



# **A Heterogeneous Thorium-based fuel design for a PWR aimed at increasing fuel cycle length**

**HB van der Walt**

**22222502**

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**Supervisor: Dr. DE Serfontein**

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## Declaration

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## Uittreksel

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Hierdie skripsie stel die leser bloot aan 'n nuwe heterogene, Thorium gebaseerde kern brandstof vir kern reaktore wat gebruik kan word om die leeftyd van die brandstof te vermeerder. Hierdie ontwerp vereis dat  $\text{ThO}_2$  tablette tussenin die gewone  $\text{UO}_2$  brandstof tablette van die reaktor geplaas word, waar die  $\text{ThO}_2$  blootgestel word aan 'n hoë termiese neutron vloed om sodoende  $\text{U}^{233}$  te kweek.

'n Heterogene ontwerp was ontwikkel omdat daar verwag word dat hierdie samestelling 'n beter kweek verhouding kan bereik as wat bereik word deur homogene Thorium gebaseerde brandstowwe. Die resultate verkry vanaf hierdie studie toon dat dit wel moontlik is om hierdie ontwerp binne 'n numeriese simulatie te gebruik, waarvan die kweek verhouding baie goed is en sodoende was die brandstof leeftyd beter as die van die verwysings modelle waarteen dit vergelyk was.

Verskillende samestellings vir hierdie ontwerp was gebruik om sodoende te bewys hoe hierdie ontwerp gemanipuleer kan word om beter resultate te lewer tydens verdere ontwikkeling. Die eerste pogings om die ontwerp te optimaliseer vir 'n beter kweek verhouding het getoon dat die ontwerp baie potensiaal wys, maar daar is omgewings binne hierdie ontwerp waar energie pieke ervaar word, wat 'n ernstige veiligheids gevaar kan wees.

Die konseptuele ontwerp wat ontwikkel was vir hierdie skripsie toon belowende resultate en daar word geglo dat hierdie ontwerp verdere ontwikkeling verdien. Enige verdere ontwikkelinge gaan baie moet fokus op die veiligheid van hierdie ontwerp, maar daar is ook ernstige teenstand teen enige Thorium gebaseerde brandstowwe wat aangespreek moet word.

## Abstract

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A new heterogeneous Thorium based fuel design has been proposed for Pressurised Water Reactors in order to increase fuel cycle lengths. This design incorporates ThO<sub>2</sub> pellets which have been included between UO<sub>2</sub> fuel pellets to breed fissile U<sup>233</sup> through transmutation of Th<sup>232</sup>.

A heterogeneous design was chosen in order to increase the conversion ratio of the fuel beyond what has been achieved with homogeneous Thorium based fuels. The results of this dissertation have shown that it is possible to introduce this design into an infinite reactor simulation, where a high conversion ratio can be achieved in order to increase the fuel lifetime and thereby increase the fuel cycle lengths.

The use of different fuel configurations have been explored to develop a concept design which can serve as a proof of concept for further development. This design has undergone preliminary optimisation steps and shows promise as an advanced fuel design. However, the occurrence of energy peaks within the fuel lattice causes some concerns for safety.

The concept design studied for this dissertation has provided positive results and due consideration for further development is strongly advised. Some safety concerns have been addressed, but the use of Thorium based fuels is still met with major challenges and concerns which could not be addressed within the given time for this study.

## Acknowledgements

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I offer this piece of work in the name of Our Holy Father, for without His power and grace we would be nothing, we would not be.

“When you call me close to tell me your body is not beautiful, I want to summon the eyes and hidden mouths of stone and light and water to testify against you.”

I wish to express my gratitude to my friends who have filled my life with moments of hope and pleasure. Thank you Marina, Maritza, Marinus and Ockert for supporting me in this endeavour even when my friendship was lacking.

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Last, but certainly not least, I would like to thank my family for the precious times I have shared with them and the support they have always offered me. Your contributions have helped me grow stronger and given me the strength to pursue my dreams.

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# Nomenclature

## DEFINITIONS

Definition	Meaning
Fissium	An alloy of 2.5wt% molybdenum, 1.9wt% ruthenium, 0.3wt% rhodium, 0.2wt% palladium, 0.1wt% zirconium and 0.01wt% niobium.

## TERMS:

## ACRONYMS AND ABBREVIATIONS

Abbreviation or Acronym	Definition
Am	Americium
ANL	Argonne National Laboratory
B	Boron
BOC	Beginning of Cycle
BP	Burnable Poison
BWR	Boiling Water Reactor
EBR-II	Experimental Breeder Reactor II
EFPD	Effective Full Power Days
FBR	Fast Breeder Reactor
FM	Ferritic-Martensitic
GWd	Gigawatt days
GWd/t <sub>HM</sub>	Gigawatt days/ton heavy metal
HM	Heavy metal

Abbreviation or Acronym	Definition
IAEA	International Atomic Energy Agency
IFR	Integral Fast Reactor
$k_{\infty}$ / $K_{\infty}$	Infinite neutron multiplication factor of a reactor fuel and moderator mixture
$k_{\text{eff}}$ / $K_{\text{eff}}$	Neutron multiplication factor of a finite reactor core, also called the eigenvalue.
LEU	Low Enriched Uranium
LMFBR	Liquid Metal Fast Breeder Reactor
LWR	Light Water Reactor
MOX	Mixed Oxide fuel
Np	Neptunium
Pu	Plutonium
PWR	Pressurised Water Reactor
SNF	Spent Nuclear Fuel
Th	Thorium
ThO <sub>2</sub>	Thorium Dioxide
U	Uranium
UN	Uranium Mononitrate
UO <sub>2</sub>	Uranium Dioxide
Xe	Xenon
Zr	Zirconium
$\eta$	Number of fission neutrons produced per neutron absorbed in the fissile fuel nuclides.

## Chapter 1. Introduction

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### Overview

In this dissertation fuel cycle optimization techniques are investigated through literature and numerical models. The insights gained are then used to develop a conceptual design that may be implemented in a physical reactor after further studies. The information gathered in this study outlines the mechanisms through which this concept design will increase the fuel cycle length of the system.

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### 1.1 Background

Although new pressurised water reactors are optimised during the system design phase, many of the reactors currently in operation have room for improvement with regards to fuel cycle length. New technology and research allows developers to improve fuel cycle lengths, but currently there are a few reactors still running on old technology, in which a cycle designed for 18 months may not be capable of running at full power for the entire 18 months.

In a case where the fuel does not last sufficiently long as required by the design it creates a significant decrease in income and may even result in a nuclear power plant creating debt. A few simple design alterations could prevent these plants from ever running below capacity and the increased income during this time would greatly outweigh the costs of these modifications.

The fuel lifetime may be increased by use of many different methods, the fuels and materials may be altered or the arrangement of differently enriched and burned fuel assemblies may be optimised in order to increase this value. In many cases it was found that inserting fuels which may have a weaker starting reactivity, but breeds some fissile material over time is the most beneficial method of increasing fuel lifetime.

### 1.2 Problem statement

Recently activists who oppose nuclear power have been using the available amount of Uranium that can be mined from the earth as a weapon against nuclear power. This information, although not frightening to those who have studied more detail about the expected lifetime of nuclear fuels, does create disarray within the general public. This disarray increases the difficulty of obtaining nuclear fuels and allowing new nuclear plants to be built.

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Regulating fuel supply is already a strenuous task and international dealings are even more difficult, therefore the increased difficulty due to public misconception is an unwelcome problem. Knowing this, it is important to make the best of the available fuel that a country, or plant has available. If a plant underperforms for a few months it does not only receive less income but it makes the effort of maintaining the plant all the more difficult.

In this regard, this study proposes that the problem of fuel lifetime shortage be researched and solved as quickly as possible. Methods of increasing fuel cycle length need to be experimented with in order to demonstrate how this can be achieved and how further development could increase this length even more.

### **1.3 Objectives of the project**

To address the problems which have been stated, various objectives were identified. By completing these objectives it is possible to conclude whether the problems can be addressed or whether further study is required.

- An initial literature survey is essential in determining the extent of research which has already been completed with regard to strategies for addressing similar problems, and are therefore applicable to the study at hand.
- Once understanding is gained on established work, a unique method may be determined or a trusted method improved upon for addressing the outlined problems.
- Numerical models of an infinite reactor should be created to determine the neutronic effects that different fuels and materials will have on such a reactor.

Numerical models can simulate infinite reactors for research purposes, this may be achieved by reflecting particles off of the boundaries of a whole assembly or a single fuel rod. The infinite reactor model can then be studied with different geometries and different fuel or material compositions to determine the effects of these alterations on the fuel cycle length.

- When the method to be demonstrated has been established the numerical models will be used to simulate the proposed design for different fuel cycle lengths.

- Results collected from the numerical models should be verified. Reference models that resemble those of other studies should be created and the results from these models should coincide with those of the previous studies. Theoretical principals can also be tested to verify that the models function correctly.
- The effects of burnup on the infinite multiplication factors ( $k^\infty$ ) of the models should be investigated to determine whether the established method can increase fuel cycle lengths.

A case study will be used for which it is assumed that a reactor designed to operate at full power for 18 month cycles cannot maintain criticality for longer than 480 days. This will be applied in the following manner:

- The  $k^\infty$  value of a reference  $\text{UO}_2$  model must be determined and set as the  $k^\infty$  value for maintaining criticality.
- The numerical models of the established design should therefore have a  $k^\infty$  value higher than the set value over the entire fuel cycle length that it will be designed for. If the model does satisfy this requirement then it may be concluded that it is sufficient for the required fuel cycle length.

#### **1.4 Project scope and constraints**

Fuel cycle lengths have been improved using various methods described by previous studies. This study does not aim to test the accuracy of previous designs, but rather their application in a PWR through the use of numerical simulations. Using the insights gained from previous research it may be possible to combine the positive effects of different designs and create a new method which is more easily implemented within commercial reactors.

An in-depth literature study will be completed in order to obtain important information about viable methods of optimisation and the theoretical principals that make them an improvement. This literature will be summarised and positive aspects of these studies will be discussed with a method of applying the acquired knowledge to develop a new design.

A numerical model of an infinite reactor, based off of a reflected fuel pin, will be created with arbitrary detail. Optimization methods will be applied and tested on this model, thereafter more detail may be added to the model and the optimisation will be repeated. After completing enough optimisations to gain confidence about the methods and programming language the researcher may alter these designs in order to maximise the efficiency and ease of use of the model.

The numerical models will be designed to be simulated using the General Monte Carlo N-Particle (MCNP) Transport Code (Goorley, 2014). This code was chosen as there were many researchers working at the North-West University with experience in using MCNP at the time of writing.

This project will not be able to physically test the practical application of the proposed solution without further interested parties, funding or time, but serves as a proof of concept for this type of design.

It would be beneficial to focus on a reactor type which is currently in operation within South Africa, thus a PWR similar to the reactors found at Koeberg. It is also beneficial to focus on research currently underway at the North-West University. Due to the University's background of research on homogeneous Thorium fuel designs this study will focus mainly on the use of Thorium based fuel designs for PWRs.

Burnable poisons (BPs) are used extensively in nuclear reactors. It would be safe to assume that any design developed for this study would require the use of BPs. The addition of BPs is considered to be a process which should be completed during the detail design phase of a project. This is due to the complex configuration of BPs within assemblies, where the poisons can be added radially or axially, homogeneously or heterogeneously, etc.

There are too many BP considerations to be investigated for the available time of this study and therefore minimal attention will be given to the investigation of BPs. This material is, however, of such importance that some research has to be included which describes the advantages and configurations possible with the use of BPs for this design.

## Chapter 2. Literature Study

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### Overview

This literature study serves as a baseline for evaluating and summarising the methods used in previous projects which have been completed in order to solve problems similar to those addressed in this study. The results obtained from the projects that have been investigated will also aid in verifying the results of this project whereas the difficulties encountered by previous experimentation will serve as a guideline of what hurdles should be avoided.

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### 2.1 Introduction

Some research papers may show inconsistencies with the findings of other articles, in such cases an in depth discussion of the research findings is provided and the inconsistencies are argumentatively compared.

A numerical model is required to address the problems stated for this project. Researching projects with similar problem statements will lend better understanding of the type of model to be created, as well as the effects that different elements will have on the model.

### 2.2 Optimisation methods

Various viable methods for optimising the fuel lifetime of a nuclear reactor have been tested, others have been theorised. This study will focus on the use of different fuels and materials inside a nuclear reactor in order to improve the fuel lifetime and efficiency of the entire system.

#### 2.2.1 Metallic fuel

Prior to the 1960s liquid-metal cooled fast breeder reactors (LMBRs) were developed to use metallic fuels, but many researchers did not believe in the potential of metallic fuels and soon interest worldwide shifted toward ceramic fuels for LMBRs. However, the Argonne National Laboratory's (ANL) Experimental Breeder Reactor II (EBR-II) continued to be fuelled with the metallic Uranium-Fissium alloy U-5F. (Hofman, et al., 1997).

The EBR-II was used to determine the performance limitations of metallic fuels for power production, during these tests additional attributes of metallic fuels were discovered. Despite the newfound benefits of metallic fuels it seemed that ceramic fuel would remain the first choice even up to the end of the 1980s, but the cancellation of the Clinch River Breeder Reactor by the U.S., due to economic and fuel cycle concerns, quickly changed this perspective (Hofman, et al., 1997).

The Integral Fast Reactor (IFR) was developed by ANL in 1983, this design offered a safe and economically strong solution to some of the technical and institutional concerns that were preventing nuclear power from making a large contribution to the world's energy demands (Hofman, et al., 1997). With this design ANL showed that there was a need to use the world's reserves of Pu<sup>239</sup> as an energy source. Thus they developed a fuel system which is capable of utilizing Pu<sup>239</sup> as its principal fuel and will breed more fuel by irradiating U<sup>238</sup> for a longer lifetime (Walters, et al., 1984).

The developers of the IFR determined that metallic fuel should be used and decided that the U-Pu-Zr system, which had been developed in the late 1960s, promised superior performance to other metallic fuel systems. By the time of development the IFR metallic fuels had demonstrated excellent neutron economies and high burnup capabilities, but during testing some additional features were realized that made metallic fuels all the more attractive (Hofman, et al., 1997).

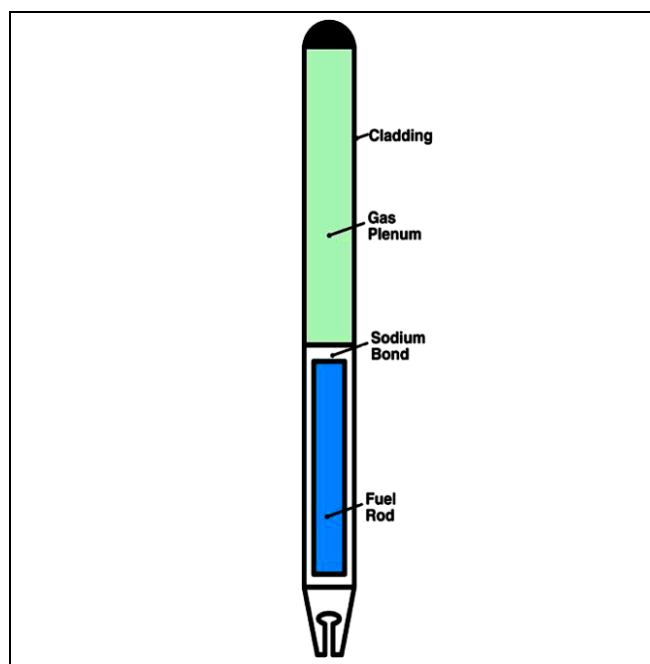
The first additional benefit discovered was that metallic fuel showed higher thermal conductivity values in comparison with oxide fuel, this resulted in significant safety benefits (Walters, et al., 1984). The EBR-II was used to demonstrate this benefit, accident scenario tests were run with the reactor at full power. One test demonstrated a loss of primary flow accident whereas the other demonstrated a loss of heat sink accident, in both cases the reactor safely shut itself down without operator or mechanical intervention (Walters, et al., 1984).

The second benefit is that metallic fuels can be safely recycled by a novel technique and this technique itself has several inherent advantages. Metallic fuel is processed through electro-refining. After refinement the cathode product contains Uranium, Plutonium, minor actinides and some residual fission products. Most of the fission products can then be separated from the cathode product and sent for refabricating and reprocessing. However, this material is highly radioactive due to the remaining fission products and therefore all refabricating steps need to be carried out remotely in hot cells (Walters, et al., 1984).

The use of this recycling technique therefore has the following inherent advantages:

- Diversion of fuel is virtually impossible due to the high radioactivity (Hofman, et al., 1997).
- The material cannot be weaponized as further PUREX-type reprocessing would be required in order to separate the Plutonium from the Uranium and the remaining fission products.
- The process involves batch operations, therefore the entire process can be scaled to meet local requirements with very specific volumes to be monitored.
- This process has been shown to be more economic in comparison to other recycling options.

Finally, and perhaps of greatest importance, this recycling method allows essentially all the actinides to remain in the fuel cycle. These actinides can then be recycled into the fuel during refabricating where they will act as fissionable material (Walters, et al., 1984). This also means that the waste produced from the system will decay to background levels within a fraction of the time required for most high-level waste.



**Figure 1: Schematic of a metallic, sodium bonded, fast reactor fuel element (Carmack, et al., 2009).**

Figure 1 demonstrates a typical metallic fuel element where the fuel rod section will contain the fissile material, this may be a fuel alloy which is stabilized by adding 10-30% zirconium. The addition of zirconium increases the melting point of the fuel and minimises chemical interaction between the fuel and cladding (Carmack, et al., 2009). Sodium is used to thermally bond the fuel rod to the cladding, sodium has a very high thermal conductivity and acts as a medium by which heat can be transferred to the cladding and the coolant.

A gas collection plenum is incorporated into the fuel element to capture the released fission product gases. Finally the fuel, sodium and cladding are sealed inside a nickel-based alloy- or stainless steel cladding, consisting of an austenitic- or ferritic-martensitic (FM) composition. Current designs prefer FM stainless steel as it has a lower thermal expansion coefficient. Future designs may have a fine oxide powder added to the steel in order to improve high-temperature strength and stress rupture properties (Carmack, et al., 2009).

Metal fuels such as U-Pu-Zr have been shown to improve the basic thermal and neutronic performance of fast breeder reactors when compared with oxide ceramic fuels (Riyas & Mohanakrishnan, 2008). It has also been shown that metallic fuels create harder neutron spectra, thus improving the breeding ratio in most breeder reactors. High breeding ratios will result in low burn-up reactivity swings, and, when coupled with a low Doppler coefficient due to the low operating temperatures will reduce the excess positive reactivity that needs to be added to reactors during start-up (Chernock & Horton, 1994).

The above mentioned factors also decrease the required fuel rod reactivity worth. Further studies have shown that the high breeding ratios may even make it possible to achieve near zero burnup reactivity swing per cycle. Metal fuelled core designs have been simulated with burnups as high as 150 MWd/kg (Dubberley, 2000).

Though there are many benefits to metallic fuels in FBRs one of the main safety concerns is a high positive sodium void worth for an unprotected loss of flow accident (Cahalan, 1990). Another accident situation which is being investigated due to safety concerns is an unprotected loss of heat sink accident, although, in pool type FBRs this type of accident is highly unlikely. Further studies have reported that a tighter packed core and flatter core shape will result in reduced sodium void worth, but will lead to a reduction of breeding ratios and also higher burnup swings (Cahalan, 1990).

### 2.2.2 Alternative fuels and materials

There are many articles which test the economic viability of using Thorium based fuel cycles, but (Du Toit & Cilliers, 2014) demonstrated more detail about the refuelling cycle, capacity factor and volumes of spent fuel and therefore this study was chosen as a first summary. The article focuses on once-through, homogeneously mixed, Thorium-Uranium fuel which is run on a 24 month cycles as opposed to the standard 18 month Uranium based fuel cycle.

Within the background theory of the above article we find information about the conversion rates of Thorium-Uranium fuels as well as the statement that Thorium based fuels show increased reactivity ( $k_{eff}$ ) stability. This statement was supported by the use of Figure 2 which shows how the breeding of  $U^{233}$  through the use of  $Th^{232}$  stabilizes the reactivity of the reactor (Du Toit & Cilliers, 2014).

For the investigation of economic aspects, an in depth study of the costs relating to the use of Thorium based fuels was completed sequentially, where the following steps are assessed: fuel cycle costs (with reference to different assumptions), raw material requirements, retrofitting, enrichment, fabrication, storage, disposal and total fuel cycle cost. The costs of refuelling downtime and income from electricity sold was accounted for, the resulting conclusion was that using Thorium based fuels will result in greater profits than their viable counterparts (Du Toit & Cilliers, 2014).

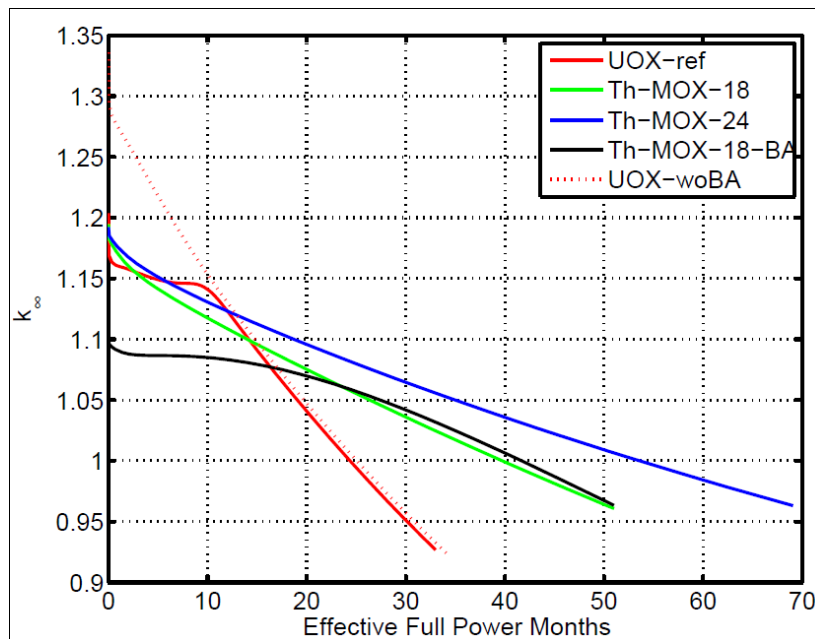


Figure 2: Infinite reactor reactivity versus full-power months for Uranium and Thorium-based fuels (Du Toit & Cilliers, 2014).

(Brown, et al., 2014) Investigated another method for increasing fuel efficiency, this method included the use of Uranium mononitrate (UN) based composite nuclear fuels. It is important to note that UN reacts chemically with water, even more so at high temperatures, and therefore the UN is “shielded” from water by another material that was homogenously mixed with the UN.

The composites UN/U<sub>3</sub>Si<sub>5</sub>, UN/U<sub>3</sub>Si<sub>2</sub>, UN/UB<sub>4</sub> and UN/ZrO<sub>2</sub> were tested using numerical models based on the Westinghouse AP1000. In these tests factors like fuel porosity, neutron flux spectrums, capture cross sections and resonance escape probability were taken into account to determine the effects of the above mentioned on the burn-up, reactivity and cycle length of the various fuel composites. The thermal conductivity of the nitride fuels is significantly higher than that of UO<sub>2</sub>. This factor, coupled with an increased fast fission factor allowed for the increased cycle lengths shown in the article.

The end results were that the UN based fuels showed increased cycle lengths and therefore increased burn up rates (Brown, et al., 2014). But the tests were not without problems, a large concern was the reduced burnable absorber and soluble poison worth inside the UN fuels due to their unique reaction spectrums.

With the above mentioned studies in mind, the investigation of the use of Thorium based fuels is deemed worthwhile for this study. The use of UN shows too many dangers in accident situations whereas the use of Thorium could have more proliferation resistance.

### **2.2.2.1 Homogeneous Thorium based fuels**

Thorium fuelled reactors have been studied for many years now, an attempt has been made by Herring, et al. (2001) to find a way in which the cost and proliferation resistance of Thorium fuelled reactors would be sufficient to sway public opinion on the use of these types of reactors.

In this study the goals were to develop a fuel which was less expensive to fabricate than the standard fuels, had a longer fuel cycle resulting in increased plant capacity factors, had high proliferation resistance and resulted in more stable, low weapons risk waste. The study used a homogeneous mixture of Thorium dioxide and Uranium dioxide with varied weight percentages of each, but UO<sub>2</sub> enriched to 19.5% U<sup>235</sup> was always used.

The results of their numerical models showed that a higher burnup could be achieved with  $\text{ThO}_2\text{-UO}_2$ , not only this, but also due to the sub-criticality of the Thorium the mixed fuel delivered lower core temperatures which means that the fuel can be safely operated at higher burnup rates without overheating. Operating at higher burnups means longer fuel cycles, increased capacity factors and less waste to be handled, stored and later, disposed of (Herring, et al., 2001).

The use of homogeneous Thorium fuel has been researched extensively with results lingering on the edge of viability (Du Toit & Cilliers, 2014) (Herring, et al., 2001) (Galperin, et al., 2000) (Thor Energy, Norway, 2012) (Blanchars & Fabrycky, 2011) (Yamamoto, et al., 2002). One method of increasing the efficiency and effectiveness of Thorium fuel cycles might be the use of heterogeneous Thorium fuels (Bae & Kim, 2005) (Dean, 2003).

#### **2.2.2.2 Heterogeneous Thorium based fuel designs**

In contrast to the benefits of using homogeneous mixed fuel as mentioned above, Ashley, et al. (2014) investigated reactor designs utilising Thorium that delivered negligible benefits to using Thorium based fuels. This study was done on open cycle Th-U fuelled reactors, but did not only look at LWRs, they added HWR and high temperature gas cooled reactor designs. The reactor designs used were those of Areva's EPR, the Indian AHWR and General Atomics' GT-MHR.

The simulations used UK National Nuclear Laboratory's fuel cycle modelling code, ORION. This code uses lattice-physics calculations from other simulations in order to model the neutronic behaviour of each model.

This study will focus on the design and results of their LWR model. The design of the reactor used was the Areva EPR and the reactor was up-scaled for the model, though most of the reactor properties were kept the same the blanket assemblies were altered in order to utilise Thorium in the cycle.

The original reactor used 193 fuel assemblies, 84 seed assemblies were modelled with annular  $\text{UO}_2$  fuel pellets enriched to 20% and axial reflector blankets of natural Uranium. 109 Blanket assemblies were added with blended  $\text{ThO}_2\text{-UO}_2$  fuel in the ratio of 87:13 and a  $\text{U}^{235}$  enrichment of 10%. The up scaled model utilised 241 assemblies, of which 105 were seed and 136 were blanket assemblies. The active length of the reactor was also increased to 4.2 meters. (Ashley, et al., 2014)

In the initial simulations it was found that the  $U^{233}$  content exceeded the 12% limit for LEU containing  $U^{233}$ . The ratio of Thorium to Uranium was then changed from 87:13 to 83:17 and the  $U^{235}$  enrichment was reduced to 7.65% in order to match the fissile fraction and to denature the  $U^{233}$ .

Due to the complexity of the model the discharge burn-ups were assumed to be the same as that of the original EPR design. This left the research open to errors and therefore better accuracy may be achieved with further full-core calculations and exact discharge burn-ups. The thermal-hydraulic feasibility of such an up-scaled design must also be evaluated.

The lifetime of the reactors considered was also increased to around 68 years in order to create a fair comparison between the different technologies, but it must be realised that this may be an over-estimation.

The sensitivity is described as a concern as it is stated that, if the average discharge burn-up and core occupancy of the U-fuelled EPR were to be increased only slightly, it would mean that the amount of Uranium ore per kWh (e) would be the lowest of all their models (as opposed to second in initial tests). The modified EPR also required the smallest amounts of separated work units per kWh (e) in the initial tests, but this was still more than the requirements of the original EPR.

The proliferation resistance was measured using the NNL proliferation resistance assessment methodology. Due to waste form calculations it was found that the TH-U fuelled EPR model showed a small advantage in proliferation resistance due to lower amounts of Plutonium being discharged per GWy. In this model it was found that the concerning factor that limits the proliferation resistance of Thorium based fuels was the score from discharged seed assemblies where the only benefits were due to the material type score, although this value was higher than that of the U-fuelled EPR. It is still important to note that these values were all on a qualitative non-linear scale and that the benefits arising due to the nature of the spent fuel from Thorium Uranium fuels should be weighed against the increased separative work capacity per kWh required for production of the fuel assemblies as well as the need for the Uranium to be enriched to 20%  $U^{235}$  (Ashley, et al., 2014).

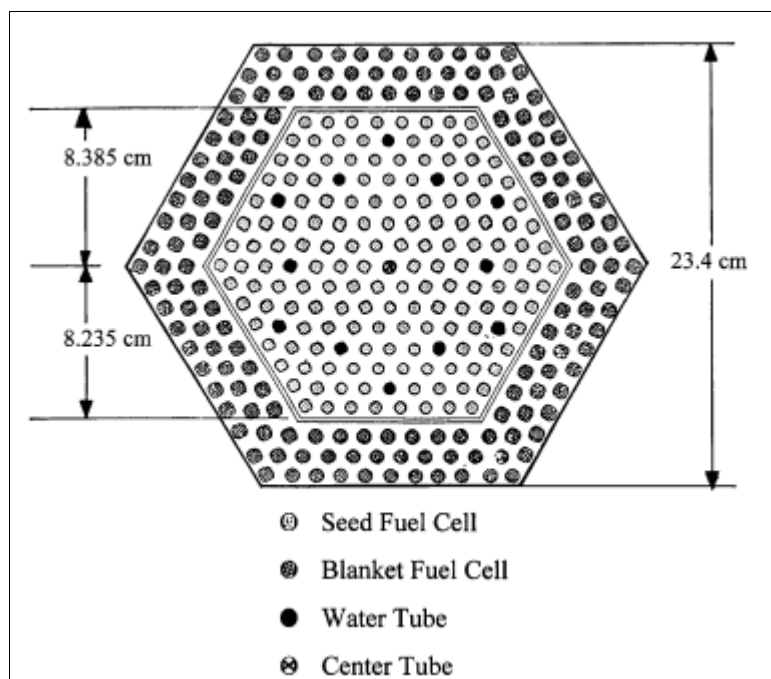
In an admittedly indicative, rather than definitive economic study the researchers found that the cost of Th-U fuel would be more than the reference, but they did feel that this difference might be negated by further studies. This was indeed the case as further studies showed that, when profit margins of electricity sales were taken into account with regards to capacity factors, refuelling outages and operational savings incurred as a result of the longer fuel cycles of Thorium based fuels, then Thorium based fuels provided a significant economic advantage (Du Toit & Cilliers, 2014).

The exciting conclusion of this study stated that it was evident to the researchers that, if lower Uranium enrichments could be used for a Th-U fuelled reactor, a notable advantage in resource utilisation could be realised (Ashley, et al., 2014).

But this does not nullify their conclusion that they feel there is little merit in using Thorium as fuel, mainly due to the need for 20% enriched Uranium which results in more separative work capacity, limited savings in Uranium ore and waste as well as inconclusive economic studies, which still do not support the use of Thorium. Furthermore, these downsides are increased with technical and licensing barriers which have not been explored yet.

In recent years heterogeneous Thorium-based fuel designs have been suggested to replace conventional PWRs. At the Ben-Gurion University in Israel researchers developed the Radkowsky Thorium Fuel (RTF) concept design, which is based on the use of blanket and seed units within a fuel assembly (Galperin, et al., 2000).

The use of blanket and seed units requires a complex reloading scheme, because the blanket and seed assemblies require different reloading strategies (Galperin, et al., 2000). A seed unit, which is placed within the central region of fuel assembly would contain 20% enriched Uranium, which is alloyed with 10% Zirconium. The blanket unit surrounding the seed would contain  $\text{ThO}_2$  mixed with 10-20% enriched Uranium. This setup therefore requires the seed and blanket areas to be divided into two physical parts within the assembly to allow independent movement of each unit. This design is demonstrated in Figure 3.



**Figure 3: Fuel assembly geometry of the Radkowsky Thorium reactor (Galperin, et al., 2000).**

If the seed assemblies are refuelled at three-year intervals and the blankets at nine year intervals it is possible to irradiate the blankets to the full metallurgical lifetime of about 100 000 MWd/T (Higatsberger, 1999).

The Whole Assembly Seed and Blanket (Wang, et al., 2000) (WASB) concept developed at MIT is another option for Thorium utilisation in PWRs. WASB used an annular fuel geometry for seed fuel that contained burnable poison material in the inner hole. An annular type of seed fuel was used to increase the thermal hydraulic safety margin. However, it is expected that the annular fuel concept will be more difficult and expensive to manufacture than conventional UO<sub>2</sub> fuel.

The analysis showed that the WASB core could satisfy the requirements of fuel cycle length and safety margins of conventional PWRs. The coefficients of reactivity are comparable to currently operating PWRs. However, the reduction in effective delayed neutron fraction required careful review of the control systems because of its importance to short term power transients.

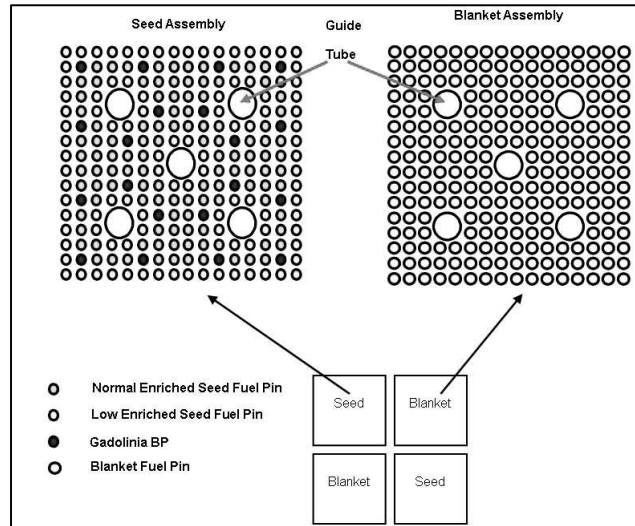
Whole core analyses showed that the total control rod worth of the WASB core was about 1/3 less than those of a typical PWR for a standard arrangement of Ag-In-Cd control rods in the core. The use of enriched Boron in the control rods could effectively improve the control rod worth.

The control rods have higher worth in the seed than in the blanket, therefore, a new loading pattern has been designed so that almost all of the control rods will be located in seed assemblies. However, the new pattern required a redesign of the vessel head of the reactor, which is an added cost in the case of retrofitting of existing PWRs (Dean, 2003).

The Kyung-Hee Thorium Fuel (KTF) concept design would consist of a whole seed and blanket assembly with a ratio of 1:3, this design was optimised to achieve a maximum conversion ratio (Kim & Woo, 2000). In most cases the seed and blanket concepts have a large power tilt between the seed and blanket units or assemblies, this resulted in a thermal hydraulic safety problem within the hot seed channel. Metallic fuels, with higher thermal conductivities than ceramics may be used within the seed channels to address this problem within the KTF design (Kim & Woo, 2000).

Blanket units were found to produce a lower power fraction than the seed by about 30% of core power, these units also required longer burnup periods than that of the seeds due to the use of a one batch fuel cycle strategy. The reason being that the blanket assemblies should remain within the core for as long as possible to maximise thermal conversion, therefore replacing the blanket assemblies only once every nine cycles is optimal. To account for the long periods of exposure the ceramic form of  $\text{UO}_2$ - $\text{ThO}_2$  was considered as a blanket fuel material instead of U-Th-Zr metallic fuel, which could encounter embrittlement problems.

The original KTF design focused on increasing the conversion ratio and has a seed-to-blanket volume ratio of 1:3. This ratio is extremely important for thermal hydraulic safety due to the high power tilt between the seed and blanket assemblies (Woo, 2000). Power peaking within the pins of the hottest seed assemblies exceeded tolerable limits when the original KTF design was simulated. The KTF design was altered to have a 1:1 volume ratio in order to reduce power peaking (Woo, 2000). Figure 4 demonstrates the revised KTF design with a 1:1 seed-to-blanket ratio, after this change the design was approved for physical testing and will be tested at the 3,983 MWth Korea Next Generation Reactor, APR-1400 (Bae & Kim, 2005).



**Figure 4: Revised KTF blanket and seed assembly geometry.**

The seed assemblies would require higher enrichments of  $U^{235}$ , when compared to typical PWR fuels, to yield the same fuel cycle length due to the low reactivity of the blanket assemblies. Blanket assemblies will remain sub-critical during the entire burnup period when installed with the same moderator-to-fuel ratio of typical PWRs, therefore an excessive amount of fissile materials will remain within the seed assemblies, even after they have been discharged

Blanket assemblies will be composed of small fractions of enriched  $UO_2$ , within the  $ThO_2$ -matrix, to compensate for their low reactivity at the beginning of burnup (until the assembly is saturated with  $U^{233}$  through conversion). The conversion ratio of the blanket assemblies can be increased by making the neutron spectrum harder within these regions.

The typical fuel cycle length could be as long as nine reload cycles, that is, 472.5 Effective Full Power Days (EFPD), although every cycle would have a different length due to reactivity variations within the blanket fuel assembly. The length of the first cycle would be longer than average due to the excess reactivity of the blanket assemblies at start-up (due to the  $UO_2$  which is added), which then decreases with burnup. The average discharge burnup of this design is 83 MWd/kgHM for the seed assemblies and 95.9 MWd/kgHM for the blanket assemblies, these values are higher than that of a conventional PWR at around 50 MWd/kgHM (Bae & Kim, 2005).

## 2.2.3 Challenges with Thorium based fuels

### 2.2.3.1 Proliferation risk

It is clear that proliferation resistance is an important factor for considering new fuels as a method of increasing the fuel lifetime. Therefore more research about the proliferation resistance of different fuel types will now be shown and controversies between these studies will be pointed out.

High burnup Thorium fuels may improve the weapons material proliferation-resistance of LWRs in three ways (Herring, et al., 2001).

- The amount of separable weapons material which is generated will be significantly less as the bulk of the fertile materials will be Thorium and the  $U^{233}$  produced by conversion will be diluted within the  $U^{238}$  fuel mixture.

Although it is true that the amount of weapons material generated will be less, it is important to note that  $U^{233/238}$  mixtures have a smaller critical mass than  $U^{235/238}$  mixtures, therefore the mixture will have to be denatured with added  $U^{238}$  (Serfontein & Mulder, 2014).

- Fuel cycles will be longer and the refuelling periods less frequent, this will make diversion of materials during refuelling less likely.

Thorium based fuels can achieve higher burnups and therefore the refuelling cycles may be extended to 24 months as opposed to the 18 month cycles of conventional fuels (Du Toit & Cilliers, 2014). Heterogeneous use of Thorium fuels allows the use of Thorium blanket assemblies which can be exposed to nine cycle lengths inside the reactor core, this reduces the refuelling outage times and increases the plant capacity factors (Higatsberger, 1999).

- The Plutonium isotopes within the fuel will be much less desirable for nuclear weapons use, when the fuel is exposed to such high burnup rates the amount of even numbered isotopes such as  $Pu^{238}$  increases. These isotopes are much more resistant to nuclear weapons proliferation (Herring, et al., 2001). 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 use of pure Pu<sup>239</sup> for weapons production would be most desirable, but super-grade and weapons-grade Plutonium is produced by irradiating natural or depleted Uranium samples with a low neutron flux. Plutonium for reactor fuel is produced at significantly larger flux values within breeder reactors, but these grades are not fixed and the isotopes produced in any fuel cycle are dependent on the neutron energy, flux value, length of the cycle and the amount of cooling or cooling periods allowed during refuelling and after discharge from the reactor (Herring, et al., 2001).

The spontaneous neutron generation rate and the amount of decay heat produced by the various Plutonium isotopes determine the desirability of a particular mixture of isotopes for use in a weapon. The destructive potential of nuclear weapons may be affected by these factors, but it is still important to note that even low yield nuclear weapons detonated in highly populated urban areas would cause significant psychological damage to satisfy the goals of many terrorist groups (Serfontein & Mulder, 2014).

Am<sup>241</sup> is produced by the 14.4-year beta decay of Pu<sup>241</sup> and will grow into separated Plutonium over time. The reasons for the desirability of Pu<sup>239</sup> and the corresponding undesirability of Pu<sup>238</sup>, Pu<sup>240</sup>, Pu<sup>242</sup> and Am<sup>241</sup> are the following:

Pu<sup>239</sup> has significantly lower spontaneous neutron generation rates and decay heat rates than its adjacent isotopes. To increase the undesirability of separated Plutonium for weapons use the fraction of Pu<sup>238</sup> and the other even numbered Plutonium isotopes should be increased (Herring, et al., 2001).

The total amount of Plutonium produced per MWd in any of the mixed Thorium Uranium test fuels is about a factor of 3.2 less than that produced in the conventional UO<sub>2</sub> fuel burned to about 45 MWd/kg. This follows from the fact that the U<sup>238</sup> content of the mixed Thorium Uranium fuels is only about 24 – 28% of that present in conventional fuels. Furthermore, the amount of Pu<sup>239</sup> is about a factor of 4 less than that of the conventional fuel, first due to the smaller amount of U<sup>238</sup> present and secondly due to the higher burnup, during which part of the Pu<sup>239</sup> is fissioned.

The spontaneous neutron production rate of separated Plutonium from Thorium Uranium fuel is about 50% larger than that of conventional UO<sub>2</sub> fuel burned to 45 MWd/kg and at least ten times greater than either of the weapons grade Plutonium's.

The amount of decay heat produced is also about 2.5 times larger than that of conventional UO<sub>2</sub> fuel burned to the same value, and up to 20 times more than either

of the weapons grade Plutonium's (Herring, et al., 2001). These factors increase the chance of pre-detonation inside an implosion type nuclear weapon and would thereby drastically reduce the yield of such a weapon. The high explosive surrounding the fuel would also be heated due by the large amounts of decay heat, this would also drastically reduce the yield of the weapon (Serfontein & Mulder, 2014).

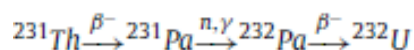
The proliferation resistance of Thorium cycles may be increased by increasing the amount of  $U^{232}$  in the spent fuel. The increased amount of  $U^{232}$  decays to  $Tl^{208}$  which is highly radioactive and produces high energy  $\gamma$ -rays when decaying. This increases the radiation and detection risk of would-be terrorists and thereby increases proliferation resistance of the fuel (Serfontein & Mulder, 2014).

$U^{232}$  also  $\alpha$ -decays with a half-life similar to  $Pu^{238}$  which produces some decay heat and decreases the usefulness of the spent fuel in bombs, but due to the very low concentration of  $U^{232}$  this factor does not add significantly to the proliferation resistance offered by  $U^{232}$ . Furthermore, there is a very low rate of spontaneous fission neutron emissions in Thorium mixtures and these can easily be used in simple high-yield gun-type nuclear weapons, which deprives this fuel of the proliferation resistance offered by  $Pu^{240}$  in Pu cycles.

Since the  $U^{232/233}$  mixtures in the spent fuel of low burn-up Thorium cycles is typically denatured by only a small amount of  $U^{232}$  the critical mass required for any nuclear reaction is lower than what is required from typical  $U^{235/238}$  cycles where the amount of denaturisation is high. This fuel can then be easily used in gun-type nuclear weapons and offers no proliferation resistance unless it is denatured with  $U^{238}$ .

The proliferation resistance of Thorium cycles may be increased using the following methods:

- By increasing the amount of fast neutrons with energies above 6 MeV, this will allow for more (n,2n) reactions to occur, these reactions create  $U^{232}$  which creates a significant radiation threat to would-be terrorists. This can be done by, for instance, burning Thorium fuels in PWRs instead of PHWRs.
- By adding  $Th^{230}$  to the Th-mixture in the fresh fuel,  $Th^{230}$  can undergo  $\gamma$ -decay followed by the reactions:



This reaction produces  $U^{232}$  resulting in better proliferation resistance,  $Th^{230}$  can be added by standard isotope enrichment processes or by using Th from mines which have a higher fraction of  $Th^{230}$ .  $Th^{230}$  is a by-product of natural Uranium decay chains and therefore mines that contain both Uranium and Thorium will most likely contain more  $Th^{230}$ .

- By increasing the burn-up of the fuel, as this will increase the rate at which  $U^{232}$  is produced, since most production routes for  $U^{232}$  require two subsequent neutron captures the rate of  $U^{232}$  production at start-up is low and increases with burn-up as intermediate isotopes in precursor transmutation chains build up in the fuel.

Although the amount of Pu produced inside a Thorium fuelled reactor would be substantially less than what is produced inside a Uranium fuelled reactor, Pu will still be produced and therefore it would be beneficial to know how to reduce the proliferation risk of Pu. A study completed by Serfontein & Mulder (2014) shows that the proliferation resistance of Pu may be increased by means which will be described in the following section.

Reactor-grade Plutonium contains approximately 23.7 wt%  $Pu^{240}$ , this denatures the  $Pu^{239}$  to the extent that the spent fuel cannot be used to create high yield nuclear weapons. This is due to the high spontaneous fission rate of  $Pu^{240}$ , which increases the spontaneous neutron flux within the fuel.

When a nuclear weapon is created from this fuel and triggered the large amount of free neutrons cause the nuclear fission chain reaction to pre-detonate, thereby blowing the imploding fuel shell apart before the optimal compression and reactivity levels can be attained. This greatly reduces the yield of such bombs, which can then be classified as “fizzle” bombs, implying that these bombs do not explode, but rather, fizzle.

Although the yield is reduced, “fizzle” bombs detonated in highly populated urban areas can still cause massive psychological damage to a large amount of persons. Due to this risk it is important to ensure that the spent fuel from U/Pu fuel cycles is extremely proliferation resistant and has low risk of being used for “fizzle” bombs.

Not only the Pu in spent fuel creates a risk of nuclear weapon production,  $Np^{237}$  has a high fast fission cross-section and very low radioactivity, as the half-life of this element is over a million years.  $Np^{237}$  is an attractive nuclear weapons fuel as it does not radiate

a high flux of spontaneous ionising rays which would pose a health risk to would-be terrorists.

$\text{Np}^{237}$  does not pre-detonate nuclear weapons as it does not emit a large spontaneous neutron flux. This element can easily be implemented in simple gun-type nuclear weapons with dangerous, high energy yields and due to low levels of decay heat it could also be used in higher efficiency implosion-type nuclear weapons.

Possible solutions to increase the proliferation resistance of Pu fuel rely on the destruction of  $\text{Np}^{237}$  and denaturation of  $\text{Pu}^{239}$  with  $\text{Pu}^{240}$  and  $\text{Pu}^{238}$ . This can be done by using  $\text{U}^{233}$  or Thorium-driven fuel cycles as these cycles produce negligible amounts of  $\text{Np}^{237}$ .  $\text{Np}^{237}$  can also be recycled from spent fuel repeatedly and burned in secondary fast breeder reactors, this will transmute the  $\text{Np}^{237}$  to  $\text{Pu}^{238}$  which has high proliferation resistance due to high levels of decay heat.

### **2.2.3.2 Barriers for Thorium based fuel assemblies**

Thorium cycles are viewed as more proliferation resistant in comparison to Uranium cycles (Serfontein & Mulder, 2014). However there are barriers restricting the use of Thorium inside most nuclear reactors at this moment and will most probably exist for many more years. The Uranium/Plutonium fuel cycles do not have these same barriers and have been favoured for reactor use.

The barriers that were found in this study are the following:

- The sustainability and cost of Uranium fuel:

This is inversely proportional to the viability of Thorium fuel cycles. At the currently low prices and high availability of U/Pu fuel there is no compelling reason to choose Thorium fuel cycles which have high fabrication and enrichment costs, with low availability due to the high U enrichment which is required. This means that unless the prices of U/Pu fuel skyrocket, the use of Th/U fuel will not be economically viable.

- The cost of reprocessing spent Thorium fuel:

Thorium based fuel cycles require the excess  $\text{U}^{233}$  in the spent fuel to be chemically reprocessed to increase proliferation resistance significantly. But current reprocessing costs are expensive which also requires Uranium prices to skyrocket before this fuel becomes economically viable.

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- The radiotoxicity of spent Thorium fuels:

As the Thorium spent fuel ages, although it has reduced radiotoxicity at first, after 1000 years this value starts to increase rapidly and, after 11000 years it surpasses that of Uranium spent fuel. This factor may increase the waste disposal costs on top of the already expensive chemical reprocessing costs which creates significant price increases associated with Thorium fuels (Serfontein & Mulder, 2014).

- Accident scenarios:

The release of radioactive particles from Thorium fuels is substantially more dangerous than what is released by Uranium fuels. Although it has been found that Thorium fuels are chemically much more stable than Uranium and will trap most radioactive fission products inside the fuel, this advantage is not infallible and nuclear regulators may not give full consideration for this fact during licensing procedures. Some changes to licensing regulations may be required to account for this benefit (Serfontein & Mulder, 2014).

### **2.2.3.3 Excess reactivity**

Considerably more control reactivity is required at start-up of a new, clean, cold core, which is loaded with fresh fuel. Most of the factors responsible are short term effects, such as low temperature and low  $Xe^{135}$  neutron poison concentration. The effects can disappear within hours or days, thereafter much less control reactivity is needed.

To reduce this required control reactivity it is common practice to place a burnable poison (BP) at selected locations throughout the core. Burnable poisons are nuclides that have large absorption cross-sections which then transmute into nuclides with low absorption cross-sections as the result of neutron absorption (Glasstone & Sesonske, 1994). Therefore, the burnup of the poison results in an increased reactivity over time, which slightly counteracts the decrease in reactivity caused by the burnup of the fuel and the accumulation of fission product poisons.

This means that burnable poisons can reduce the amount of control rods required in reactors, which use control rods for control, and could reduce the cost of such reactors. Burnable poisons added to reactors which are controlled by chemical shim would decrease the necessary Boron concentration, meaning that the Boron concentration of these reactors can be decreased over time. By reducing the required chemical shim

these reactors can ensure that the moderator temperature coefficient is always negative.

This coefficient can only stay negative as long as the water and Boric acid mixture moderates neutrons at a higher rate than it absorbs them, if too much Boron is added to the water the moderator coefficient could become positive (Glasstone & Sesonske, 1994).

Many materials have been utilised as BPs, the first was Boron in various forms, including Pyrex glass containing approximately 12wt% Boron Oxide. Further development led to the use of Gadolinia ( $Gd_2O_3$ ) which was mixed within the  $UO_2$  in several fuel rods of each fuel assembly. Advanced fuel designs utilise Gadolinia which has been zoned both axially and radially (Glasstone & Sesonske, 1994).

Core power and performance can be increased drastically with the use of sophisticated core designs which utilise higher enriched fuel, usually 5% enriched Uranium, and significant amounts of burnable poisons such as Gadolinia. By zoning the Gadolinia and the Uranium correctly it is possible to produce very uniform burnup and power. By utilising such advanced core designs in both BWRs and PWRs cycle lengths can be increased up to 24 months and a power uprating of up to 20% can be achieved for some reactors (Glasstone & Sesonske, 1994).

Burnable poisons used in light water reactors include Boron, Hafnium, Europium, Gadolinium, Samarium and Cadmium. In most cases, Boron is the burnable absorber of choice and a variety of placement schemes are exercised. These include homogeneous mixtures with the fuel or localised placement to flatten the neutron flux and increase reactor operational lifetime. These materials are usually dissolved into the coolant of the reactor, sometimes alloys or ceramic forms of the absorber are dispersed throughout the reactor core (Washington, et al., 2014). The rate of burnup of the BP can also be controlled by its positioning with respect to the reactor's neutron flux levels.

Homogeneous mixtures with burnable poisons have several disadvantages (Washington, et al., 2014). First, the decomposition effects experienced by the poison exaggerate those of the fuel, which could exacerbate fuel swelling and the build-up of fission gas products. Secondly, adding the material to the fuel matrix often degrades the mechanical properties of the fuel or fuel alloys, which are already being degraded due to irradiation effects.

Correct placement of BPs can result in the mitigation of some disadvantages when compared with homogeneous mixtures of fuel and BPs. This can be accomplished by, for instance, coating the fuel pellet with a BP.

Seven different BPs were evaluated by Jo, et al. (2009) in a modified General Atomics Gas Turbine-Modular Helium Reactor (GT-MHR) design, these materials were: Boron carbide, Erbium oxide, Europium oxide, Gadolinium carbide, Gadolinium oxide, Samarium oxide and Dysprosium oxide. The natural isotopic compositions of each material was sintered inside a mixture of the BP and graphite. For this study the BPs were placed, in pin form, at the six corner positions of the hexagonal fuel assemblies and also at six internal pin positions inside the fuel block.

The fuel blocks were arranged in an annular configuration and a three batch fuel shuffling scheme was utilised. Three of the burnable poisons; Boron carbide, gadolinium oxide and gadolinium carbide; improved cycle lengths significantly and higher fuel discharge burnups were reached (Jo, et al., 2009). The power reactivity coefficient was negative for all of the burnable absorber cases, this decreased reactivity swing and added inherent safety features.

The use of burnable poisons is one of the conventional approaches to controlling excess reactivity in HTGRs. The use of particle-type burnable poison in both pebble bed reactors and prismatic HTGRs have been reported to effectively control the high excess reactivity and flatten the reactivity swing throughout the whole burnup operation (Trinuruk & Obara, 2015). These results were also confirmed in HTGRs using Uranium nuclear fuel. Trinuruk & Obara (2015) investigated the use of burnable poison particles in HTGRs using Thorium-based fuels to determine whether these particles could effectively improve the safety features of Thorium-based fuel loaded in a small, long life prismatic HTGR. The effects of suppressing excess reactivity during operation and the effect on the temperature coefficient were of primary importance for this study.

It may be shown that the use of Thorium fuel in a prismatic HTGR can have advantageous neutron economics because of the higher neutron absorption cross section of  $\text{Th}^{232}$  compared to that of  $\text{U}^{238}$  in the thermal energy region. This quality results in a higher production of additional fissile  $\text{U}^{233}$ , but could lead to extended periods of high reactivity and a positive temperature coefficient (Trinuruk & Obara, 2015). This study found that the use of particle-type burnable poisons effectively minimises the excess reactivity and flattens the reactivity curve, resulting in a lower burden on the control rods. The use of burnable poison particles was also useful in

reducing the positive moderator temperature coefficient and led to the achievement of a negative core temperature coefficient (Trinuruk & Obara, 2015)

In terms of the neutron economy, Thorium has about a three-fold larger absorption cross section than  $U^{238}$  in the thermal energy region. Therefore,  $Th^{232}$  can convert to fissile  $U^{233}$  more readily than  $U^{238}$  can convert to  $Pu^{239}$  in the Uranium-based fuel cycle. In addition,  $U^{233}$  has an eta-value (ratio of neutrons produced per neutrons absorbed in the fuel for each fission reaction), at thermal energies higher than those of the fissile material  $U^{235}$  and  $Pu^{239}$ . This high eta-value makes the use of Thorium fuel even more attractive from the neutron economy standpoint (Trinuruk & Obara, 2015).

To design a prismatic HTGR under the concept of long-life reactor operation, the loading of large amounts of fissile material was exercised. This resulted in large amounts of excess reactivity at the beginning of operation. This design therefore required large amounts of burnable poisons in order to compensate for the excess reactivity.

### **2.3 Summary**

Various methods of increasing fuel cycle length have been researched and any inconsistencies have been addressed by cross referencing different studies. The studies investigated can be used to predict the effect of different design alterations and the numerical models can be used to verify these predictions or vice versa.

The difficulties experienced by studies which have attempted to address proliferation, political and environmental concerns have been investigated and the difficulty of solving these problems has been demonstrated clearly.

## Chapter 3. Methodology

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### Overview

This chapter provides a detailed description of the methods followed in order to achieve the required objectives of this study. This study will develop a concept design that may be used as a basis for further development if the design proves its worth. The best way of testing a conceptual design is the use of numerical models, for this project the software MCNP will be used in order to numerically predict the outcomes of different variables.

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### 3.1 Development of a concept design

This project was initially started with the simple goal of finding a method which would improve the fuel lifetime of a nuclear reactor. Most of the literature which was studied was done with that goal in mind, until the project could be defined more clearly. Therefore the bulk of the literature studied describes different methods used for increasing fuel lifetimes, conclusions drawn from this research was then used to help further define the project.

Once a few viable methods of achieving the required goal were discussed the scope of this project was expanded. Where it was determined that it would be beneficial to focus on a reactor type which is currently in operation within South Africa, thus a PWR similar to the Koeberg reactors, and to focus on research currently underway at the North-West university.

Due to the university's background of research on homogeneous Thorium fuel designs the scope of this project was altered to focus on Thorium based fuels for PWRs. It became abundantly clear that a lot of research has been done on homogeneous use of Thorium to increase the fuel lifetime of reactors, but research into more complex, heterogeneous designs was limited. A new advanced fuel design was also discussed and it was decided that this dissertation would focus on the study of this design.

This idea was to develop a heterogeneous fuel design by adding Thorium pellets between the Uranium fuel pellets, this could increase the chance for breeding by allowing more thermal neutrons to enter the Thorium. One of the expected benefits of this design is that it could be implemented within any PWR during refuelling as the Thorium pellets can be added to the fresh fuel rods before insertion.

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The above mentioned design was then developed into a concept design which could be numerically modelled and tested. But it was important to keep in mind exactly what could be achieved for this study and the scope and limitations was expanded to accommodate for the available time and resources of this project.

The concept design was developed to determine a system specification for a preliminary design, this design requires geometrical, neutronic and some thermal hydraulic specifications. The concept design could not be developed in a manner by which it is capable of addressing political and legal challenges faced by Thorium-based fuels.

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**

Using numerical models to simulate what would happen in this type of design allows the simulation of arbitrary designs within short amounts of time. Physical testing would cost fortunes and require vast amounts of time. The scope of this project is also not to develop a design which could go directly to physical testing, but rather to determine the possible benefits of the proposed design, further studies will be required to ensure the safety, economic feasibility and practical application of the design.

It was determined that the use of the simulation software MCNP would be the most beneficial for this study as there were many researchers with experience on this software at the time of writing. The accuracy of this program adds to the benefits, although the simulation times are longer than many other codes.

It was decided that the numerical model would simulate only one fuel rod and surrounding materials up to halfway to the next fuel rod, these materials are enclosed within a square geometry as though it were placed within a square fuel assembly. Reflective boundaries would then be created on the outside surfaces of the model, this will simulate an infinite amount of these rods with infinite length to form an infinite reactor with a fuel rod design of our own making.

To decrease calculation times the above mentioned models were modified to include only an eighth (1/8) of the geometry. This was done by cutting a 'pie' shaped section of the fuel rod, when viewed from above, and once again adding reflective boundaries, thereby simulating the entire circumference of the fuel rod.

### **3.2.1 Reference cases**

Reference models were used to verify the results from the numerical models created for this study. The results of the reference models should resemble results obtained from other studies done by other researchers in order to show that the models developed for this study compare well with those developed for previous studies.

For the heterogeneous design good practice would be the use of a homogeneous model to verify the use of Thorium in the system as well as a UO<sub>2</sub> fuelled model to determine the effects of adding the Thorium. The extensive studies completed previously on homogeneous designs and conventional fuels makes it easy to cross reference results from this study with those from previous studies. Verification of the results from models where BPs were implemented have also been done to ensure that the models where these materials were used deliver desirable results.

Once the reference models had been created and tested for verified the knowledge gained from these designs could be used to develop a heterogeneous case with trustworthy results. The results of this model cannot be cross referenced with results from previous studies as this design has not been studied before.

Verification of the heterogeneous models will require some ingenuity, though the use of a homogeneous case increases the accuracy of the results some statistical variations can occur. In most cases the accuracy of the models depend on the ability of the researchers to predict what the expected outcome would be, and if the results differ greatly from what is expected the literature studied should be used to determine validity of the results. Until further tests can be compared with results from this study the verification of results is promoted by theoretical explanations, the use of reference models and the use of neutronic principals.

### **3.3 Optimization**

As expressed in the scope of the project it is not necessary for this design to be optimised up to the point where it can be introduced into physical reactors, but rather to improve on the knowledge of heterogeneous designs. This does include the study of some optimisation concepts which can be used to prove important design factors.

Optimisation steps include verification of the model, the use of the correct data libraries, temperatures, materials, dimensions, statistical parameters as well as the use of the correct burn values.

Iteration is key, statistical variations can occur with the use of too few source points, but too many source particles would require too much time to complete. Testing what level of accuracy is required improves the quality of results and can be used in the verification of the results.

### **3.4 Summary**

The steps that will be followed in order to address the problems stated for this project have been explained. Ultimately it is important to develop a conceptual design which can improve fuel cycle lengths and this design should be tested and verified through the use of numerical models that can be simulated using MCNP.

## Chapter 4. Concept design

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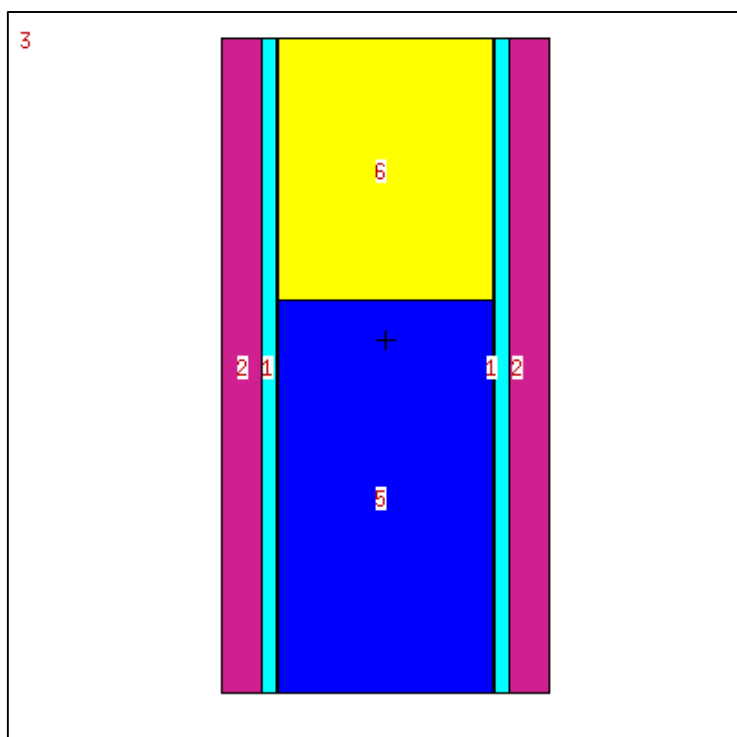
### Overview

A new design has been proposed which utilises heterogeneous Thorium based fuel and further research is required to determine the efficiency of such a design. This chapter introduces the proposed design and attempts to address the expected challenges that have been predicted for this type of design.

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#### 4.1 Proposed concept, Thorium pellets between Uranium pellets

The proposed design is shown in Figure 5:

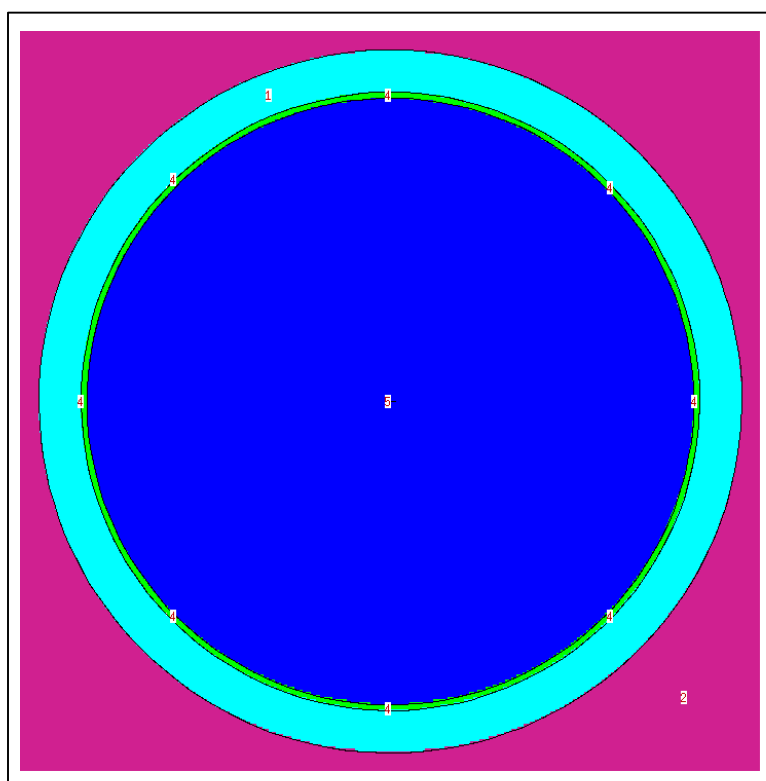


**Figure 5: Front view of numerical model used for MCNP simulations**

The front view of the model shows the six different cells, please be aware that cell 4, the Helium filled gap between the fuel and the Zirconium cladding, is not numbered in this picture due to the size of the image. The following numbers represent the specified materials and parts:

1. Zircalloy-4 cladding at 600K
2. Clean water, H<sub>2</sub>O, at 600K

3. Outside boundary, this cell is required to enclose the model.
4. Helium filled gap between fuel and cladding
5. Enriched  $\text{UO}_2$  fuel (enriched with  $\text{U}^{235}$ )
6.  $\text{ThO}_2$  for breeding, with pure Thorium<sup>232</sup>

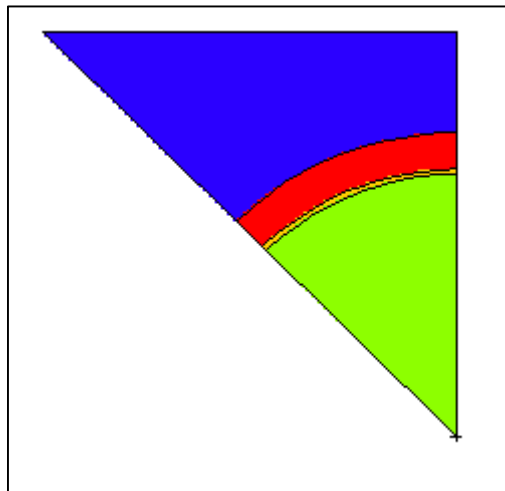


**Figure 6: Bottom view of the numerical model proposed for MCNP simulations**

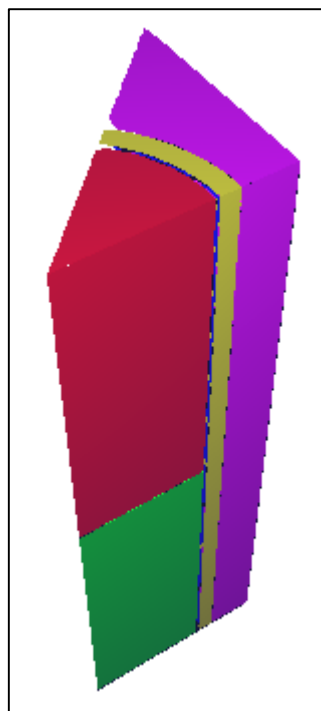
The bottom view of the model shows how the fuel rod is circular, but that the reflective boundaries are rectangular, this creates a more realistic assumption of how a fuel rod would be affected inside a fuel assembly as the assembly is rectangular with even spacing between the rods. The reflective boundaries will therefore simulate this model as an infinitely large fuel assembly inside an infinitely large reactor.

To decrease simulation times the model was divided into an eighth sized section (when viewed from above or below) as demonstrated in Figure 7 and Figure 8. The use of reflective boundaries makes it possible to use such a 'pie' shaped section to simulate the entire circumference of the fuel rod. Furthermore, the reflective surfaces will not only simulate the entire fuel rod, but will infinitely multiply this area in all directions,

which will result in an infinite reactor design. Verification of the results of the full rod versus the eighth model will be done to ensure this method is accurate.



**Figure 7: Top view of eighth sized model proposed for simulations.**



**Figure 8: 3D display of the eighth sized model that is displayed in Figure 7**

Ultimately the numerical models will recreate an infinitely large reactor, the lengths and compositions of the  $\text{UO}_2$  and  $\text{ThO}_2$  pellets can then be altered to change the design of the entire reactor.

The proposed design creates a region of Thorium which can interact with the neutrons in this region without competing against Uranium. In the homogeneous case the atoms of Thorium are scattered within the  $\text{UO}_2$  and the chances of Thorium absorbing a neutron decrease rapidly as neutrons have to pass the U atoms without reacting with them.

At thermal energies the chances of a neutron colliding with a Uranium atom are relatively large, luckily the amount of  $\text{U}^{235}$  is low which increases the benefits of homogeneous fuel, but the breeding potential of homogeneous fuel is still limited due to this competition.

By placing a region of Thorium outside the Uranium it is possible to ensure that more Thorium reacts with thermal neutrons whilst also enhancing the burnup of  $\text{U}^{235}$  as there is no more Thorium to compete with for neutrons.

Beginning of cycle (BOC) excess reactivity is a problem usually solved by adding Boron to the reactor coolant, in a homogeneously mixed Thorium breeder the same counts, but the Thorium decreases the excess reactivity significantly. The same can be achieved with heterogeneous designs, but now with added benefits.

Adding Thorium between the Uranium creates a kind of void between the fuel pellets, this void reduces BOC reactivity, but then uses the neutrons inside this void to breed  $\text{U}^{233}$  fuel. As the reactor operates the amount of  $\text{U}^{233}$  increases whilst  $\text{U}^{235}$  is burned, the burning of  $\text{U}^{235}$  decreases reactivity, but the  $\text{U}^{233}$  compensates for this loss over time, together with some amounts of  $\text{U}^{235}$  which are bred from the  $\text{U}^{238}$  in turn.

For this design the following terminology will be used, x cm Th and y cm U. This depicts the use of x cm Thorium pellets placed inside the fuel rod between y cm Uranium fuel pellets. Therefore the model 2cm Th 5cm U consists of 2cm Thorium pellets placed between 5cm Uranium fuel pellets. Some simplifications have been used, where the "cm" may be omitted in graph legends.

## **4.2 Challenges affecting the concept design**

To further develop the concept design into a workable, practically applicable design certain challenges have to be overcome, these challenges include optimisation steps as well as safety concerns which have to be addressed for final designs. Determining the optimal lengths of Thorium and Uranium as well as the optimal ratio between these

two is the first step, but safety studies provide a much larger and more time consuming challenge that cannot be addressed within this study.

#### **4.2.1 Optimal length of Thorium**

The first variable to consider for this design would be geometry, where the lengths of both the Thorium and Uranium pieces can change. To accurately determine the effect of changing the dimensions it is best to change the length of only one piece at a time.

The effect of the length of Thorium is considered to have the largest effect on the operation of the reactor. As the Thorium creates a void between the Uranium where neutrons can be slowed to thermal energies or absorbed the length of the Thorium has a significant effect on the reactivity of the system.

The most dramatic effect is expected to be shown when the Thorium disk is too long, this would mean that neutrons cannot pass through this area, thus all neutrons which would have passed between the Uranium pieces disappears. Though this means that a lot of neutrons will be absorbed with the possibility of breeding it also has the massive drawback that the reactor cannot maintain criticality.

When the Thorium is too short it would mean that the neutrons can pass freely between the Uranium, this increases the excess BOL reactivity and would require more Boron within the coolant and more control rod control worth. A short Thorium piece would also allow most of the neutrons to pass through without being slowed and the probability that the neutrons will be absorbed in the Thorium for breeding decreases drastically.

This makes it extremely important to determine which length of Thorium would allow sufficient amounts of neutrons to pass through in order to maintain criticality, whilst also allowing some neutrons to be slowed to thermal energies or get absorbed by the Thorium.

#### **4.2.2 Optimal ratio of Thorium/Uranium**

In order to breed a large amount of  $U^{233}$  Thorium has to be exposed to neutrons over a long period of time, if the reactor cannot maintain criticality breeding would be impossible as the reactor would never be capable of producing the required amount of neutrons. Due to the absorption of neutrons inside the Thorium the amount of fuel, i.e. the amount of source neutrons, should be sufficient.

This would mean that, if the reactor has too much Thorium relative to the amount of Uranium, then the reactor would not be capable of maintaining criticality until sufficient amounts of breeding have taken place. Whereas having a reactor with too much Uranium would mean that the breeding effect is minimalised and the amount of excess reactivity is difficult to reduce.

An important factor to consider is that when there is more Thorium, there is more fissionable material which can be used for breeding, one method of using more Thorium with less Uranium would be to increase the enrichment of the Uranium. This would allow the reactor to maintain criticality with an increased breeding ratio, but increasing the amount of enrichment can be a very expensive task with lot of legal hurdles.

A best case scenario would be a ratio of Thorium/Uranium that does not require excessively high enrichment whilst allowing for the maximum amount of Thorium to be added.

#### **4.2.3 Excess reactivity and energy peaks**

One of the bigger challenges for a practical design in this project is the appearance of energy peaks in the regions where the Thorium and Uranium are in contact, in this region thermalized neutrons pass from the Thorium into the Uranium and immediately get absorbed within approximately the first centimetre of Uranium. If the neutrons which are absorbed undergo fission it creates a large energy- and thus temperature spike in the contact area. These energy peaks can cause considerable side effects if they are large enough, if the heat is transferred to the water it could create spots where local boiling is experienced. The resultant voids created would drastically affect the moderation of neutrons and the reactor's inherent safety features should shut it down at that moment.

The first solution to this problem that comes to mind is the use of burnable poisons, at the beginning of a reactor life cycle there is still no  $U^{233}$  inside the Thorium. Due to the small absorption cross section of Thorium compared with that of  $U^{235}$  or  $U^{233}$  neutrons get scattered rather than being absorbed. But when this region is filled with  $U^{233}$  the chances that a neutron will be absorbed are significantly higher, thereby decreasing the energy peaks.

Therefore controlling the BOL movement of neutrons by adding burnable poisons inside the Thorium one could possibly decrease the energy peaks whilst still allowing sufficient amounts of breeding to decrease these peaks after a short operation time. Alternatively burnable poisons (BP) could be added to the first centimetre of Uranium which is in contact with the Thorium to absorb the neutrons which could create the peaks.

Even a balanced solution could be proposed where a centimetre of BP is added which is centred over the contact area between the Thorium and Uranium pieces. A final solution to this problem could not be developed within the given time for the project, although some tests were run to investigate the initial proposals, further testing is of utmost importance.

One more solution could be the addition of a cone shaped Uranium region, this region would penetrate the Thorium and add to the length of the Uranium. The benefits of this proposal require much more research, but a few tests were run to determine the effects of this design.

The cone addition came to mind during testing and evaluation of the thermal neutron flux within the fuel rod, the flux distribution itself makes a cone-like profile inside the Thorium region. Filling this profile with Uranium could be more effective for breeding  $U^{235}$  out of  $U^{238}$  than breeding  $U^{233}$  out of the Thorium, but only for this small region. It should be noted that the practicality of the fabrication of such a design is not taken into consideration and falls outside of the scope of this study.

Challenges which will not be approached in this project are those of political, economic, legislative or environmental background. Solving, or even simply discussing these challenges together with designing and testing different models would require far more time and resources.

### **4.3 Summary**

The proposed design which has been created is shown here, this design has been adapted into a numerical model which can be simulated within MCNP as an infinitely large reactor by using reflective surfaces. An eighth sized model been developed to reduce simulation times. Some challenges opposing the use of this design have been addressed. Furthermore these challenges have been converted into objectives by designing the model to reduce the negative effects of these challenges.

## Chapter 5. Results

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### Overview

The results of many numerical models and tests are shown in order to demonstrate the effects of the proposed design. The use of different fuel cycle lengths, coupled with the set  $k^\infty$  value for criticality is displayed in order to determine design parameters which can be used for further development.

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### 5.1 Reference cases

The following reference cases were used. By completing reference studies we can determine the benefits/weaknesses of the heterogeneous models. Reference models can easily be matched with models from literature to help verify the results from this project.

All of the models which were created have been modelled with dimensions similar to that of models previously tested by other researchers, but due to time constraints the models could not have too much geometric complexity. The designs chosen were those of She, et al. (2014) and Thor Energy, Norway (2012). The article by She, et al. (2014) describes geometric data efficiently and shows results of their burnup over time tests, which is exactly what is required for this project, therefore the geometry of their model will be used.

The simulations of Thor Energy, Norway (2012) are based off the Ringhals 3 reactor in Sweden, of which, the geometry is not specified and further details could not be obtained. But the power density of their model is included and will be used for this projects "burn" function. Thor Energy, Norway (2012) researched the use of homogeneous Th-MOX fuels and describes enough detail about the design that this study can be used for reference models, with the added benefit of BP models also being included.

The concept design specifications which have been used for all of the simulations (except the homogeneous reference model) are listed in Table 1.

**Table 1: Design specifications used for numerical models**

Parameter	Value and units
Fuel pellet radius	0.4096 [cm]
Cladding inner radius	0.4178 [cm]
Cladding outer radius	0.475 [cm]
Pin pitch	1.26 [cm]
Fuel density	10.2 [g/cm <sup>3</sup> ]
Cladding density	6.55 [g/cm <sup>3</sup> ]
Coolant density	1.003 [g/cm <sup>3</sup> ]
Power density	105.5 [W/cm <sup>3</sup> ]
Enrichment	3.1wt% U <sup>235</sup>

The homogeneous reference case which was modelled has some slight alterations with regard to the design specifications of all other models, these alterations are shown in Table 2.

**Table 2: Design specifications employed by the reference homogeneous model (only those that differ from the other models are displayed)**

Parameter	Value and units
Fuel pellet radius	0.556 [cm]
Cladding inner radius	0.5642 [cm]
Cladding outer radius	0.6214 [cm]

In many cases the temperatures of different materials were not the same for all reference models or heterogeneous models, therefore this parameter could not be included in Table 1. The temperature values for the reference cases are described in Table 3 and the respective values for the different materials inside the heterogeneous design are demonstrated in Table 4. Cross section data was evaluated at the specified temperatures in accordance with MCNP data tables.

**Table 3: Temperatures of all materials inside the various reference models**

Model	Temperature
UO2 first reference	300 K
UO2 reference with BP	600 K
Th-MOX reference	600 K

**Table 4: Temperatures of materials utilized in heterogeneous models**

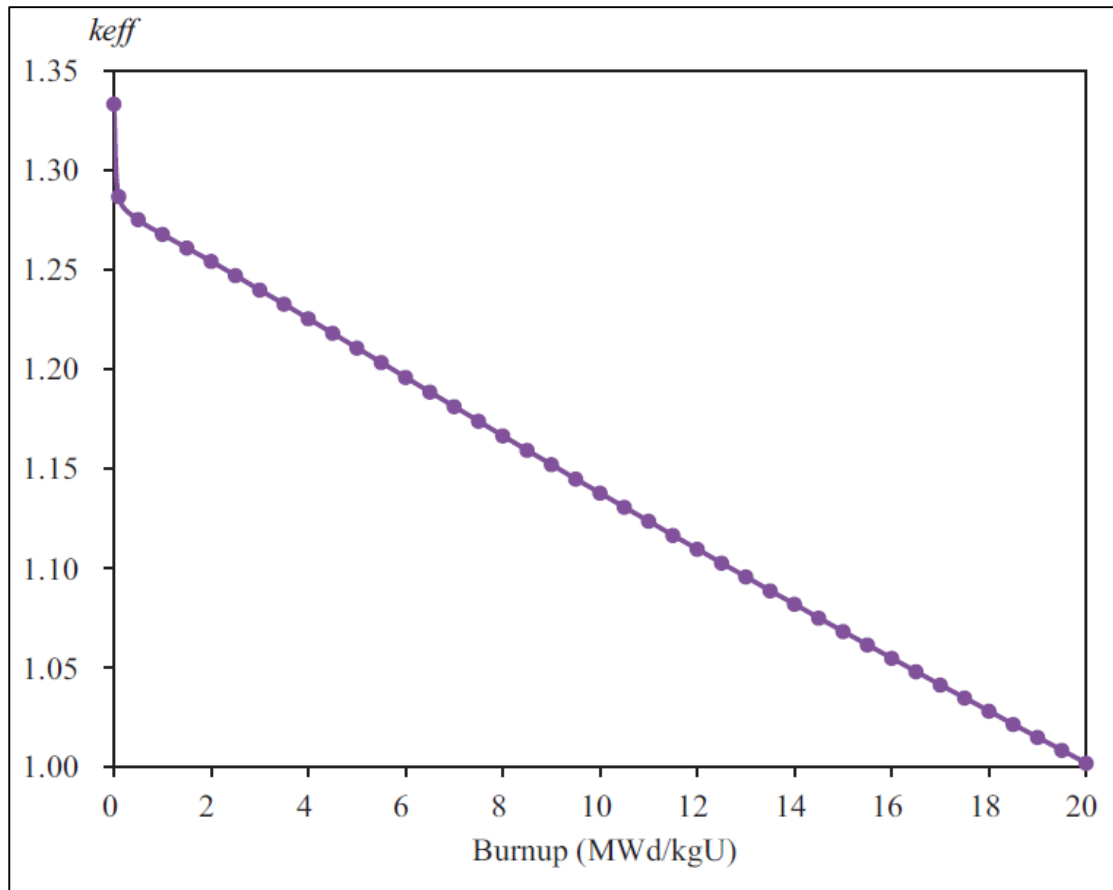
Material	Temperature
Coolant	600 K
Cladding	600 K
Helium gas	600 K
Fuel	900 K

The material libraries which were used for all models were developed in such a manner that each material contains the isotopes which are found to be the most abundant in natural mixtures of the material, except in cases where the material has been enriched with a certain isotope. Isotope information was gathered from (Winter, 1993-2015).

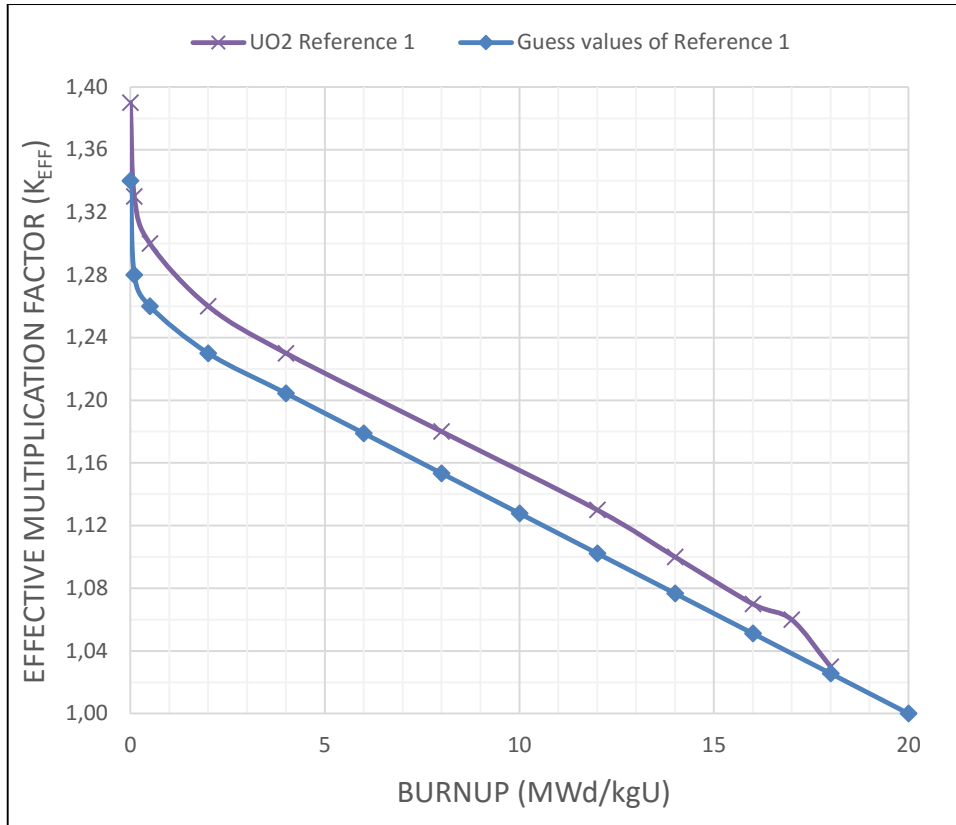
### 5.1.1 Uranium dioxide (UO<sub>2</sub>) reference

A reference model which contains UO<sub>2</sub> fuel with no Thorium or Boron was created as well as a model which does contain Boric acid as well. By determining the infinite multiplication factor ( $k^\infty$ ) which such a reactor would have at any specified time it is possible to set an operational limit for each Thorium model. That is, if the reactor power has to be reduced on day 480 due to the  $k^\infty$  value of the UO<sub>2</sub>, then the Thorium fuel should maintain a  $k^\infty$  value higher or equal to the  $k^\infty$  value of the UO<sub>2</sub> model on day 480.

The first reference model was set up to be compared with the results of She, et al. (2014). It is important to note that these model used full core calculations, the relevance of using this reference is that, if the models developed for this study compare well with those of She, et al. (2014), then it may be assumed that the use of an infinite reactor is sufficient for preliminary tests.



**Figure 9: Dependence of  $k_{eff}$  over time due to burnup evaluated by (She, et al., 2014)**



**Figure 10: Comparison of results from UO<sub>2</sub> reference model with those of (She, et al., 2014). Values were adapted from Figure 9 to better compare the graphs.**

By comparing the above figures it is clear that the forms of the graphs are the same, but that the infinite reactor model starts at a higher multiplication factor. This is due to the zero leakage experienced by an infinite reactor, opposed to the full core simulation which allows neutron leakage out of the system.

The second reference model was modelled with the same geometry, but with 600 ppm Boric acid added to the coolant, the same as that of the tests run by Thor Energy. There is a slight temperature difference between the temperatures used, where Thor Energy, Norway (2012) used 575 K, but the temperature closest to this within the MCNP data tables is 600 K, therefore 600 K was used for the reference models (Thor Energy, Norway, 2012).

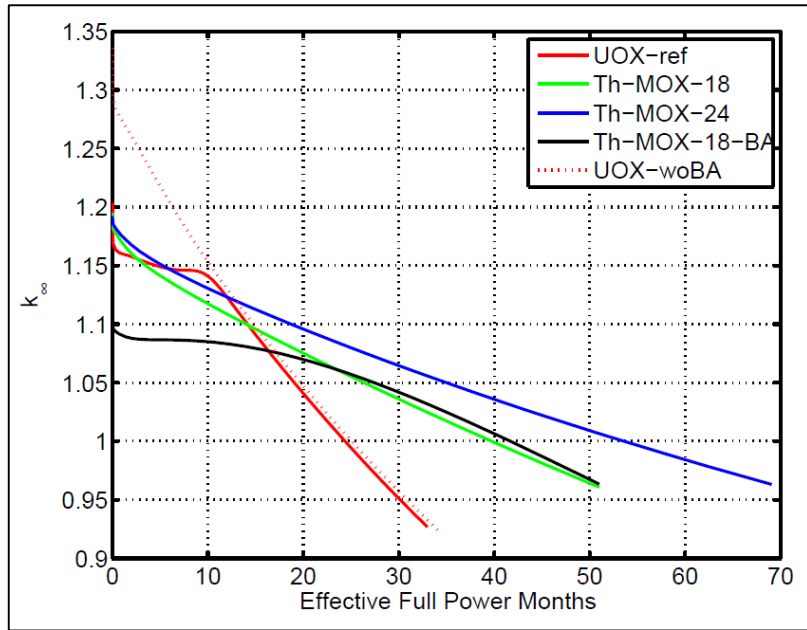


Figure 11: Dependence of  $k_{\infty}$  over time due to burnup evaluated by (Thor Energy, Norway, 2012)

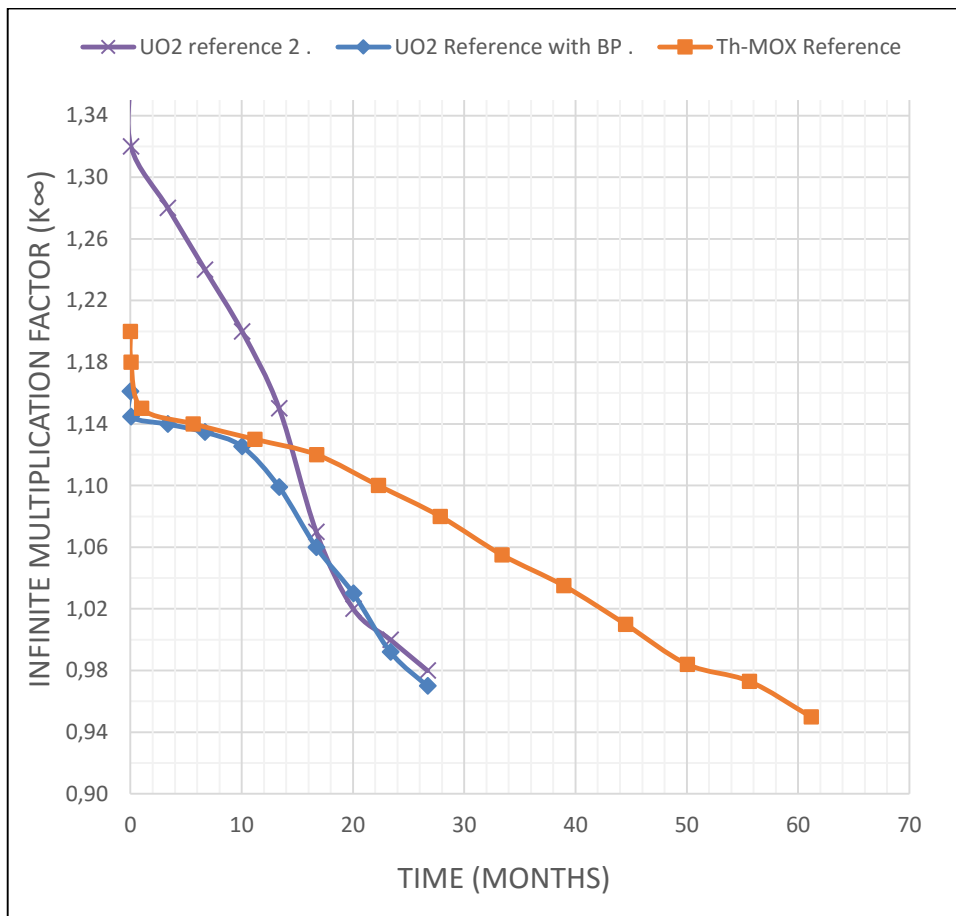


Figure 12: Results from UO2 and Th-MOX Reference models.

By comparing Figure 11 with Figure 12 one can determine that the models created for this project are accurate as the results are closely related, some statistical deviation is expected and could be the reasons for the small differences in the  $k^\infty$  values of the different models. The use of Boric acid also looks successful.

### **5.1.2 Homogeneously mixed Thorium dioxide (ThO<sub>2</sub>) reference**

The homogeneous Thorium reference model can be used to determine the benefits/weaknesses of the heterogeneous designs. The use of reference models is required to determine the validity of results from models developed for this study. The results of this model are displayed in Figure 12 and should be compared with those of Figure 11.

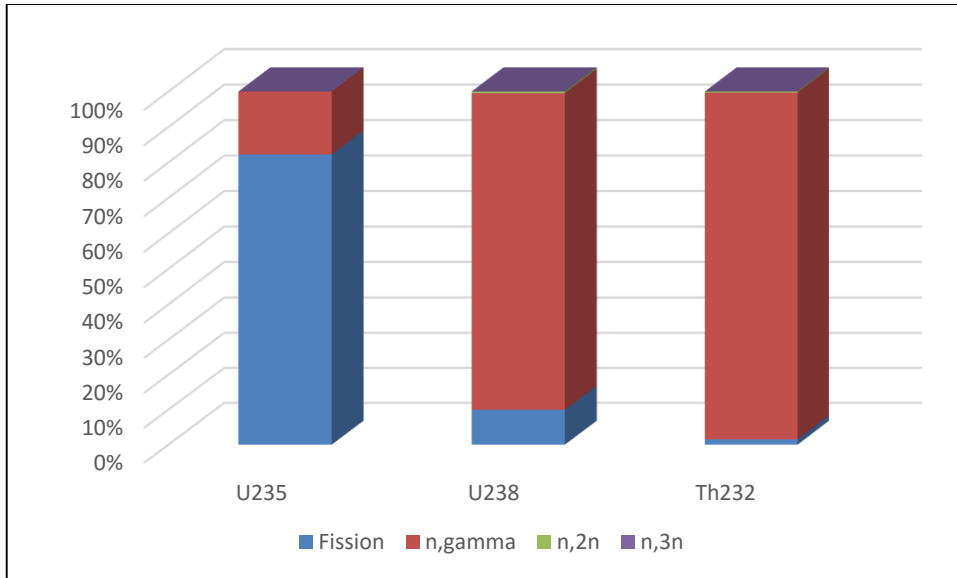
The reference model created for this study is similar to the Th-MOX-24 model simulated by Thor Energy, Norway (2012). The reference model was not burned for the same amount of time, but rather only for 60 months, which should be sufficient for the required verification.

The correlation between the models seems sufficient to assume that the Thorium interactions of our reference model are acting as required and that this knowledge can be applied to heterogeneous models.

One benefit of using heterogeneous designs would be that the Uranium and Thorium atoms do not compete for neutrons, in the homogeneous design this is not the case. Rather the Thorium competes with U<sup>238</sup> as the fission cross section of U<sup>235</sup> is exponentially larger than the absorption cross section of Th<sup>232</sup> at thermal energies.

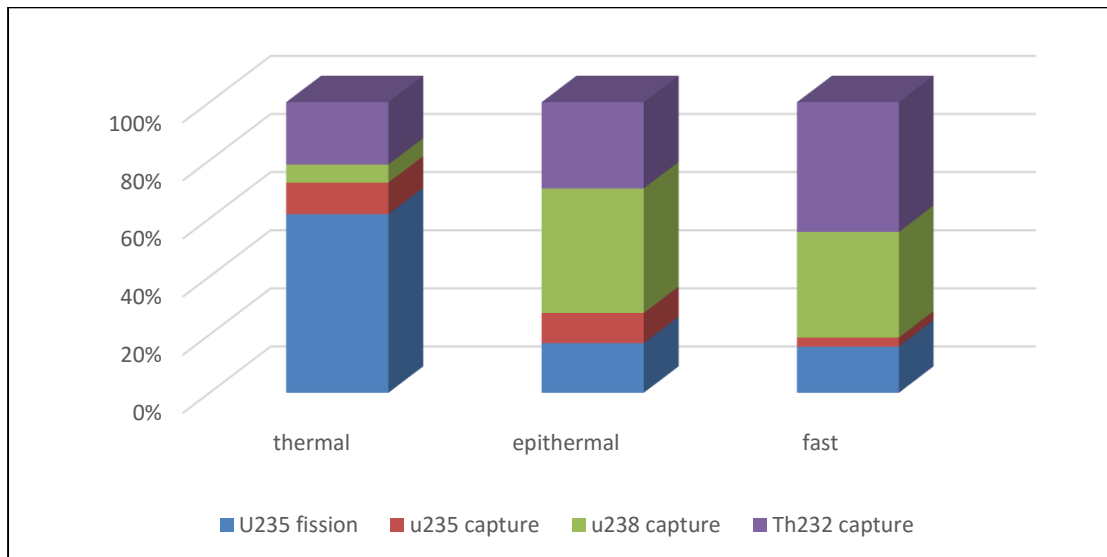
By using isotopic reaction rate tallies it is possible to determine the probability that reactions will take place in the materials, this information can be expanded to different energy levels for the different materials and reactions. These tallies were set up to measure reaction rates inside the ThO<sub>2</sub>-UO<sub>2</sub> homogeneous mixture

The following figures describe the percentage chance for reactions to take place within the homogeneous model, this information is normalised to 100% in order to show the isolated effects of the materials and reaction rates rather than values. In essence each bar shows the contribution of each reaction inside a material or vice-versa.



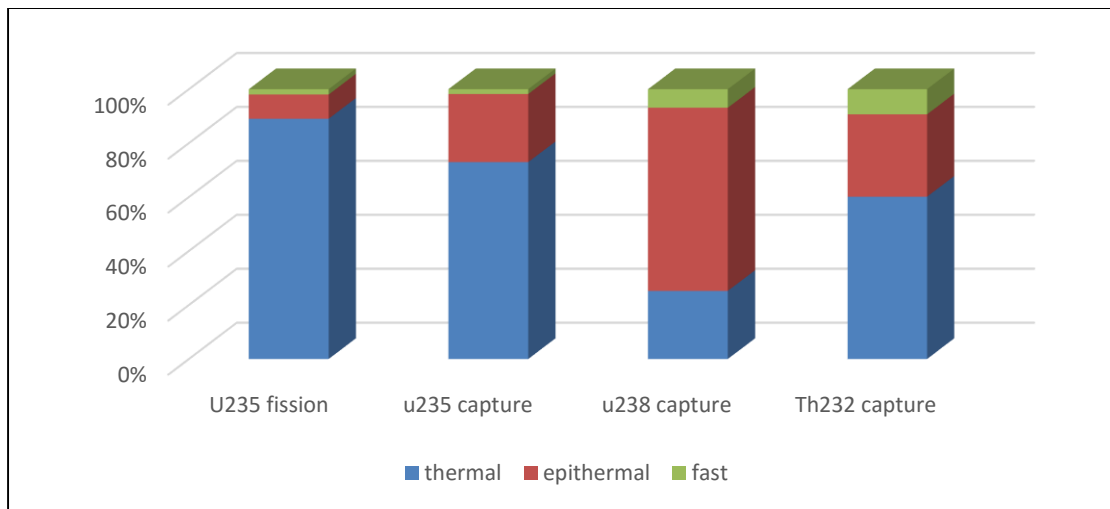
**Figure 13: Reaction rate tallies for the homogeneous reference model, the most important materials are listed and their different rates for reactions are graphed.**

Figure 13 shows that the chance for  $U^{235}$  to fission is significantly larger than the chance that it would capture neutrons.  $U^{238}$  would most likely capture neutrons, but there is a chance for fission reactions, whereas it seems that  $Th^{232}$  would virtually always capture neutrons in a (n,gamma) reaction.



**Figure 14: Reaction rate tallies for the most important materials, the neutron energies are listed and the different reactions for each material are graphed.**

Figure 14 shows how, in the thermal region (defined as any energy below 0.625 eV, the same that MCNP uses)  $U^{235}$  will absorb most neutrons in fission reactions. The epithermal region (0.625 eV – 100 keV) is dominated by  $U^{238}$  captures where the Th-232 leads the fast neutron (any energy above 100 keV) consumption. It is important to note that, judging by the graphs, the total probability that  $Th^{232}$  will capture neutrons over all energies is slightly larger than the probability that  $U^{238}$  will do so, but the values can be orders of magnitude different and this should not be accepted as the case without further research of the tally count values.



**Figure 15: Reaction rate tallies for material reactions, these values are dependent on the energy groups of the neutrons**

Figure 15 demonstrates the probability that a reaction will take place at a specified energy level. This shows that  $U^{235}$  fissions will most likely occur in the thermal energy group, but this is also true for  $U^{235}$  captures.  $U^{238}$  captures will occur most at epithermal energies whereas  $Th^{232}$  captures dominate in the thermal energy range.

This makes it important to take note of the probability that a certain reaction will take place, such as how the chance that  $U^{235}$  fission will take place rather than a capture reaction due to the difference in cross sections, this is demonstrated in Figure 13. Ultimately it supports the theory that exposing  $Th^{232}$  to high thermal flux values will promote conversion through capture reactions.

The following table describes the values of the isotopic reaction rate tallies (units are tally count / source neutron / cm<sup>2</sup>). By analysing Table 5 it is clear that U<sup>235</sup> fission reactions will dominate the thermal energy range, but second to these, Th<sup>232</sup> captures will take place. These results strengthen the requirement that Uranium and Thorium be separated instead of competing for neutrons.

**Table 5: Isotopic reaction rate tally counts for the different material reactions at different neutron energies.**

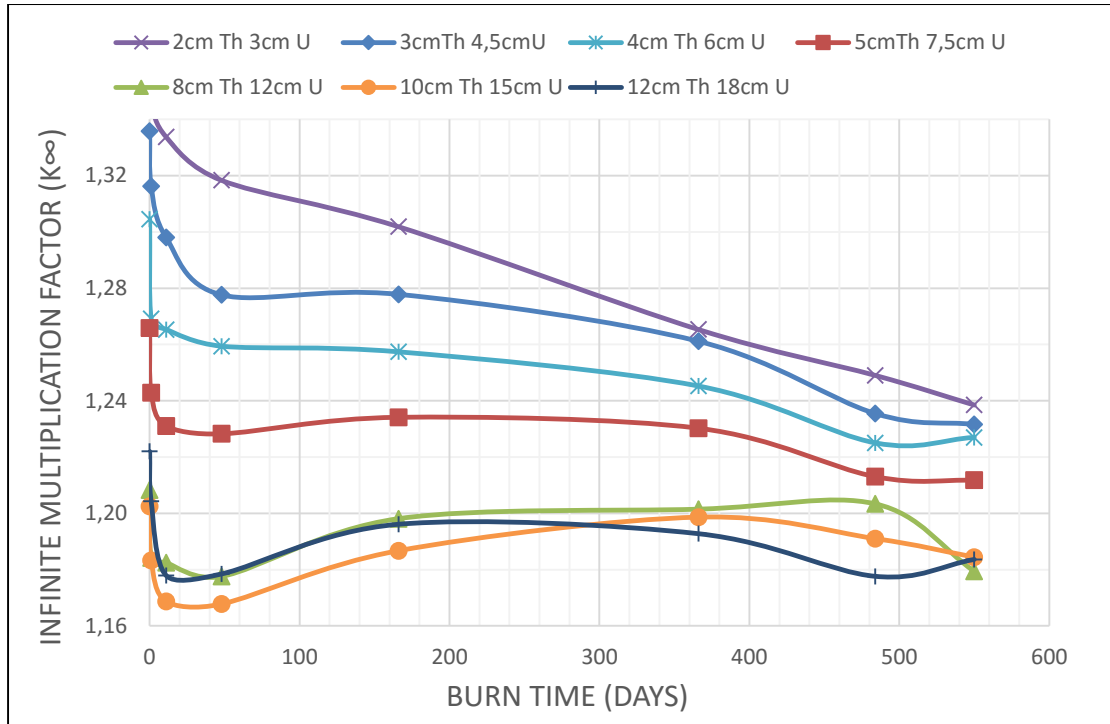
Energy range	U-235 fission	U-235 capture	U-238 capture	Th232-capture
Thermal	0.5153	0.0911	0.0527	0.1818
Epithermal	0.0520	0.0316	0.1418	0.0924
Fast	0.0114	0.0022	0.0144	0.0282

## 5.2 Determining the optimal length of ThO<sub>2</sub>

A simple procedure can be followed to determine the optimal length of Thorium, simply use the same ratio every time and model different lengths. To be thorough it would be beneficial to iteratively cross reference optimal length tests with optimal ratio tests.

This would require determining a satisfactory length of Th, finding a satisfactory ratio of Th/U and then using this ratio in further tests to determine a better Th length and this process can be repeated until the researchers are confident in the values. For the purpose of this project, to design and explore a concept, iterative tests will not be done, but further tests could be beneficial for a detailed design.

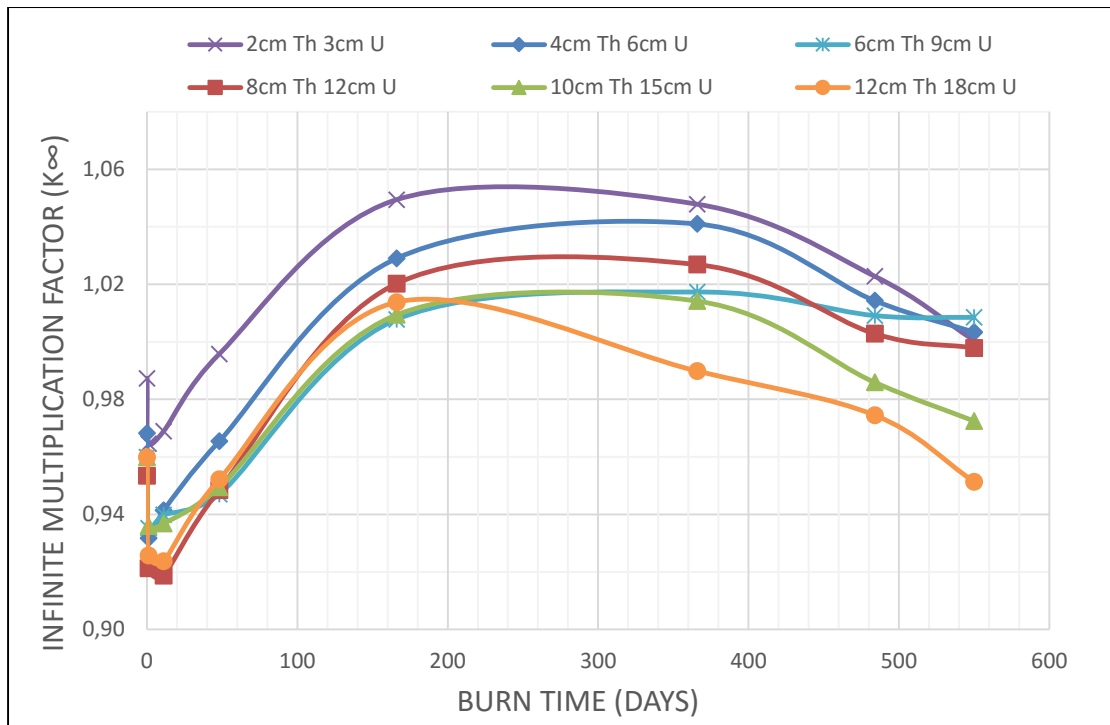
For the first attempt at finding the optimal length an arbitrary ratio of Th/U was chosen, this would be 2Th/3U, which is the smallest ratio that has been tested within this study. Different lengths of Thorium were modelled with this ratio and the enrichments were set to 4.5wt% U<sup>235</sup>, initially no Boron was added but further tests used Boron to decrease the excess reactivity at BOL.



**Figure 16: Burnup over time for different Thorium lengths with a ratio of 2Th/3U, equal enrichments and no Boron.**

The results shown in Figure 16 were used in conjunction with those of Figure 17 to determine a conceptually optimal length for the Thorium. Analysis of Figure 16 shows that 5cm Thorium would be the best choice as the difference between the day 11 and day 550 values for this model were the smallest of all the models. There were also no drastic reactivity swings as in the cases of models with 8cm or more Thorium.

Due to the high excess reactivity at BOL and the possibility that the addition of Boron would affect the optimal length of the Thorium, the next tests were modelled with Boron homogeneously mixed inside the ThO<sub>2</sub> region. The amount of Boron to be used was difficult to determine without any previous tests and iterative tests were run, starting at 0.1% Boron and doubling this value. When a value of 0.4% Boron was reached it had become clear what the effect of Boron would be on the system and this concentration was used for the results demonstrated in Figure 17.



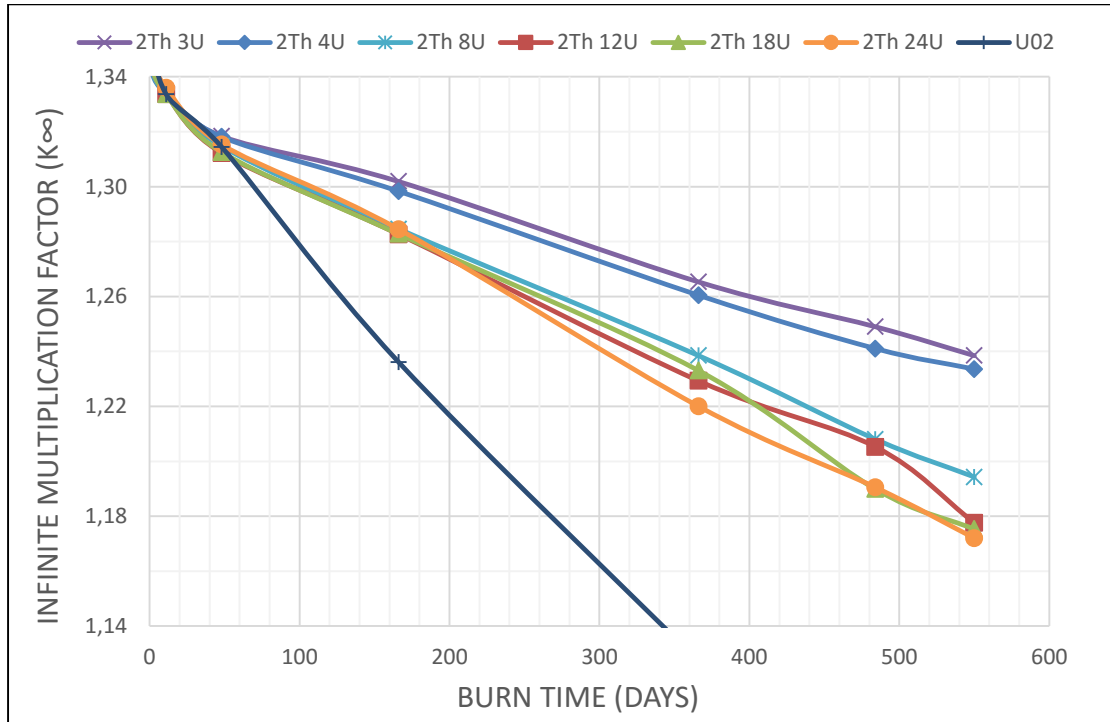
**Figure 17: Burnup over time for different lengths of Thorium with ratio of 2Th/3U, equal enrichments and Boron concentrations, the Boron is homogeneously mixed within the ThO<sub>2</sub>**

The results of these models showed that having more than 6cm Thorium would negatively affect the reactor, whereas less than 4cm would also reduce the lifetime. The median value of 5cm Thorium, which also showed promise in the previous test was chosen as the conceptual optimal length of Thorium until further development is required.

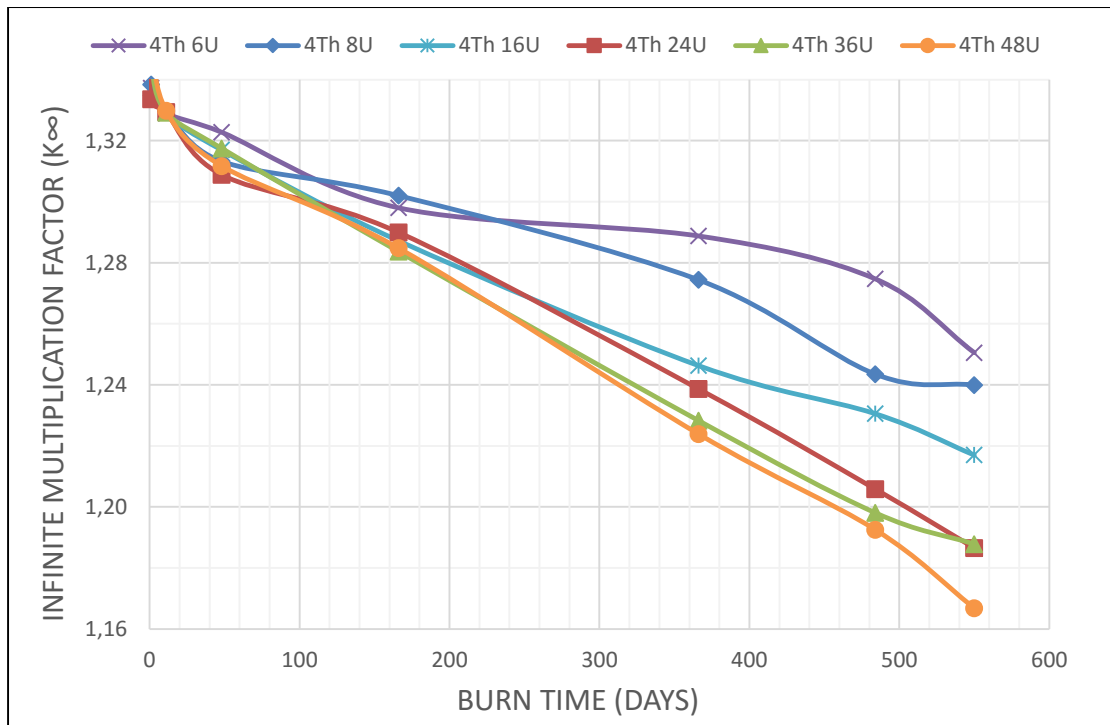
### 5.3 Determining an effective ratio of Thorium to Uranium

Two methods of determining which models are more effective have been used in this project, the first was the use of average gradients, i.e. looking at the difference between the day 11 and day 550  $k_{\infty}$  values. A model which has a smaller average gradient, therefore a smaller difference between the two values stated would be more efficient as it would mean that that specific model either burned less fuel or converted more material to fuel than the ones with larger differences. This method was used in the above tests.

The second method is the use of normalization, where instead of determining or looking at the gradients of each graph one could alter the models to have the same  $k^\infty$  values at a specified time. This can be done by changing the enrichment of each model, once this can be achieved it is easy to determine which model has the best burnup as this would be the model with the highest  $k^\infty$  value at the end of burnup.



**Figure 18: Burnup over time for models with 2cm Thorium and different lengths of Uranium, therefore different ratios of Th/U. No Boron was added but the enrichments were altered to normalise the  $k^\infty$  values of each model on day 11**

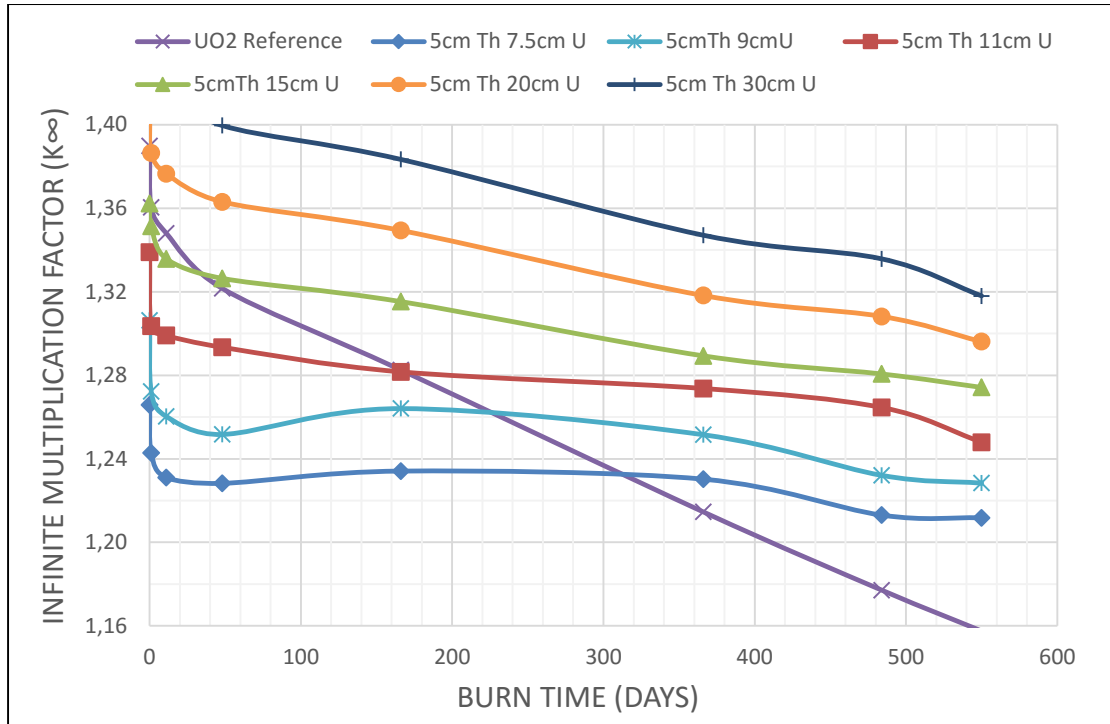


**Figure 19: Burnup over time for models with 4cm Thorium and different lengths of Uranium, therefore different ratios of Th/U. No Boron was added but the enrichments were altered to normalise the  $k_{\infty}$  values of each model on day 11**

Simple tests were run with arbitrary lengths of Thorium (these tests were run before it was determined that 5cm Thorium should be used) and varied lengths of Uranium in order to determine the effects of altering the ratio between the materials. It soon became clear that the solution to this question was quite simple, more Thorium equals more breeding.

The enrichments of the above models were altered iteratively until their day 11  $k_{\infty}$  values were approximately equal to that of the reference  $\text{UO}_2$  model on day 11. Day 11 was chosen as this value would be significant in tests which include Boron as it is expected that most of the Boron would have burned away by day 11.

It is assumed that changing the enrichments of the fuel will not have an effect on the gradients and therefore, the final  $k_{\infty}$  values of the models. This assumption can be made as long as the amount of Thorium is not exaggerated. All of the models tested could maintain criticality for at least a month at low enrichments. If the model has too much Thorium to maintain criticality then increasing the enrichment to the point where it can continue operating would be a futile exercise.



**Figure 20: Burnup over time for 5cm Thorium and varied Uranium sizes (12.7 a/o% U and no Boron)**

Increasing the length of Uranium increases the reactivity at BOL, this increase coupled with a slow reduction of  $k_{\infty}$  value would then result in higher  $k_{\infty}$  values at the end of life. Using the average gradient approach and looking at the difference between day 11 and day 550  $k_{\infty}$  values one can determine which model has the best breeding.

Although it is possible to use the design with 5cmTh and 7.5cm U for its breeding potential it is still important to consider that this design would require a high enrichment in a real reactor. We believe that an enrichment of above 15% would be required, using this value would be political suicide and a design which requires lower enrichments should be chosen.

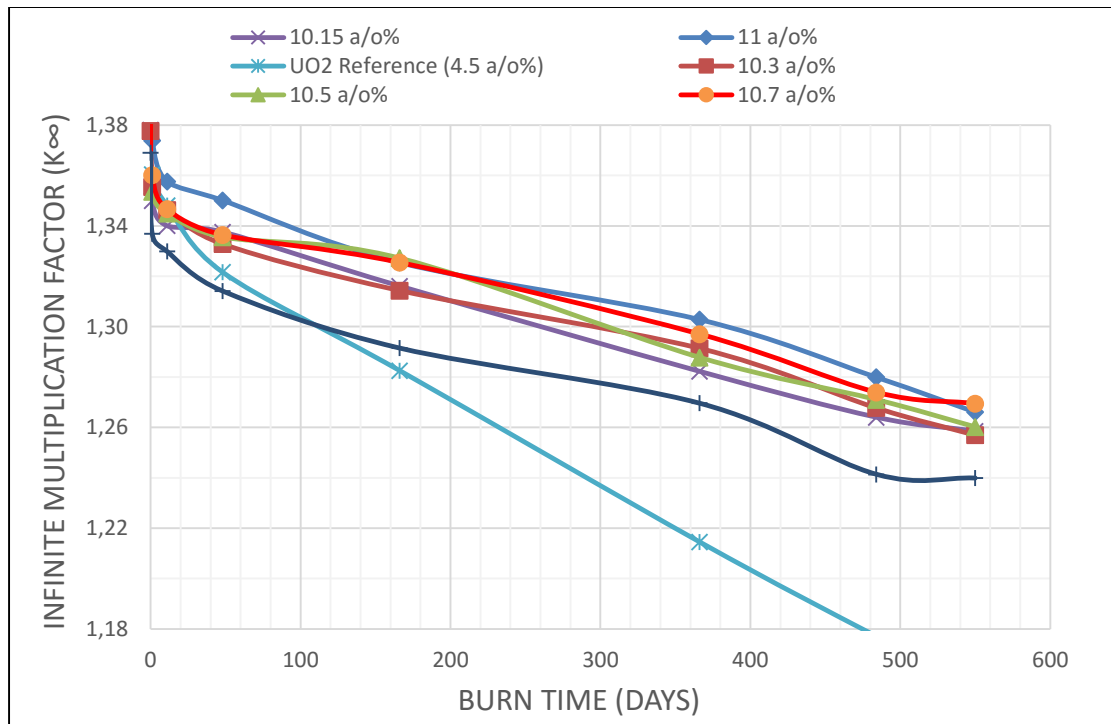
The designs considered are 20 and 30cm U as these designs would require the least enriched Uranium, but still have at least half the slope of the reference. For the purpose of this project no further research as to which of these models would be best was completed and 20cm U was arbitrarily chosen to allow more time for continuing other tests which may have more importance and academic value

### 5.4 Determining enrichment required for a conceptual design of a 18 month cycle

With the lengths being conceptually optimized it is time to move on to the goal of the project, determining whether this design can be used to increase fuel lifetime. The reference UO<sub>2</sub> design is extremely important for this outcome.

In accordance with the case study provided in section 1.3 on day 480 the UO<sub>2</sub> reactor power level has to be decreased. This means we can make the assumption that the  $k^\infty$  value of the reference model on day 480 resembles a value which is too low for operation. Looking at Figure 21 of the UO<sub>2</sub> reference model this value can be determined to be approximately 1.18.

This means that, in order to ensure full power operation for 18 months, the conceptual heterogeneous design should have a  $k^\infty$  value of 1.18 at month 18. To achieve this value is easy if any enrichment can be used, but determining the lowest required enrichment now becomes a priority as it is difficult to use enrichments above 10%.



**Figure 21: Burnup over time of 5cm Thorium and 20cm Uranium model. The enrichments were iteratively altered to attempt to determine what enrichment would deliver the required  $k^\infty$  value at day 550**

The results of Figure 21 demonstrate that the enrichment can still be lowered below 9% and the  $k_{\infty}$  value is expected to be sufficient with this design. But before these tests were run it seemed more beneficial to push the design further, developing a 24 month cycle would prove more beneficial. As a first outcome for this study it can be stated that using a design of 5cm Thorium placed between every 20cm of Uranium one could achieve an 18 month cycle with excess reactivity to spare with Uranium enriched to 9wt%.

### 5.5 Increasing fuel reloading cycles to 24 months

Expanding upon the outcomes of the project it would be beneficial to design a 24 month cycle. The 5cm Th 20cm U design has been modelled with different enrichments to determine what enrichment would be required to achieve 24 months of operation.

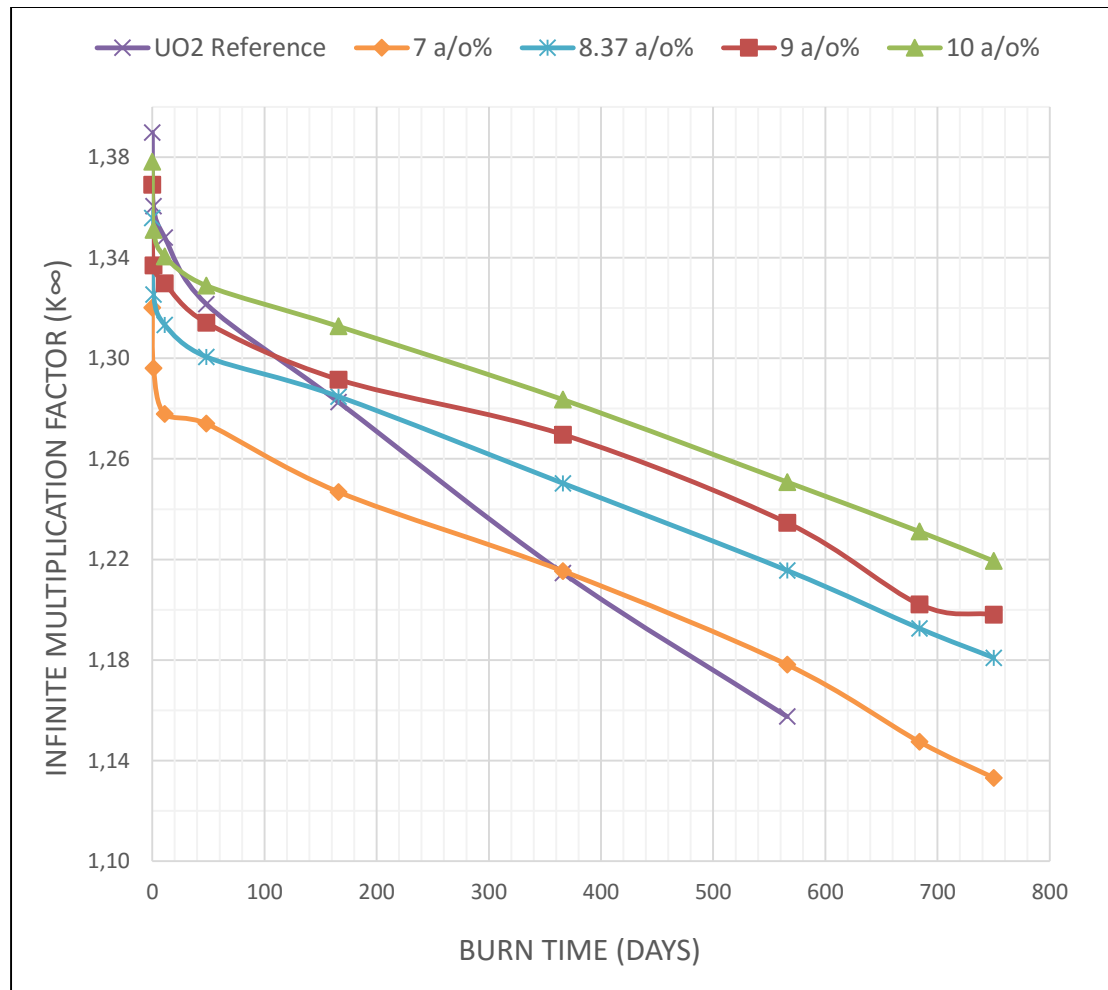
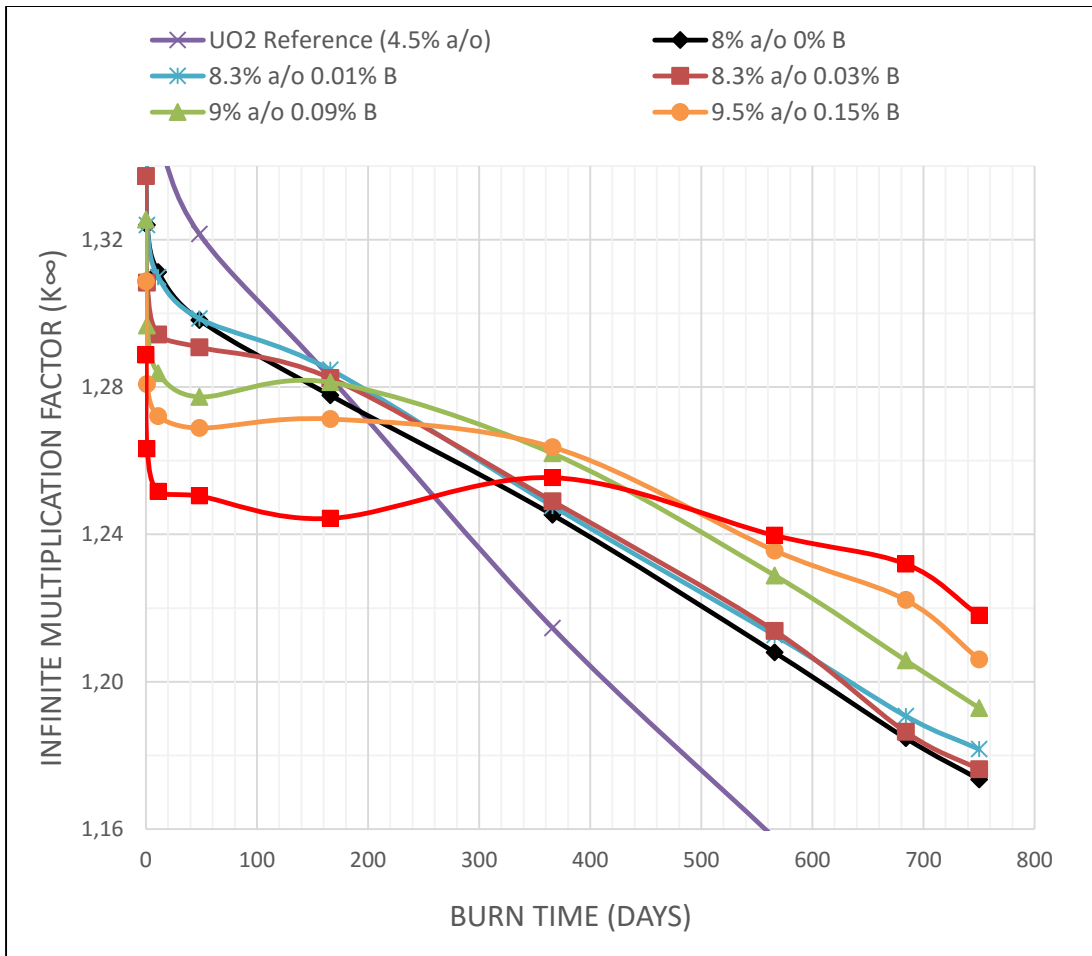


Figure 22: Progression of  $k_{\infty}$  with burnup for 5cm Th and 20cm U model with different Uranium enrichments over a 24 month duration

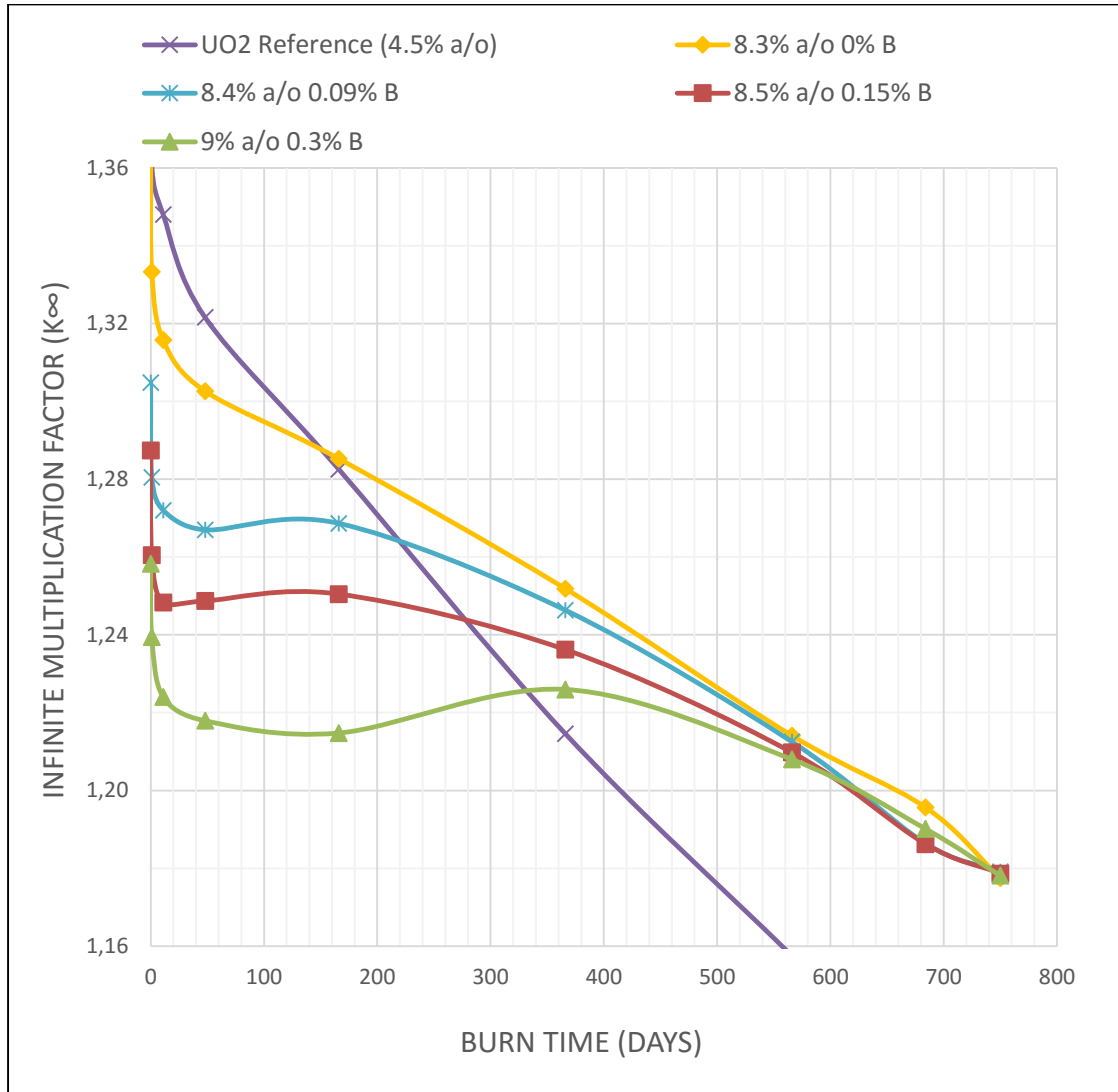
Figure 22 demonstrates that a 5cm Th 20cm U design with 8.37wt% U<sup>235</sup> can be used to achieve a 24 month fuel lifetime, but excess reactivity could pose a problem for further design. Tests with Boron poisoning were completed to determine the effects of Boron on the final k<sup>∞</sup> value and which amount of Boron would be required. Different amounts of B<sup>10</sup> was homogeneously mixed within the ThO<sub>2</sub> of the 5cm Th 20cm U design. Boron can still be added to the water as is done with most reactors, but this negatively affects the reactivity coefficients of water and therefore having the Boron inside the fuel rod could be more beneficial.



**Figure 23: Progression of k<sup>∞</sup> with burnup for 5cm Th and 20cm U model with different Uranium enrichments and Boron concentrations**

At first it was expected that the Boron poisoning would greatly affect the reactivity at the end of the fuel cycle, but the results show that only excessive amounts of Boron had significant effects on the k<sup>∞</sup> value at day 750. In the models with excessive amounts of Boron, the Boron was not completely burned after a few days and kept poisoning the reactor for long periods of time.

Enrichment values were guessed at this stage, but overcompensating for the Boron poisoning led to different  $k^\infty$  values at the end of life. Further studies were required to determine Boron concentrations and enrichments which would have the required  $k^\infty$  values at end of life



**Figure 24: Progression of  $k^\infty$  with burnup for 5cm Th and 20cm U model with different Uranium enrichments and Boron concentrations (second iteration)**

Further studies were completed to determine the enrichments which resulted in the same end of life  $k^\infty$  value with different Boron concentrations and U enrichments. These results show that Boron has very little effect on end of life reactivity when used in small concentrations, but large quantities of Boron do not burn out fast enough and the amount of enrichment required grows exponentially.

Beginning of life excess reactivity is decreased drastically, even with very small Boron concentrations and therefore more research could be beneficial, but within the scope of the project this research will be omitted and focus is placed on the k value of the models on day 750, which is approximately 1.18 as required, therefore, success!

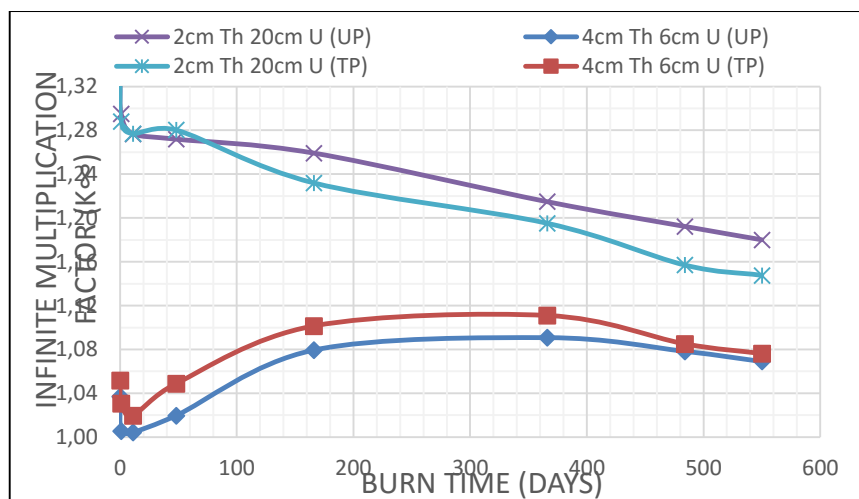
The above results can be further explored to determine which amount of Boron would be necessary, then the amount of Uranium can be adequately adjusted. But as a project outcome it can be stated that the use of a heterogeneous fuel design comprising of a 5cm Thorium pellet placed between 20cm Uranium fuel pellets with 8.5wt% U<sup>235</sup> enrichment and 0.15wt% B-10 inside the Thorium pellets would be sufficient for increasing the fuel cycle lifetime drastically.

## 5.6 Burnable poison usage

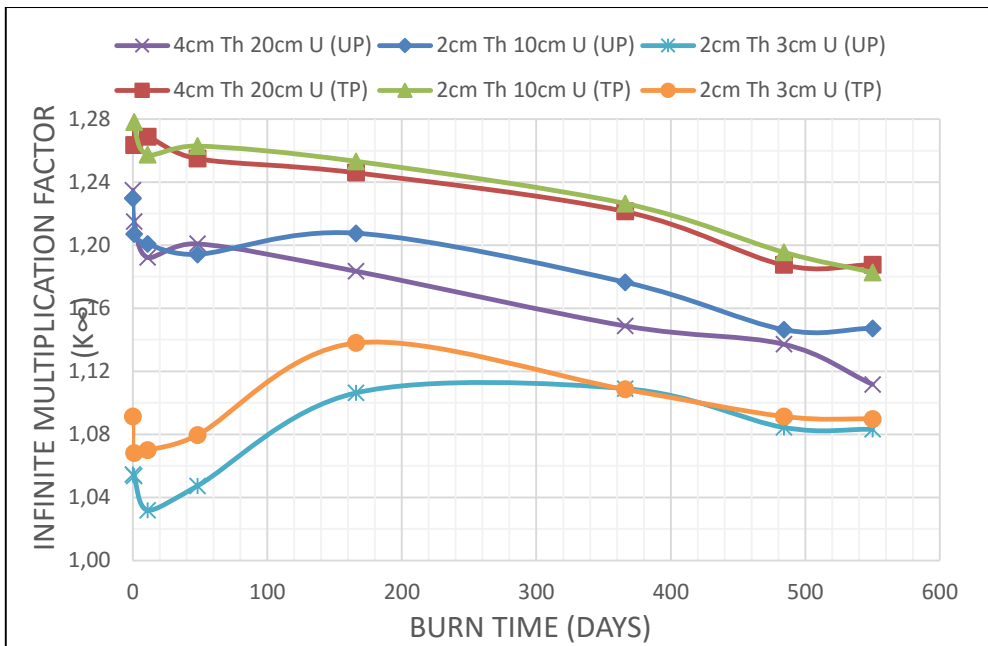
Further testing is required to determine how much Boron is required to reduce energy peaks and where the Boron should then be placed, but the above results show that there is some room for rather high concentrations of Boron to be used. These questions have been touched upon and the tests are shown in this section.

### 5.6.1 Placement of Boron inside the Thorium, Uranium or both

One of the challenges presented within this project is where to place the Boron if it is placed within the fuel rod. To determine what difference in effect this placement would have models were set up with different, arbitrary, lengths and ratios of material.



**Figure 25: Burnup over time of different models with equal enrichments and Boron concentrations, but with the Boron placed in either the Thorium or Uranium. UP = Boron placed within Uranium and TP = Boron within Thorium**



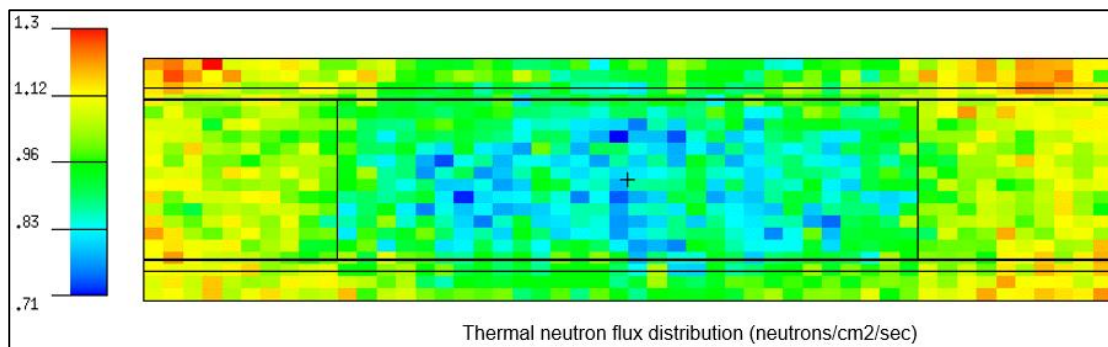
**Figure 26: Burnup over time of different models with equal enrichments and Boron concentrations, but with the Boron placed in either the Thorium or Uranium. UP = Boron placed within Uranium and TP = Boron within Thorium. (Second batch)**

The models show only one instance where the poison inside the Uranium case has a longer lifetime (2cm Th 20cm U). Therefore it may be concluded that adding the Boron to the  $\text{ThO}_2$  would be preferred in virtually all cases.

Further research will be required to determine under which circumstances it would be more beneficial to include the Boron inside the Thorium alone. Testing of different placements of Boron is also suggested, but within the scope of this project further assessment will not be completed.

### 5.6.2 Decreasing energy peaks with Boron

Neutron tallies are a very beneficial feature of MCNP, these tallies can be set up in many different ways and measure many different parameters. For these tests a symmetrical model was created with mesh tallies of different discretization sizes, this allows detailed measurements in small grid blocks across the entire model as would be seen in many CFD simulations. This model is shown in Figure 27 where the left and right blocks are  $\text{ThO}_2$  sections and the middle block is  $\text{UO}_2$ , no Boron was added.

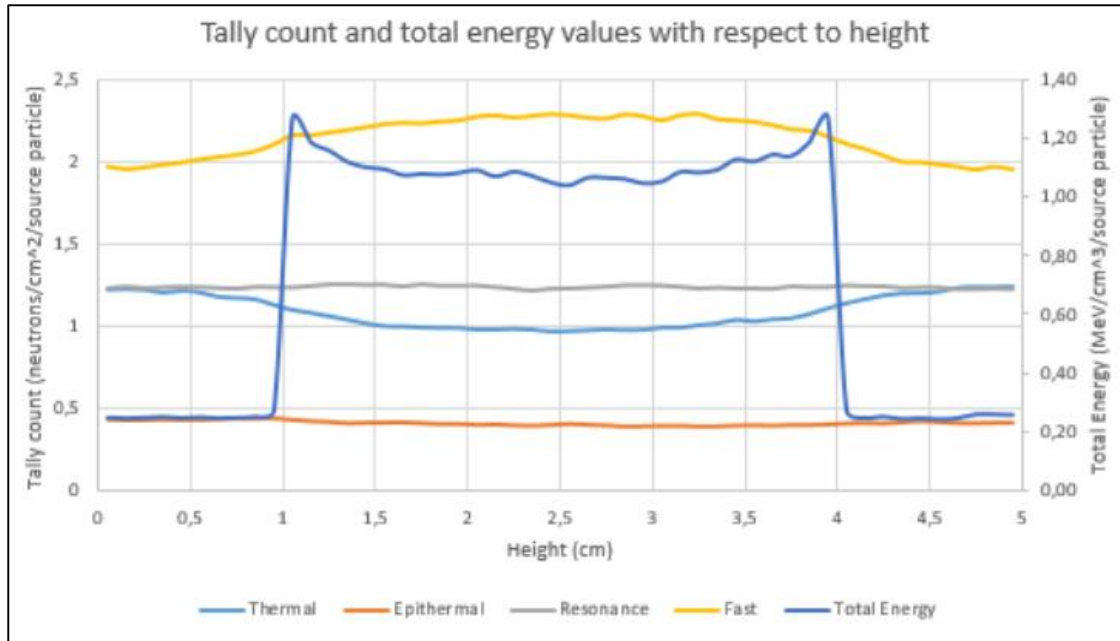


**Figure 27: Contour plot of tally count for thermal neutron flux within the symmetrical model. Scale units are tally counts/source neutron. Figure is rotated by 90 degrees therefore the x-axis is height.**

Figure 27 visually displays the large differences in thermal neutron flux within the model, the large values for thermal flux within the  $\text{ThO}_2$  regions can be explained through two factors.

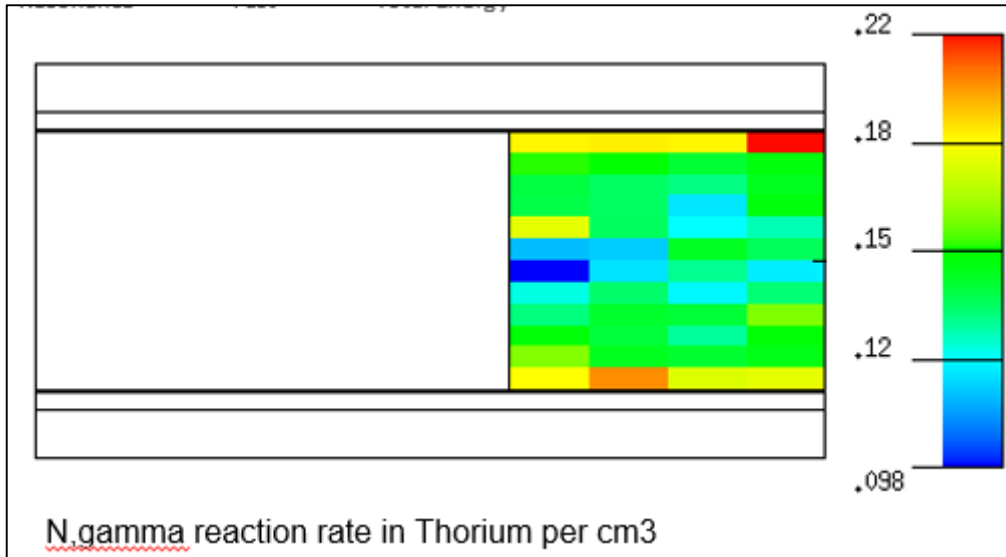
Firstly, the fission cross section of  $\text{U}^{235}$  for low energy neutrons is exponentially larger than the total absorption cross section of  $\text{Th}^{232}$ , therefore low energy and especially thermal neutrons are easily absorbed within the  $\text{UO}_2$  region. Secondly, neutrons with low energy enter the  $\text{ThO}_2$  region and are scattered around until they reach thermal energies without leaving this region.

This shows some good news for the theory of this design, as we wish to have large amounts of thermal neutrons within the  $\text{ThO}_2$  to maximise the probability that the Thorium will absorb neutrons in capture reactions, thereby breeding  $\text{U}^{233}$  over time.



**Figure 28: Graphs of tally counts for different parameters. The first four are neutron tally counts at different energy levels. The last, Total Energy, shows the energy deposited by neutron reactions. Note that the x-axis shows the height of the symmetrical model, this can be compared with Figure 27.**

It can be seen that the thermal flux is higher within the Thorium sections and that the expected energy peaks appear in the Th/U contact areas. These peaks should be controllable by reducing the thermal flux within the Thorium region by adding Boron. At BOL the thermal flux within the Thorium will be relatively low, but enough exposure over time will allow the Thorium to be saturated with  $U^{233}$  due to conversion. Once there is enough  $U^{233}$  within this region it should act as a separate fuel, which does not have such a high thermal flux due to the large amount of neutrons being absorbed for fission.



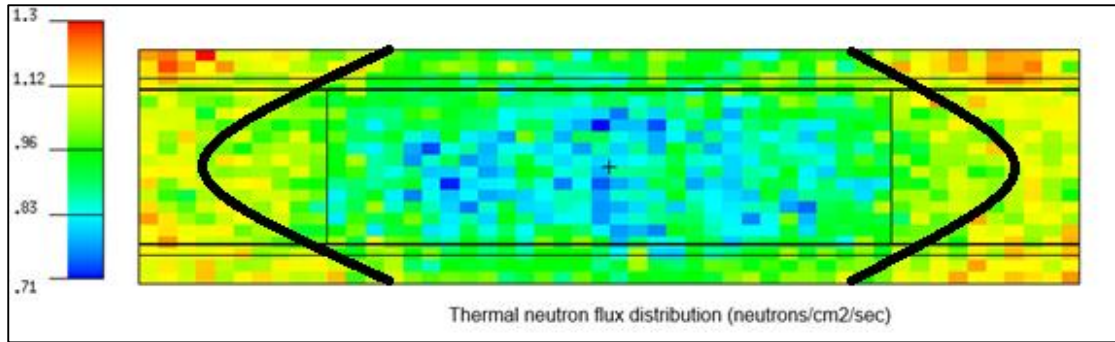
**Figure 29: Reaction rate tallies describing the neutron capture reactions within the ThO<sub>2</sub>.**

The reaction rate tallies of the ThO<sub>2</sub> demonstrate how thermal neutrons which enter the Thorium from the water are readily absorbed, neutrons which are not absorbed, most likely those which have low energy but have not reached “thermal” energies yet, are scattered around some more. These neutrons either end up in the middle of the Thorium region where they are most likely absorbed by the Thorium or make their way to the Uranium where they are readily absorbed for fission.

Figure 29, Figure 28 and Figure 27 demonstrate how the neutron flux has a large impact on all other reactions within the system, where the energy peaks that are seen are caused mainly by the thermal neutrons which are not absorbed within the ThO<sub>2</sub>. These neutrons enter the UO<sub>2</sub>, where they are absorbed almost immediately due to the large fission cross section of U<sup>235</sup> and then the resulting increase in fission reactions creates an energy peak.

### 5.7 Addition of a Conical region

When any one of the heterogeneous models is divided into mesh sections and neutron flux tallies are recorded within these blocks an interesting profile appears within the thermal neutron flux. If Figure 27 is inspected closely it is possible to draw an almost cone shaped line between some high neutron fluences and much lower fluences within the Thorium, this is visually demonstrated in Figure 30.

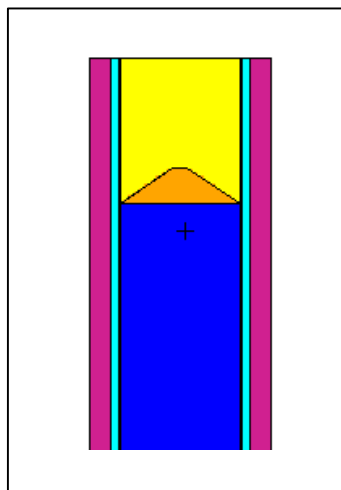


**Figure 30: Thermal neutron flux tally results, with profile lines added**

Due to these profile lines it was theorised that the addition of an alternate material may be capable of better utilization of the reduced fluxes. Having the correct material could reduce the chance that a neutron moving from the Thorium into the Uranium would be absorbed almost immediately, therefore the energy peaks may be reduced by this method. Burnable poisons could also be added to this region for the same effects.

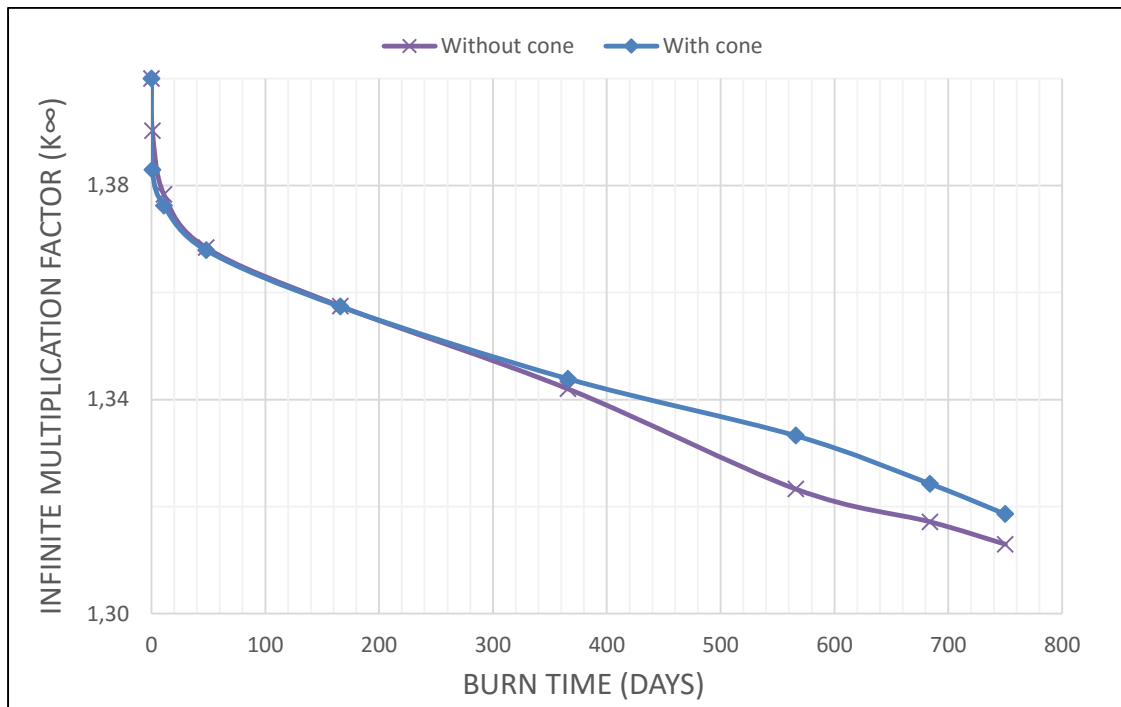
A model was designed with a cone shaped cell between the Thorium and Uranium sections, this design can be manipulated by changing the material within the cell arbitrarily. This model is demonstrated in Figure 31.

The model was then tested with the same design specifications as the 5cm Th and 20cm U model with 8.3 a/o% and zero Boron, but in order to compensate for the increased amount of fuel the volumes were normalized, this resulted in a  $k_{\infty}$  value similar to that of the original model, but the cone model did not lose as much reactivity over time. The results of this test are shown in Figure 32



**Figure 31: Heterogeneous model with cone shaped region added**

The choice of which material should be included within this region would require large amounts of time, but the test which was run simply extended the Uranium fuel into this region. The use of Uranium is thought to be beneficial due to the high probability that  $U^{238}$  will capture neutrons within the intermediate energy region. If the neutrons have not been sufficiently slowed down before reaching this region the chances could be quite large that the  $U^{238}$  is converted to  $Pu^{239}$ .

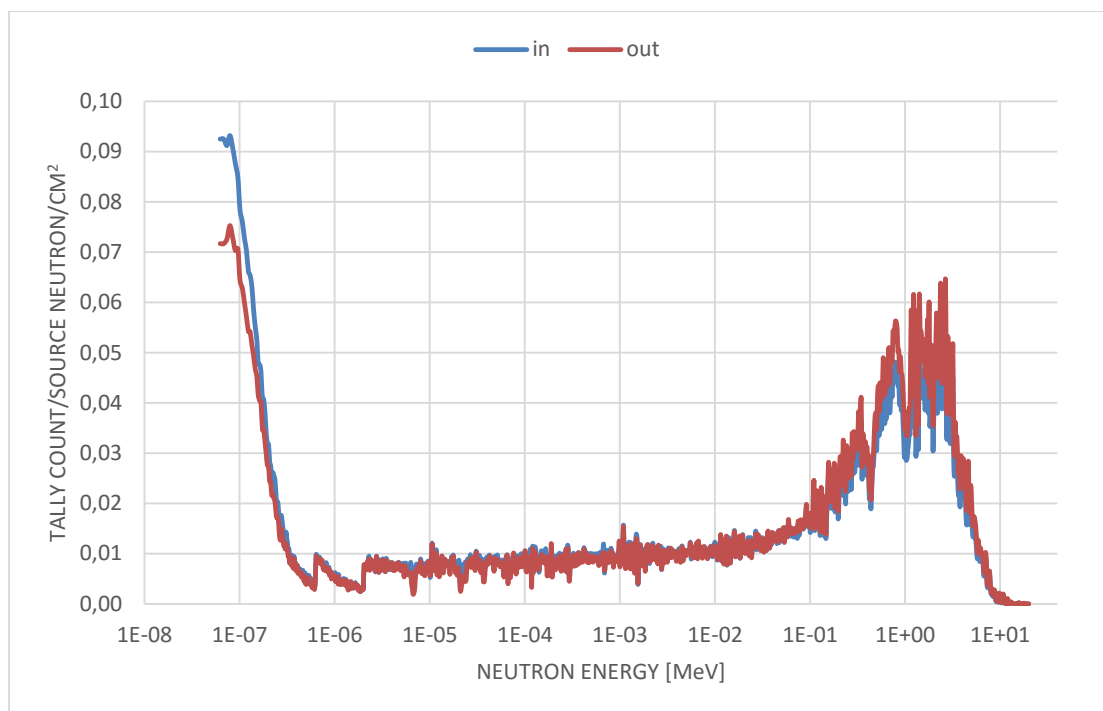


**Figure 32:  $k^\infty$  change over time due to burnup for the original 5cm Th 20cm U design vs. the modified cone design with the same Th and U volumes.**

## 5.8 Verification of results

Verification of the results from the heterogeneous models will require some ingenuity. Some creative ideas have been used and are shown in this section, as well as some general information about verifying results obtained using MCNP tallies.

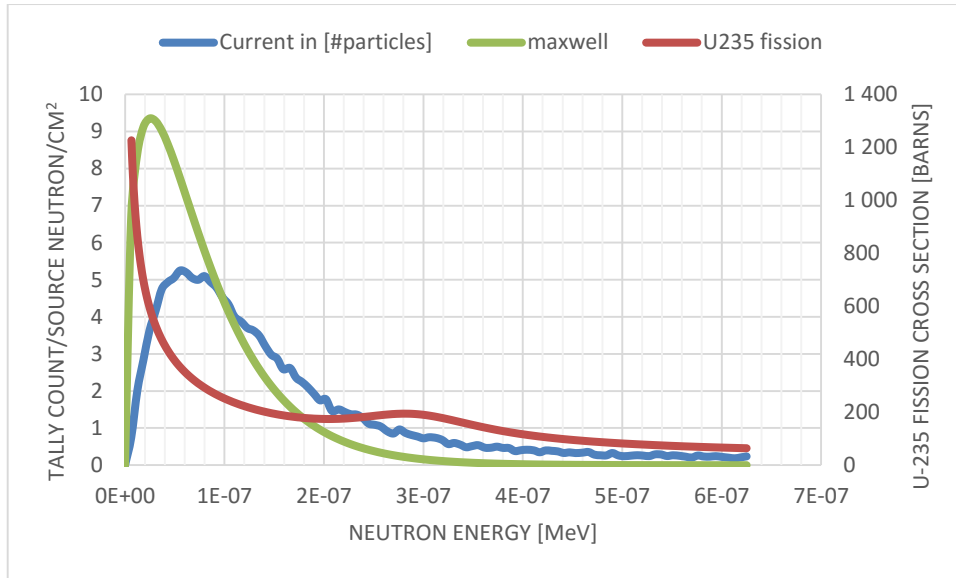
To determine whether the moderation of the model is correct neutron tallies were created to determine the amount and energies of neutrons entering or leaving the Uranium region. This is important because the correct process of moderation would be if neutrons created during fission inside the fuel leave the fuel with high energy, are then moderated by the water or Thorium and then re-enter the Uranium with less energy, preferentially thermal energy.



**Figure 33: Neutron flux tallies for a continuous spectrum of neutron energies with two vectors, in or out of the Uranium region.**

Figure 33 demonstrates exactly that, the flux, i.e. the amount of neutrons per area, is larger for high energy neutrons leaving the region, whereas the flux of low energy neutrons is significantly higher for neutrons entering the region. This verifies that neutrons are sufficiently moderated within the water before re-entering the Uranium region.

Another theoretical principle which can be tested with these tallies is the Maxwell thermalization theory that thermal neutrons will reach an equilibrium within a moderator (Lamarsh & Baratta, 2012). Due to the presence of materials which will absorb the neutrons it is expected that this equilibrium will be affected, but only in value, the shape of the distribution should not be greatly altered.



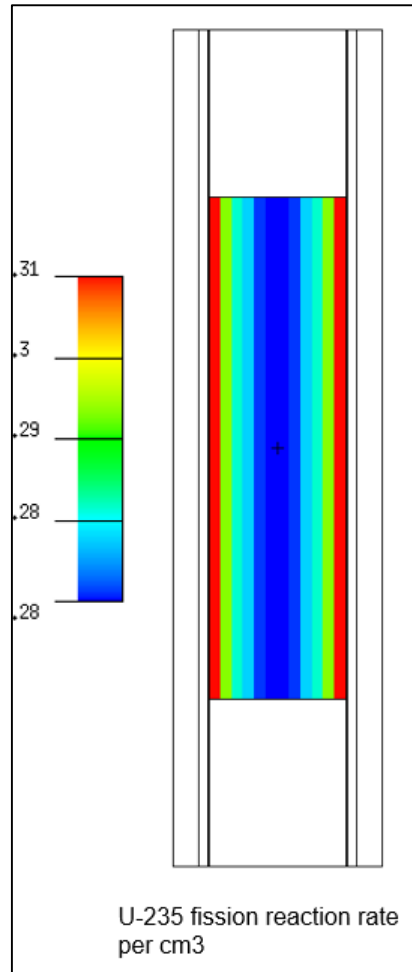
**Figure 34: Neutron current tallies for neutrons entering the Uranium region.**

**The Maxwell distribution is plotted for comparison. The fission cross section of U-235 is shown to demonstrate the increasing likelihood for neutrons to be absorbed.**

It can be concluded from Figure 34 that the distribution of neutrons inside the water, i.e. the neutrons entering the Uranium region, is correct, the shape of the graph is as required, but due to the materials which easily absorb thermal neutrons the values of the distribution are greatly affected. This absorption is greatly increased as the energy of the neutrons decreases due to the increasing reaction cross sections of most materials at lower neutron energies, the fission cross section of  $U^{235}$  is an example of one of these.

### 5.8.1 Sensitivity of results

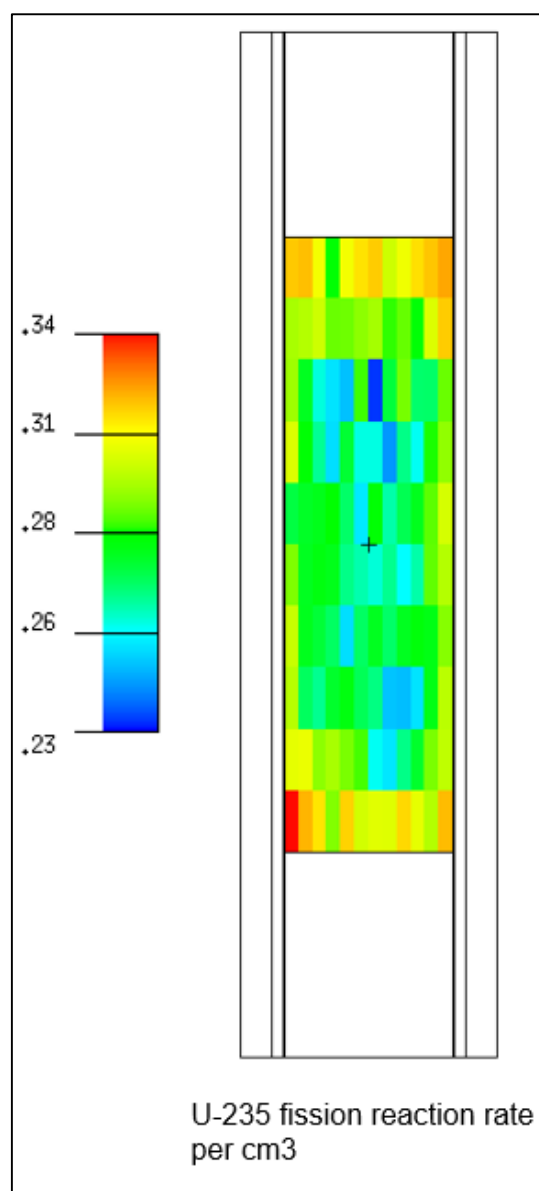
Using large discretisations, or meshes, forces tally data to be averaged over a large area. This average shows symmetrical results without any statistical anomalies. But when more detail is added and individual areas are inspected some statistical spikes occur, due to the nature of the calculations, that is, using probabilities and the chance that neutrons would collide or react in certain ways, creates leeway for such statistical fluctuations.



**Figure 35: U-235 fission reaction rate tally count averaged over a large area, i.e. the mesh is divided over the x-axis only.**

Increasing the amount of neutrons or the amount of cycles reduces statistical fluctuations, but at a certain point the accuracy does not increase enough to justify the computing time required. Figure 35 and Figure 36 demonstrate the same reaction rate tallies, with the same amount of cycles but different discretizations were used and drastically differing conclusions can be made from both.

This serves to show that analysing different levels of detail can give different answers in some cases and the results of the models should be carefully inspected as the results are extremely sensitive to small changes. But not only the method of perceiving the results is so sensitive to change, but the inputs of the models themselves are drastically affected by the simplest of changes. Keeping this in mind, this study has attempted to verify all results as thoroughly as time could allow.



**Figure 36: U-235 fission reaction rate contour plot with small discretization blocks, the mesh is divided in many x- and y-axis grids.**

## 5.9 Summary

The results have shown that the concept design is expected to easily increase the fuel cycle length, this design may even be implemented in 24 month cycles. The challenges for the concept design have been discussed in further detail and some recommendations for addressing these problems have been mentioned. Further research and development may be capable of completing a safely implementable practical design for industry testing. Verification of the results has been demonstrated with the use of reference models and some tests which showed that the neutrons behaved as would be expected from theoretical principles

## Chapter 6. Conclusions and Recommendations

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### Overview

It may be concluded that the conceptual design was a success and that the results of this study are verifiable with the literature stated in this dissertation. Further studies and some very time consuming hurdles will have to be faced and overcome to increase the efficiency and safety of this design, but the initial results show that this design could have great potential as a future improved fuel design in PWRs.

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### 6.1 Conclusions

The literature study which was completed identified work which contributes to the background of this project and was used to predict and support the results of the study.

A numerical model which simulates an infinitely large PWR has been successfully created and the model is capable of determining what effects different fuels and materials will have on the burnup of the system over time. A concept design which is capable of increasing the fuel lifetime of PWR's and is easy to implement into any existing system during shutdown was developed.

The results provided can be used to sufficiently determine that this design should work in practice, but only if the design's safety concerns can also be addressed. This concept design can be further optimized and enhanced to achieve 24 months of full power burnup. Verification of the results has been conducted through the use of reference models and the application of theoretical principals.

Ultimately, a new design has been developed and tested and this design has achieved the required outcomes of this project, where the  $k^\infty$  of the 5cm Th 20cm U model with 8.5wt%  $U^{235}$  enrichment and 0.15wt%  $B^{10}$  inside the Thorium pellets would be sufficient for increasing the fuel cycle lifetime drastically.

## 6.2 Recommendations for further design development

Further optimisation and simulations are recommended to determine aspects of the design which could not be investigated. Simulation of an infinite reactor is beneficial for preliminary design, but further simulations with more detail are required. The use of other numerical modelling codes can be used to further verify the results of this study and to further develop the design.

This design does show some safety concerns due to energy peaks which arise due to the increased thermal flux inside the Thorium region. These energy peaks could lead to local boiling of the coolant or even local meltdown of the fuel in extreme cases. Further studies of the configuration of the design as well as the use of Boron inside the fuel should be completed to address safety concerns.

Other great concerns which will prove time consuming and politically challenging are the proliferation risks as well as the 'barriers for Thorium' described in this dissertation. These challenges will require more time as simply modelling designs which have more benefits than drawbacks will not be sufficient, time consuming tests and regulatory changes will have to be completed.

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