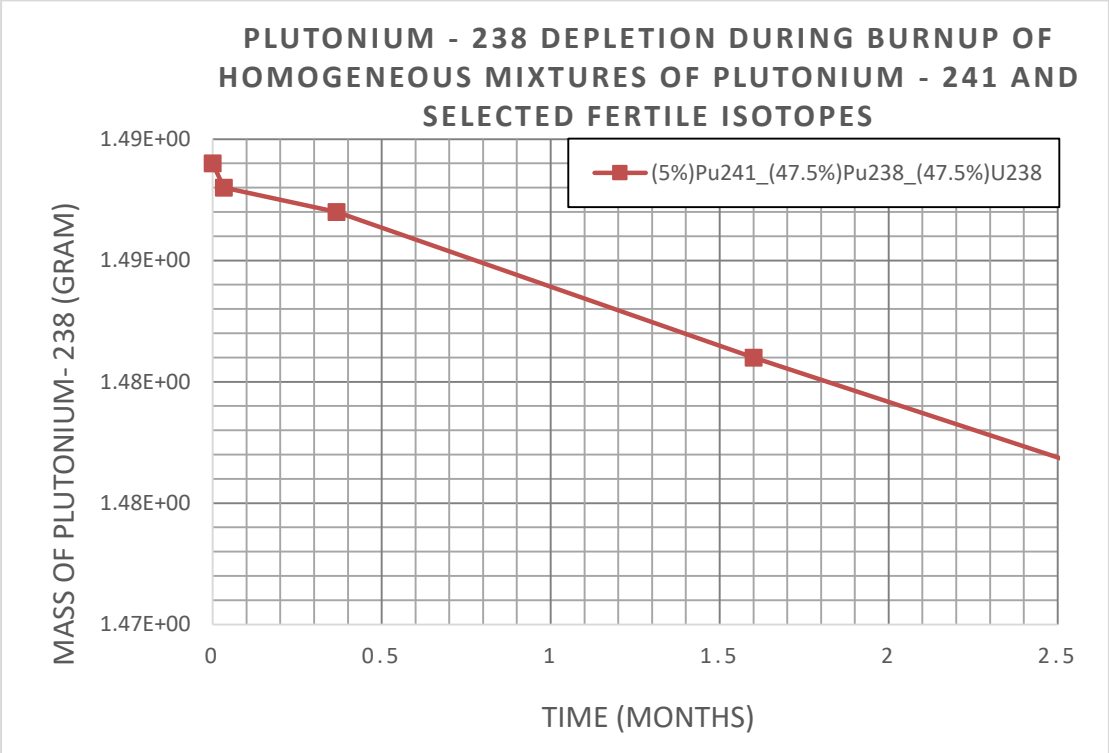

Figure 78: Depletion rate of ^{238}Pu during burnup of homogeneous mixtures of ^{241}Pu and selected fertile isotopes

5.5.3.4 Section results

Figure 79, displays a compilation of the computed data from the evaluated fuel compositions, and will serve as a further feasibility analysis, of the proposed fuel compositions, with regard to the constraints specified in section 5.5.1.

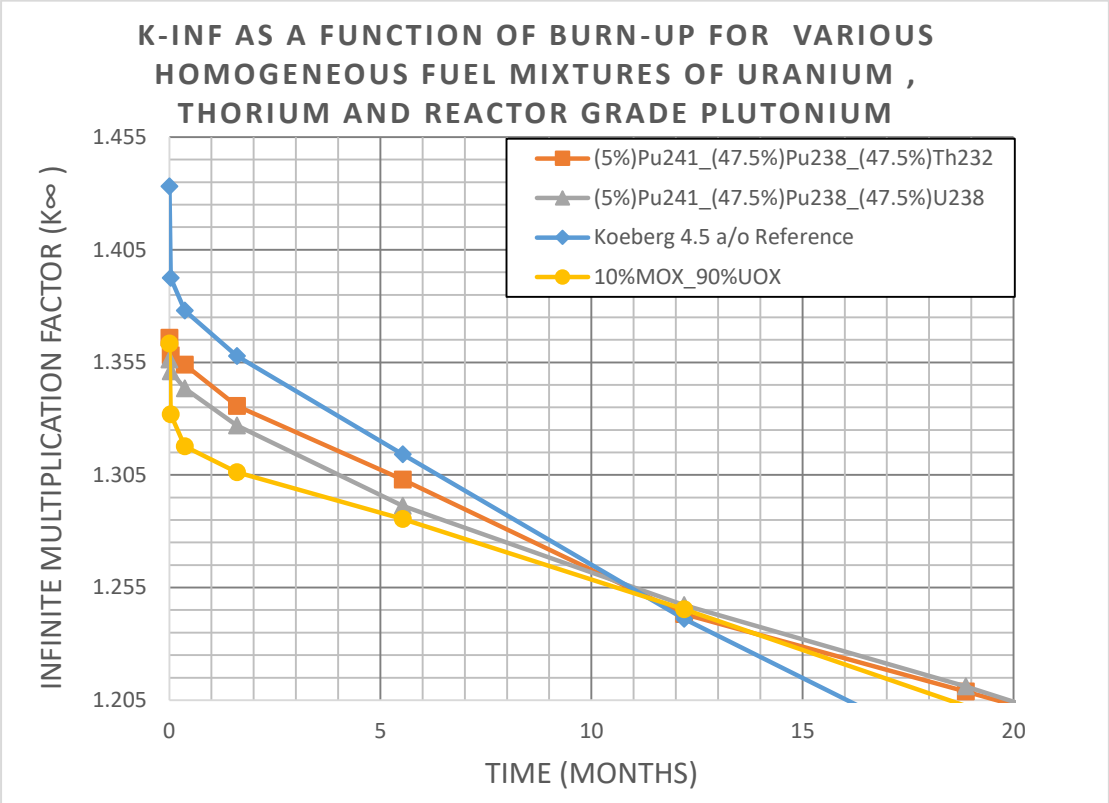

Figure 79: Comparison of the Infinite multiplication factor over time due to burnup of various mixtures of uranium, thorium and plutonium

All of the fuel compositions displayed in Figure 79, successfully increases the fuel cycle length, to varying extents, without any geometric alterations to the fuel pellet or reactor. A comparison of the isotopic neutron captures are displayed in Table 40.

Due to the reduced heat transfer capacity involved, with the addition of large amounts of plutonium, as discussed in section 5.5.3.3.2, the conceptual ^{241}Pu compositions will not be a feasible solution to use as substitute for the standard UOX fuel composition currently implemented in Koeberg nuclear power plant.

Table 40: Section comparison of neutron captures on day zero of burnup

	Isotopic composition			
Neutron captures	**4.5% U235 _95.5% U238**	**10% MOX _90% UOX**	**5%Pu241 _47.5%Pu238 _47.5%Th232**	**5%Pu241 _47.5%Pu238 _47.5%U238**
Moderator (H_2O)	2.2845E+11	1.7444E+11	9.5762E+10	9.3511E+10
Oxygen (in fuel)	9.3704E+09	1.4063E+10	1.2561E+10	1.3090E+10
Uranium – 235	7.4449E+11	6.4319E+11	0.00E+00	0.00E+00
Thorium - 232	0.00E+00	0.00E+00	6.60198E+11	0.00E+00
Uranium - 238	1.4762E+12	1.4044E+12	0.00E+00	7.7771E+11
Plutonium - 238	0.00E+00	3.5021E+10	2.4917E+12	2.4801E+12
Plutonium - 241	0.00E+00	2.3536E+11	7.3659E+11	4.8881E+10
Helium	0.00E+00	0.0000E+00	0.0000E+00	0.0000E+00
Zircaloy-4	3.2863E+10	3.3157E+10	2.6032E+10	2.6032E+10

Table 41: Section comparison total of neutron captures on day zero of burnup

Isotopic composition	**Total captures**
4.5% U235_95.5% U238	2.4914E+12
10% MOX_90% UOX	2.9921E+12
5%Pu241_47.5%Pu238_47.5%Th232	4.0228E+12
5%Pu241_47.5%Pu238_47.5%U238	4.1079E+12

Table 42: Section comparison total fissions in fissile and fertile isotopes on day zero of burnup

	Fissions	
Isotopic composition	**Fissile isotopes**	**Fertile isotopes**
4.5% U235_95.5% U238	3.3142E+12	1.6764E+11
10% MOX_90% UOX	3.2490E+12	1.8333E+11
5%Pu241_47.5%Pu238_47.5%Th232	2.1748E+12	1.1662E+11
5%Pu241_47.5%Pu238_47.5%U238	2.0849E+12	1.2633E+11

5.5.3.5 Conclusion

The drag on the economic feasibility induced by, the heat removal equipment upgrades required to ensure safe reactor operation, will outweigh the benefit of an extended fuel cycle length.

The only viable option, is the 10% MOX: 90% UOX fuel composite, due to the fact that it complies with all the feasibility prerequisites, includes the use of stockpile plutonium, and delivers a reasonable time extension with regard to fuel cycle length.

5.5.4 Summary of computed results

Figure 80, displays a compilation of the computed data from all the UOX and MOX fuel conceptual fuel compositions, and will serve as a further feasibility analysis, of the proposed fuel compositions, with regard to the constraints specified in section 5.5.1.

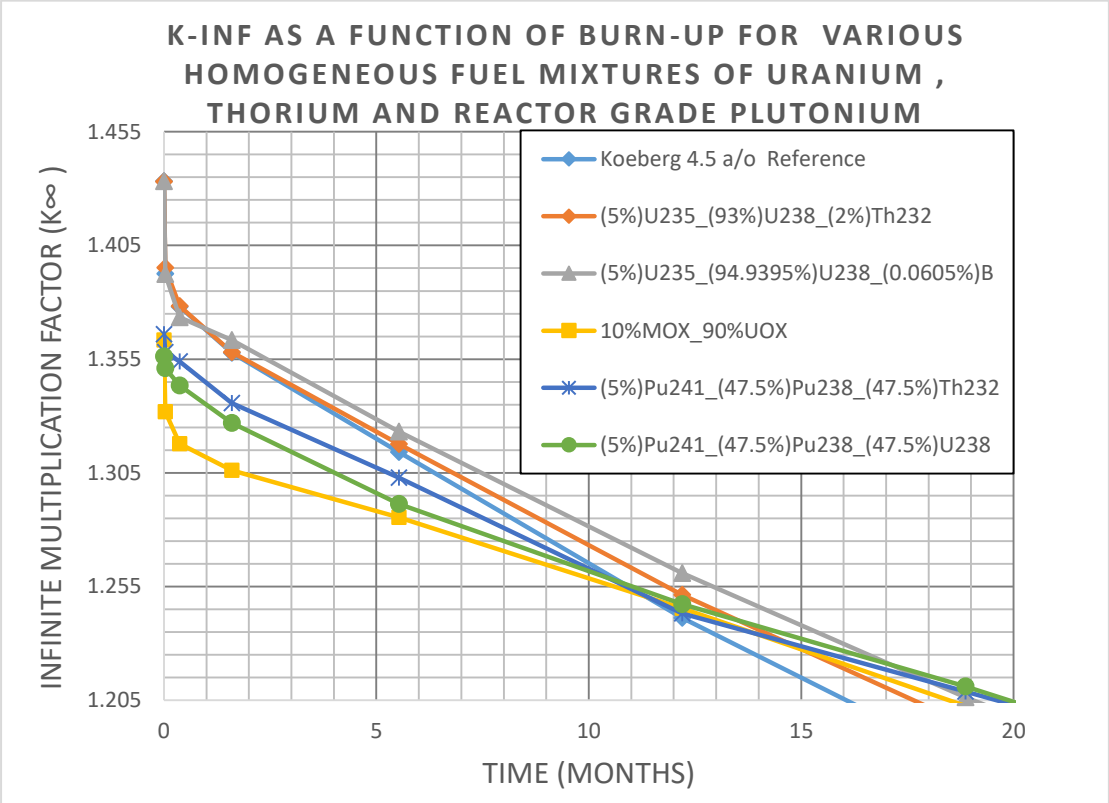

Figure 80: Comparison of the Infinite multiplication factor over time due to burnup of various mixtures of uranium, thorium and plutonium

The various fuel compositions deliver excellent results, all of which extend the conceptual, fuel cycle length of Koeberg nuclear power plants 900 MW PWR, operating on a full core loading of the conceptual fuel compositions. All of the fuel compositions, have pros, and cons, some more severe than others, but none the less all succeeding in their main objective of extending the operation length of the reactor.

From Figure 81, which is an amplified version of Figure 80 depicting the infinite neutron multiplication factor (k_∞), between 15 and 20 months of the burnup period. This enabled the distinction, of the various fuel compositions, and the magnitude to which they prolonged the fuel cycle length of the reactor.

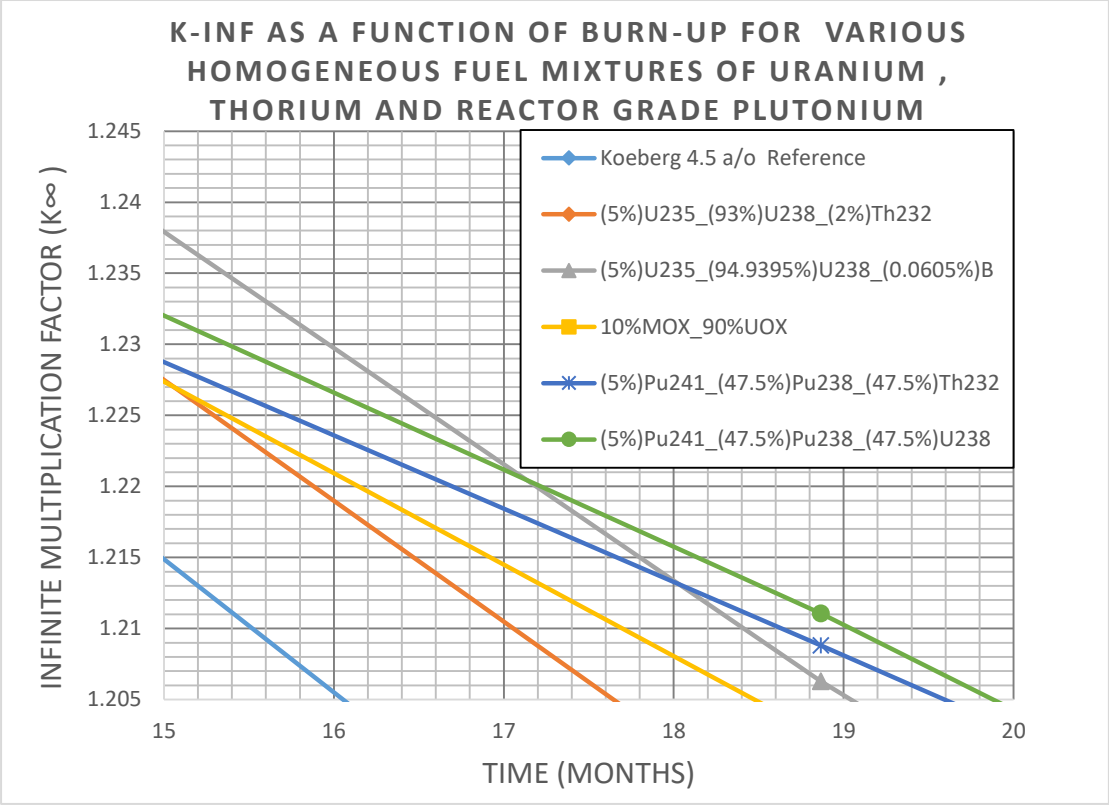

Figure 81: Comparison of the Infinite multiplication factor over time due to burnup of various mixtures of uranium, thorium and plutonium

5.5.5 Conclusion

By analysing the data displayed in Figure 81, three fuel compositions stand out with regard to feasibility, performance and implementability: 5% ^{235}U_94.9395% ^{238}U_0.0605% B, 10% MOX_90% UOX, and 5% ^{235}U_93% ^{238}U_2% ^{232}Th. The aforementioned are the fuel compositions, are the recommended fuel compositions, to use as a substitute for the current UOX fuel composition, currently implemented in Koeberg nuclear power plant.

The proposed fuel compositions, successfully delivered an extended fuel cycle length without, increasing the initial infinite neutron multiplication factor (k_∞), or reducing safety characteristics with regard to reactivity coefficients. The heat transfer capabilities, were also uncompromised, eliminating costly upgrades. The conceptual fuel compositions did not affect the thermal neutron distribution, and therefore ensure safe operation, without increased reactivity control. Some challenges will be discussed in section 6.2

5.5.6 Sensitivity of results

A fundamental paramater to take into account, when analysing the accuracy of MCNP 6.1 Beta results, are the use calculations with statistical charachteristics, for instance the standard deviations present on most calculated values.

Accumulation of statistical errors can occur during compound calculations, the magnitude of the accumulated errors percentage, can be minimized by increasing the number of active cycles, and using an increased number of neutron source particles. If uncertenty, with regard to fundamental parameters occur, a limit can be placed on the maximum allowable stadard diveation, this increases the accuracy of all calculated paramters substantially.

Unfortunately, increased accuracy will induce computing time restraints on burnup simulations, thus increased computing capabilities will be required to run simulations within the same timeframe. The effect of reduced accuracy, is evident from the ridget nature of the generated curves, but for the pupose of this disseratation, it will suffice.

With large discretization, or mesh intervals a computed average of tally data over a significant area is obtained. The obtained data, will provide symmetrical results with reduced statistical anomalies.

During analysis of isotopic and neutronic interations, a probalistic approach is applied, where a neutron/isotope can have a number of possible interations. The interaction likelihood, is obtained from the neutrons energy, and the specific isotopes cross section at the specified energy, to undergo said reaction. The aforementioned calculations are statiscally based and, have a inclination to become increasingly inaccurate with smaller samples sizes.

By increasing the initial neutron seed, or active cycles, statistical anomalies can be decreased substantially, to a certain extent. However this contrivance, does reach a limit, where the increased accuracy is not justifiable, due to the increase in computing resources required.

Figure 82, and Figure 83 were obtained from a similar analysis done by (Walt, 2015), where, ^{235}U fission reaction rate tallys were set up with varying discretization sizes, but a constant number of active cycles were used. As evident from the displayed data, the result varied significantly.

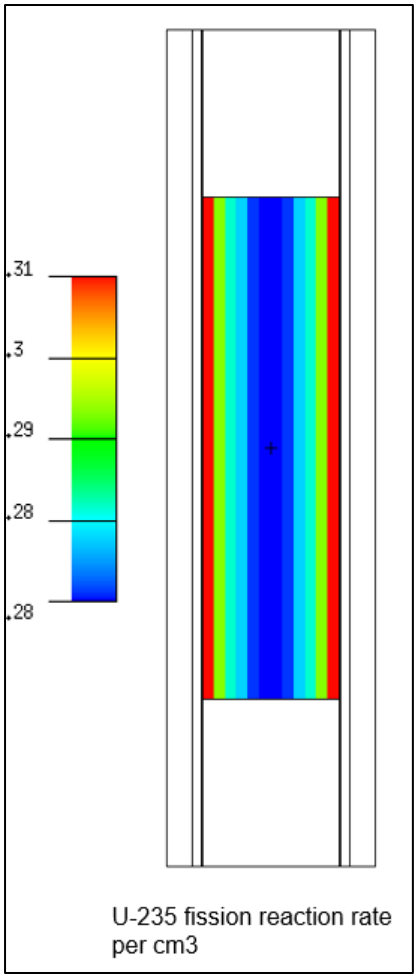

Figure 82: ^{235}U fission reaction rate tally count averaged over a large area, i.e. the mesh is divided over the x-axis only. Scale units are tally counts/source neutron (Walt, 2015)

As evident from Figure 82, where the model was only discretized only along the x-axis, the data varies greatly from the data displayed in Figure 83, where x and y direction mesh discretization was used. If the mesh geometry or number of iterations are insufficient, large statistical deviations can occur in the obtained data.

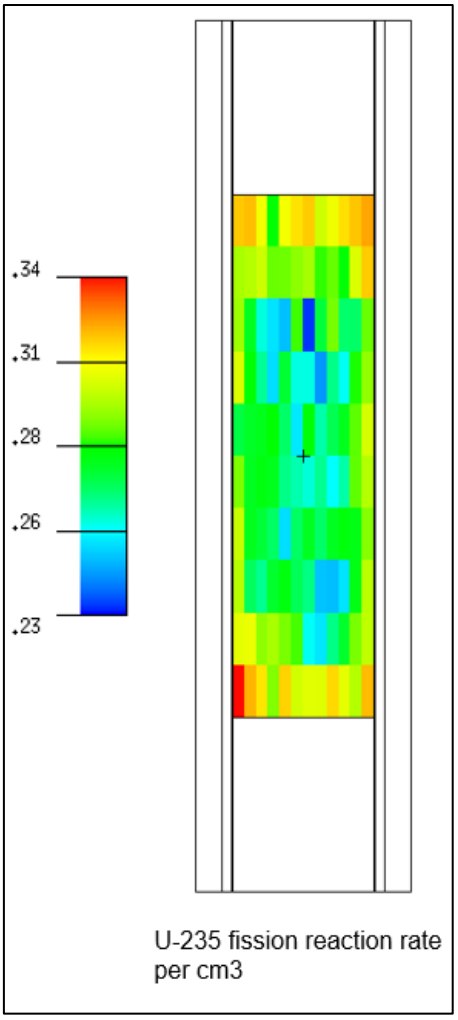

Figure 83: ^{235}U fission reaction rate contour plot with small discretization blocks, the mesh is divided in many x- and y-axis grids (Walt, 2015)

Chapter 6. Conclusions and Recommendations

Overview

The research has conclusively conceptualised, various conceptual fuel compositions that successfully extend the fuel cycle length of a PWR. The obtained results are accurate, and verifiable with the literature contained in this document. Further research and development, are required to determine the practical implementability, and safety characteristics of the conceptual fuel compositions. The identified areas, for proposed further investigation, and analysis are described.

6.1 Conclusions

The literature survey, identified a theoretical basis for the investigation, of conceptual fuel amalgamations, which could possibly increase the fuel cycle length of a PWR. The aforementioned served as the background for this study, and aided in verification of the computed results.

By successfully creating a numerical model, capable of determining the isotopic, and neutronic interactions during burnup simulations, of an infinite fuel pin, an in-depth analysis could be done, on any homogenous conceptual fuel composition. The data can be extrapolated, and used as an estimate for the conceptual fuel compositions, behaviour over time, during burnup, in a full core.

The proposed conceptual designs, successfully sustained a fission reaction chain, for a period greater than the standard UOX fuel composition, currently implemented in Koeberg nuclear power plant. The proposed designs, reduced the reactors dependency on burnable absorbers / poisons, and supplied increased inherent safety, with regard to various temperature reactivity coefficients.

The conceptual designs, are immediately implementable, and would not require any geometric alterations, or increased reactivity control. The heat transfer capacity of the conceptual fuel compositions, are in close correspondence with the currently implemented UOX fuel composition, and will not require upgrades to heat extraction capacity of the reactor.

The most attractive options, as determined by this dissertation, to increase the fuel cycle length of Koeberg nuclear power plant, is to increase the enrichment of the standard UOX fuel to 5 a/o, and add a neutron absorber or superior fertile isotope to the fuel composition. In this study the feasibility of natural boron, and small amounts of thorium-232 were evaluated, both of the aforementioned successfully increase the fuel cycle length of the reactor, within the prerequisites of feasibility, as described in section 5.5.1.

MOX – UOX composites, reduce the plants environmental impact, by utilizing reprocesses reactor grade plutonium, from spent fuel depositories, without dependency on additional water rods for increased moderation.

The data analysis provided a knowledge basis with regard to the isotopic and neutronic interactions, of conceptual fuel compositions consisting of the predominant fissile and fertile isotopes, currently found in nuclear reactors and/ or their spent fuel depositories. The aforementioned, can be used for further optimizations, and development of the proposed alternatives, to determine the possibility of even longer fuel cycle lengths, at higher burnups.

6.2 Recommendations for further design development

Increase accuracy, with regard to isotopic and neutronic interaction behaviour, during burnup simulations can be achieved, by systematically increasing the complexity of the simulated geometry. The first step would be to simulate an infinite fuel assembly, proceeded by an infinite full core burnup simulation, and ultimately a finite full core burnup simulation.

The feasible conceptual compositions, can be optimized even further, by conducting a thermodynamic analysis of the composite, during burnup conditions, as well as a material property analysis, due to fatigue, as a direct result of the extreme operating conditions.

Further simulations are recommended to fully determine and analyse the effect of certain characteristics of the design. Simulation of an infinite reactor, suffices for preliminary design evaluations, but further simulations with more complex are required. Other numerical reactor modelling codes can be used to further verify the results of this study, and to optimize the design.

This design does show some theoretical safety concerns with regard to the temperature reactivity coefficients. This was especially postulated for the MOX fuel and reactor grade plutonium fuel compositions. However, these effects were not actually simulated. Method should be conceptualised to mitigate these effects, as the proposed fuel compositions showed promising results.

The proliferation risk of the fuel, is an area of fuel design that most certainly requires more research, and analysis. The mitigation of proliferation risks will prove to be extremely time consuming, and politically challenging may arise, but the basis of conceptual fuel design is rooted in the alleviation of the aforementioned problem.

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