URANIUM-THORIUM FUEL MIXTURE ON REACTOR TRIGA PUSPATI (RTP) CORE KINETICS BY A SIMULATION APPROACH

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During the early stages of nuclear energy development in the year 1960's, Uranium and Thorium was being considered as possible fuel sources, but as researchers found that uranium and the by-products of the reaction had other uses, especially in the weapons industry, thorium study research was sidelined to allow the full research and development of uranium as an energy source for electricity generation and weapons manufacturing.

Recently, research on thorium as a nuclear fuel source is starting to regain popularity. Nevertheless, thorium has its drawbacks compared to uranium. The main problem researchers have found out about uranium is that Thorium fuel is fertile instead of fissile [1]. This means that it can only be used as a fuel in conjunction with a fissile material such as recycled plutonium. They also stated that, Thorium fuels can breed fissile uranium-233 (U-233) to be used in various kinds of nuclear reactors.

As for the nature of thorium, it is a naturally-occurring and slightly radioactive material. Thorium exists in nature in a single isotopic form – Thorium-232 (Th-232) – which decays very slowly. The decay chains of natural thorium and uranium give rise to minute traces of Thorium-228 (Th-228), Thorium-230 (Th-230) and Thorium-234 (Th-234), but the presence of these in mass terms is negligible. It decays eventually to lead-208 (Pb-208). In its pure state, Thorium is a silvery white metal that retains its lustre for several months. However, when it is contaminated with the oxide, thorium slowly tarnishes in air, becoming grey and eventually black. When heated in air, thorium metal ignites and burns brilliantly with a white light. Thorium dioxide (ThO_2). The most common source of thorium is the rare earth phosphate mineral, monazite, which contains and average of 6%-7%.

Since Thorium is not fissile, it cannot be used directly in a nuclear reactor to produce energy. However, because it is fertile, upon bombarding it with a neutron, the Thorium (Th-232) will transmute to uranium-233 (U-233) which is an excellent fissile fuel material. All thorium fuel concepts therefore require that Thorium-232 (Th-232) is first irradiated in a reactor to provide the necessary neutron dosing. Thorium fuels therefore need a fissile material as a 'driver' so that a chain reaction (and thus supply of surplus neutrons) can be maintained. The only fissile driver options are Uranium-233 (U-233), Uranium-235 (U-235) or Plutonium-239 (Pu-239) [2]. Unfortunately, none of the stated fuels are easily accessible.

Nevertheless, it is possible (but very difficult) to design thorium fuels that produce more uranium-233 (U-233) in thermal reactors than the fissile material they consume. (This is referred to as having a fissile conversion ratio of more than 1.0 and is also called breeding) [3]. Thermal breeding with thorium requires that the neutron economy in the reactor has to be very good. The possibility to breed fissile material in slow neutron systems is a unique feature for thorium-based fuels and is not possible with uranium fuels.

Energy is now considered as a major requirement for the continuous existence of humans on this planet. Energy is required to power basic amenities like healthcare, public safety, local businesses, small to large scale factories and many other, considered basic, human needs. Ever since the industrial revolution in the 18th century, the use of fossil fuelled power plants has also grown exponentially in order to meet the requirements of energy. At that time, it seems like fossil fuels was the ideal energy source. As the world population is continuously growing exponentially, so does the requirement of energy. As of 2007, the world consumption fossil fuels is at 11.1billion tonnes [4] and as the days go by when the energy requirement increases, fossil fuels are receding at an alarming rate.

Nevertheless, the supply of fossil fuel is said to last for another 100 over years. Even then, that does not mean that human should sit back and relax until the supply of fossil fuels dry out. Instead, alternative fuel sources should be researched and applied and take the place of fossil fuels. Nowadays, green energy and alternative fuel is becoming more popular. Ranging from small scale renewable energy like personal sized solar panel and wind turbines to power up a medium sized household and all the way to large scale green energy projects such as hydroelectric turbines, solar [5]. and wind farms [6] dedicated to power up small cities are being researched and some are currently being applied at a considerably large scale such as the Thorium Molten Salt Reactor [7], in the light water reactor [8]. and used in a pressurised water reactor [9].

As nuclear energy is gaining popularity, so is its demand for nuclear fuel, specifically Uranium-235 (U-235) and Uranium U-238 (U-238). Even though uranium is the most popular element used to obtain the required energy, there is still an alternative to the alternative, which is the use of Thorium-232 (Th-232) as a fuel source.

The reasons to opt for Thorium fuel cycle [10]. over other radioactive fuel cycles are due to the following reasons: [11]

	The presence of Thorium – fuelled ADS[1].	Minimizing radio toxicity of nuclear waste. Uranium fuel required 30 000 years cooling time compared to Thorium which is 30 times less than that.
	Abundant in nature and easy to mine for.	Thorium is widely distributed (average concentration of 10 ppm) in earth's crust. Compared to uranium, thorium is more abundant by 3~4 times. Mining of thorium from monazite is simpler compared to mining for uranium from its ore.
	Thorium-232 has better nuclear characteristics compare to uranium-235	Thorium-232 is more 'fertile' than U-238 in thermal reactors because of Th-232 has a higher thermal neutron absorption rate which is trice as more compared to Uranium-235. (7.4 barns as compared to 2.7 barns). This makes the conversion of Th-232 to U-233 more efficient than U-238 to Pu-239 in the thermal neutron spectrum.
	More chemically stable and stable radiation resistance.	Thorium dioxide is chemically more stable and has higher radiation resistance than uranium dioxide. The fission product release rate for Thorium dioxide (ThO_2)–based fuels are one order of magnitude lower than that of Uranium Dioxide.
	Excellent past performance of Thorium dioxide (ThO_2), (Th,U)O2, ThC2 and (Th,U)C2 fuels in HTGRs.	The use of thorium-based elements used in the nuclear reactor core had demonstrated excellent performance in the past in the high temperature gas cooled reactors (HTGR) in several countries such as Germany, USA and the UK.
	Non-proliferative nature of the fuel cycle [12].	Because of the nature of Thorium and its by-product, it is not suitable to be used as a nuclear war head. Therefore, the chances of it being misused and breaking Malaysia's non-proliferation treaty is very small.
	Less problematic in handling the trans-uranium (TRU) waste.	There are much less plutonium and Minor Actinides (MA: Np, Am and Cm) produced as compared to the Uranium-238 fuel cycle. Minimizing the toxicity problems. Minimizing the decay heat problems.

Many works on the neutronic simulation of the Thorium Dioxide-Uranium (232Th, 235U)O_2 fuel was

carried out by using the MCNPX2.6 software. Some of the research conducted was to study the behaviour of the fuels in the nuclear reactor, Reactor TRIGA-Puspati. For this study, a light water moderator was used because during its years of commercial operation, it has proven itself to be a successful nuclear based reactor in the energy generation sector. However, compared to light water, heavy water has a moderating coefficient which is 80 times smaller. The uses of water acts both as a moderator and a coolant to the reactor. Also, graphite and beryllium is commonly used as the reflector [2], even though there are other alternative moderators. Compared to other materials, Beryllium Oxide (BeO) will act as a much better reflector [3].
By using the MCNP2X Monte Carlo code that was developed by the Los Alamos National Library, the simulation, calculation along with the analysis was conducted. The code is a general-purpose Monte Carlo Code [9], which will facilitate independent or coupled neutron, photon and electron transport calculation [13] s. The code will treat it as an arbitrary three-dimensional configuration of material and geometric cell. At the same time, the software will provide a versatile description of the source, the variance reduction methods, a flexible tally structure, and a vase collection of cross-section data in never-ending energy representation. Also, the software will cover the energy that ranges from $1X10^5$ all the way to 20MeV.
The neutron-induced cross-sections at 293K was applied using the ENDF/B-VI nuclear data library. In this research, the researchers considered the following two processes;(1) Inelastic scattering occurs with the cross section σ_{in} and a coupled energy-angle representation which was derived from ENDF/B S(α, β) scattering law. (2) elastic scattering with no change in the outgoing neutron energy for solids with cross-section σ_{el}. and an angular treatment derived from lattice parameters.
The simulation was conducted with the thermal region being defined in an energy range of $10^{-5} < E < 0.025$ eV and the core materials was selected based on table 1 when a KCODE card with 5000 neutrons and 250 active cycles along with 50 inactive cycles.

The calculations conducted was specifically targeting at obtaining a suitable neutron flux and having a reduced enrichment value within the compact core. In order to find the optimal geometry setting, an initial set-up was used and the geometry was gradually optimized until the set requirements is achieved. For this research, the design was considered to be at a diameter and height of 120 cm and 140cm respectively. The core was configured to have 19 fuel elements with 19 assemblies of 100cm height in each assembly. A 5cm thick Beryllium Oxide (BeO) reflector was considered around the core. [10]. The fuel elements, a $(Th,U)O_2$ fuel element, with the diameter of 2cm and 2.2% U-235 enrichment was used. Also, acting as the moderator was heavy water. There were 0.5cm, 1 cm and 2 cm gaps in between the assemblies and fuel pins respectively and a 0.2cm stainless steel covering the Be) reflector.

To reduce the neutron leakage, a method used was to select a reflector which has a proper composition and thickness. If the neutrons diffuses far enough into the reflector, there is a high chance that some will diffuse back into the core. Therefore, the reflector was optimized by varying the Beryllium Oxide (BeO) thickness from 5 cm up to 30 cm.

Six silver alloy control rod was used [14], in order to avoid criticality accidents,. The reactivity was defined using the following formula:

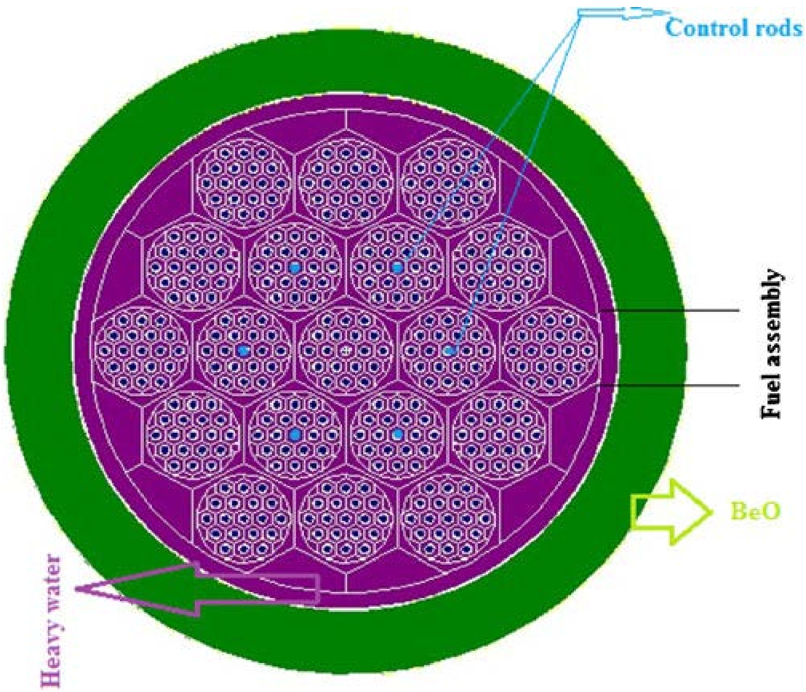
$$\boldsymbol{\rho = \frac{K_{eff} - 1}{K_{eff}}}$$

The effective delayed neutron fraction was the unit used to when the reactivity was measured in fractions. A unit of ρ/βeff is called a dollar [15], where βeff is the effective delayed neutron fraction

Material	Composition (wt%)	Thickness (cm)	Density (g/cm3)
Fuel	(U,Th)O 235U:2.2, 232Th: balance	2.00	10.00
Cladding	Zircaloy-4 Sn:1.4, Fe:0.23, Cr:0.1, and Zr SS304	0.04	6.50
Cover plate	Fe:69.5, Cr:19.0, Ni:9.5, Mn:2.0 side	0.2 variable	7.92 3.00
Reflector	Be:36, O:64 Top & Bottom	2.00	2.00
Control rods	Cd:4.9, Ag:80.5, In:14.6	2.08	9.32

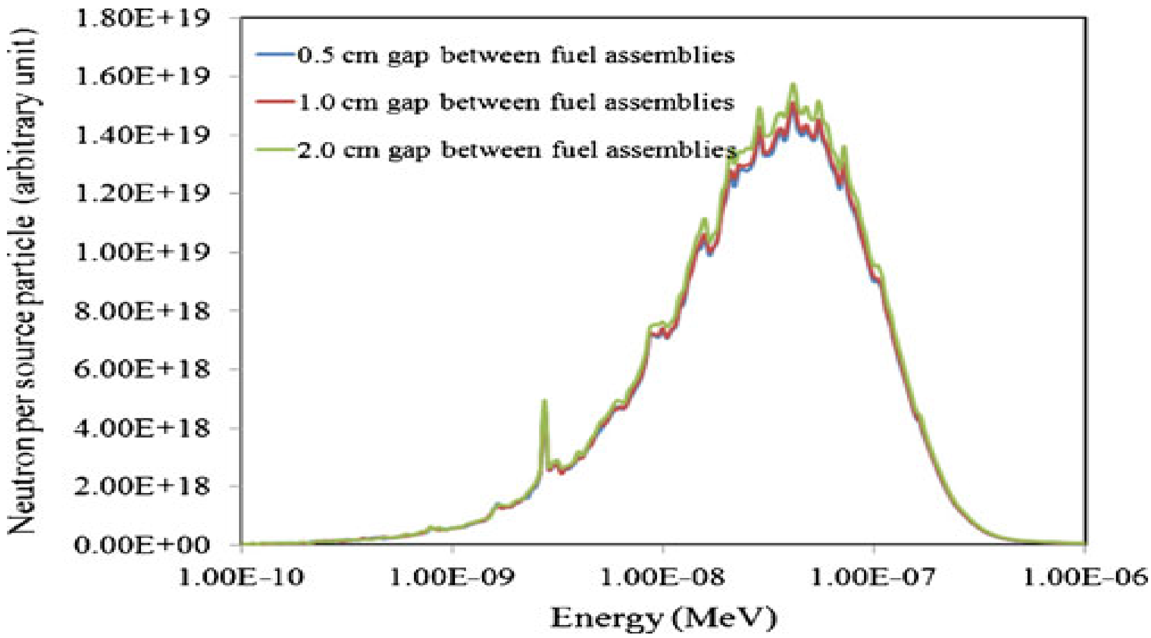
Core Material Composition

In the simulations that was carried out, the Neutronic parameters of the fuel setup; hexagonal, 10-assembly core, Thorium-235 and U-235 mixture, 2.2% fuel enrichment, enrichment was considered. A k_{eff} value of 1.00026 was obtained for the configuration of 19 fuel elements in each of its 19 assemblies, where each fuel was interspaced of 0.5cm and was arranged in a hexagonal shape in a core of surrounded by a 274,750 cm^3 heavy water moderator and is 120 cm in diameter. By increasing the gap between the assemblies to 1 and 2 cm, a decrease of $k_{eff}$to 0.99680 and 0.97491 had occurred, respectively, while still using a 5 cm Beryllium Oxide (BeO) reflector.



Critical core which is 15 cm thick of Beryllium Oxide (BeO with configuration consisting of 19-assemblies.

The calculations showed relative discrepancies when using the 2 cm fuel assembly gap in comparison with 1 cm gap as shown in the following figure. Thus, 0.5 cm gap seems to be most suitable.



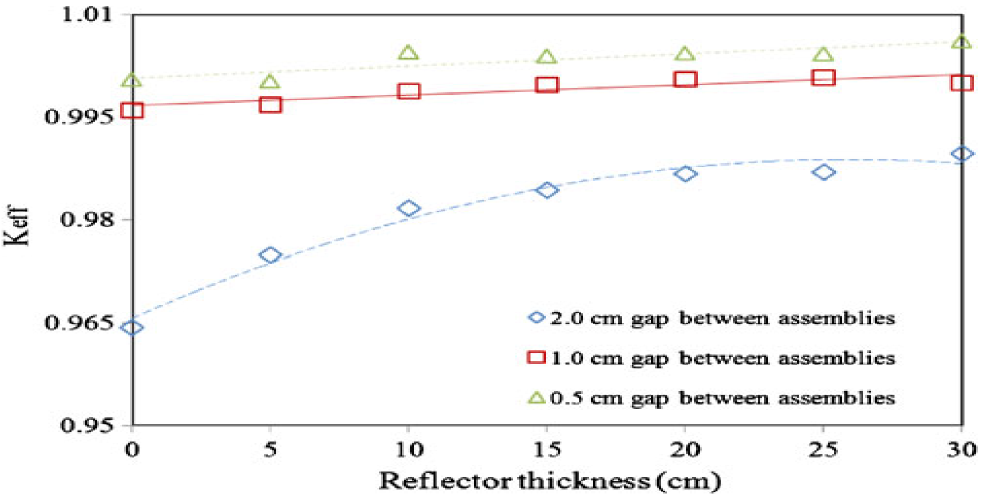
Neutron spectra Comparison of core with various gaps between fuel elements.

The uses of different Beryllium Oxide (BeO) thickness also cause some fluctuations in the k_{eff} value as tabulated in following table.

Effect of different thickness Beryllium Oxide (BeO) on k_{eff}

BeO thickness (cm)	0	5	10	15	20	25	30
2 cm gap between fuel assemblies							
K_{eff}	0.96432	0.97491	0.98171	0.98435	0.98676	0.98701	0.98971
SD (pcm)	53	49	51	48	47	42	45
1 cm gap between fuel assemblies							
K_{eff}	0.99607	0.99680	0.99883	0.99977	1.00052	1.00079	0.99995
SD (pcm)	49	47	50	48	47	50	45
0.5 cm gap between fuel assemblies							
K_{eff}	1.00052	1.00026	1.00454	1.00396	1.00437	1.00428	1.00618
SD (pcm)	49	49	49	47	48	51	48

The k_{eff}value were more stable around the 2cm gap between assemblies compared to 1cm and 0.5cm. When the gap was 0.5 cm, k_{eff} fluctuations were less compared to the rest. As a matter of fact, additional volume of water can itself act as a reflector and reduce the presence of thermal neutrons in the Beryllium Oxide (BeO) reflector. However, by increasing the thickness of the reflector will make the reflector act like a shield for neutrons and will decrease the scattering of neutrons which is aimed to the centre of the core. Thus, the simulation was conducted to observe the most suitable reflector thickness.



Comparison of reflector neutron spectra with different reflector thicknesses.

By using the Monte Carlo MCNP software, a 3-dimensional simulation developed a versatile and accurate full model of the TRIGA core and its fuel elements. The script was compiled in order to run a simulation in the MCNP software to obtain the neutron flux distribution.

Using the MCNP software, neutron flux distribution had predicted that the thermal flux values seem to be higher than the experimentally determined values. This difference in values was discussed to be due to error in physical model or the temperature effect, which was neglected in MCNP calculation. Nevertheless, the magnitude of this effect is believed to be neglect able. In order to calculate the neutron flux distribution, the following equation, was used.

$$\Phi_{total} = \Phi F_4 \times (Power\ Level \times \upsilon) \div (Q_{value} \times k_{eff})$$

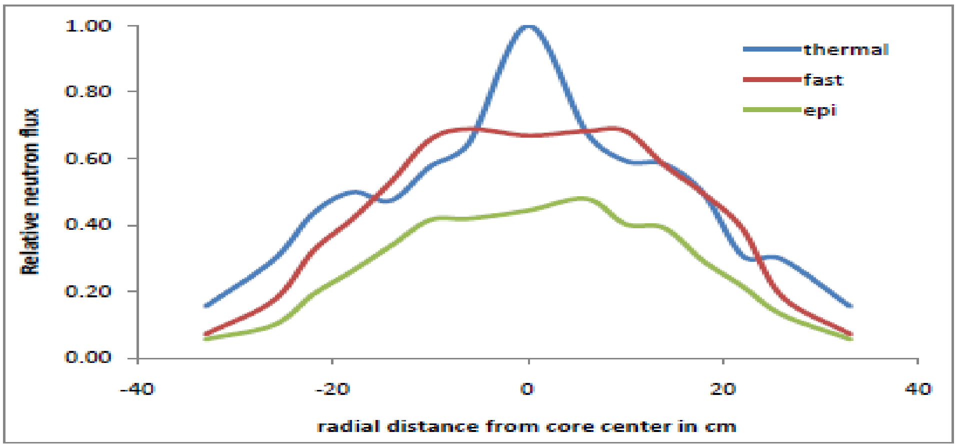
-where; **Φ** is neutron flux

υ is average neutron emitted per fission

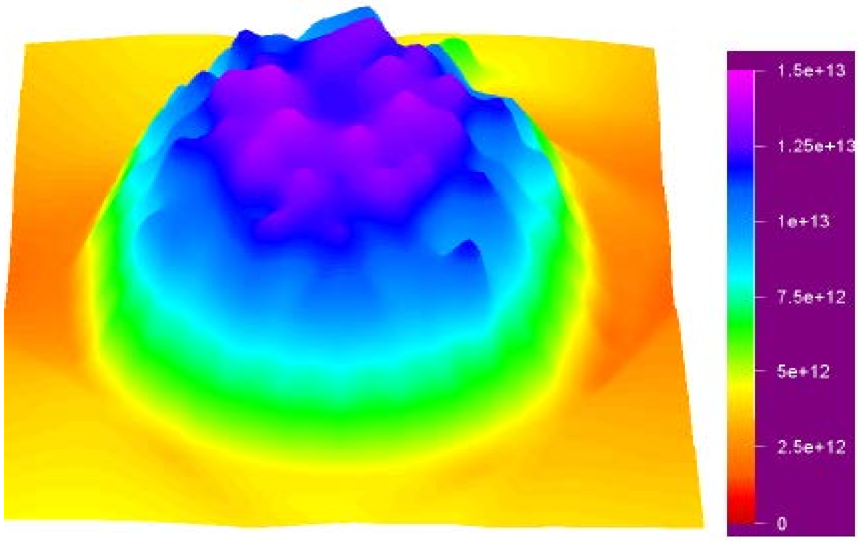
Q is recoverable energy per fission

The thermal neutron energy considered to be all energy below 0.5 eV which is the energy cut-off for Cadmium that was used in neutron flux measurement. The k_{eff} predicted by MCNP was 1.12728 ±0.00071 which is higher than the measured one which is 1.091036, this is expected since the MCNP does not taking into account the fuel burnup.

The neutron flux distribution inside the reactor core was determined to be dependent on the different types of elements in it. The maximum neutron flux will be distributed towards core centre. Actually, it was found that the maximum thermal neutron flux was at the Central Thimble location. Since this area has been filled with a moderator, which is water, the fast neutrons were thermalized. But at the edge of the core, the thermal flux was relatively higher than the fast flux because of the graphite reflector effect.



Radial Flux Distribution

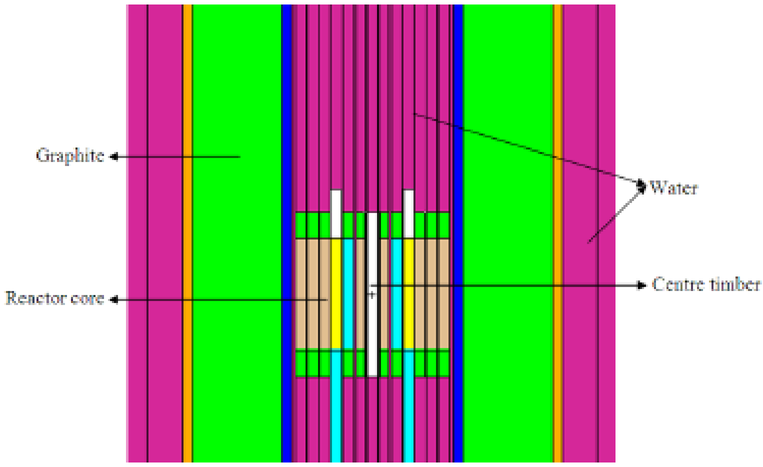


Fast Neutron flux distribution

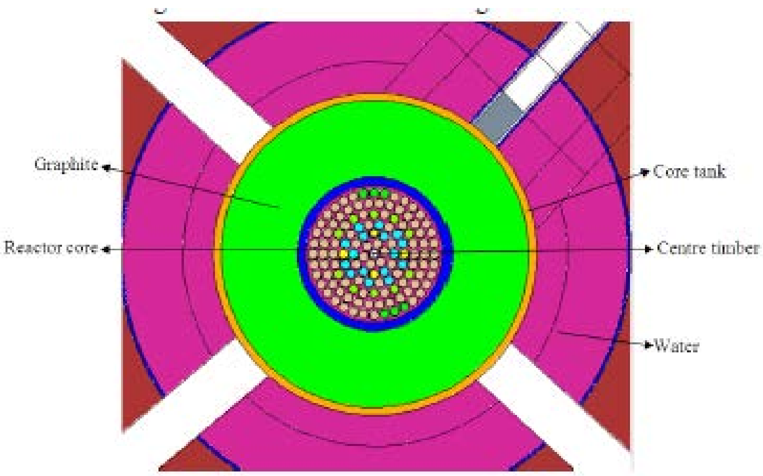
Based on the experiment conducted, it was said that the Radial and axial neutron flux distribution was much more depends on the fuel loading pattern and location in the core. Also, the result obtained reinforces the reliability of the MCNP software for the design verification and reactor core parameters calculation.

The Monte Carlo MCNP software can be used to calculate the criticality of the Triga Mark II Pool Type Reactor. This research paper provides the required information regarding using the Monte Carlo simulation to simulate the capabilities of that reactor in fulfilling its safety function.

Using the MCNP5 software [14], a complete model of RTP which was constructed. The constructed core was based on the 12th core configuration which is made of of 114 correctly positioned fuel rods, 10 of flux holes, 6 dummy fuel rods, 3 control rods of fuel-follower type are used i.e. regulating, (R), Shim (C), and safety (S), 1 air-follower control rod (transient rod), reactor tank, graphite reflector and centre timber. The fuel elements constructed was represented as cylinders with the respected dimensions and materials, at the exact locations. The core centre was assumed as the origin with the coordinates; (0, 0, 0) in the x-y plane. In the 12th configuration, 88 fuel elements of 8.5wt%, 16 fuel elements of 12wt% and 10 fuel elements of 20wt% was used.



Axial Model for the RTP configuration in MCNP5

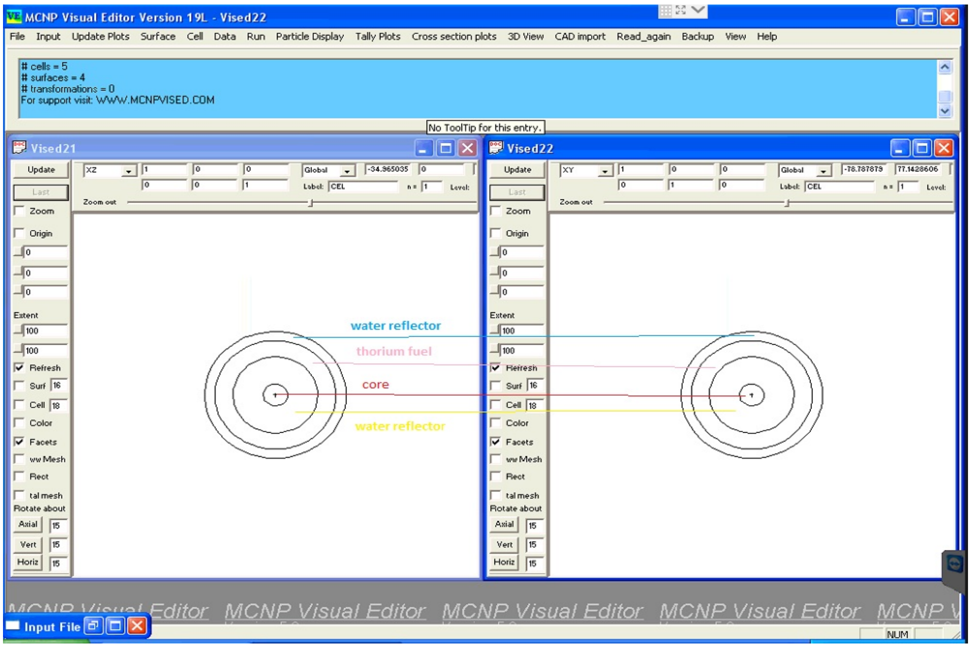


Radial Model for the RTP configuration in MCNP5

Based on the conducted simulation, it can be concluded that the physical parameters such as the k_{eff}, flux distribution, dose and several other parameters was obtained and was tabulated in following table.

Comparison of the MCNP5 calculation and SCRAC calculation

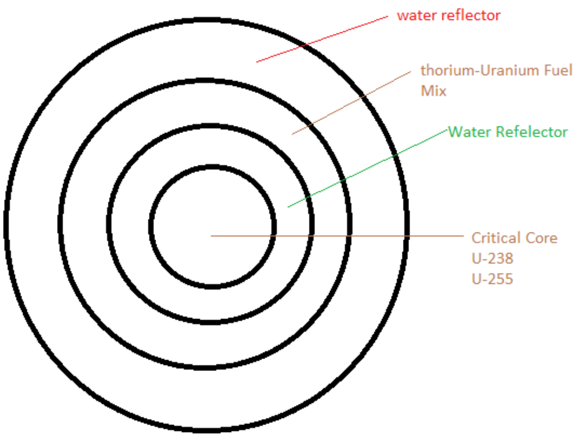
Effective multiplication factor (Control rods fully withdrawn) by MCNP5 code	1.10773 ±0.00083	Effective multiplication factor (Control rods fully withdrawn) by SRAC code	1.0876
Effective multiplication factor (Control rods fully inserted) by MCNP5 code	0.98370 ± 0.00054	Effective multiplication factor (Control rods fully inserted) by SRAC code	0.8435



Reactor Core Design MCNP Visual Editor. Front view (left), Top View (Right)

It was concluded that by using the MCNP5, it was an advantage compared to using the deterministic methods. This is because the MCNP5 software is powerful code for the criticality calculation which may be hard to be achieved by deterministic calculations.

For the first core design, the first core is known as the critical core. In this first core, it will be the source Uranium-238 (U-238) and Uranium-235 (U-235) particles. The 2nd sphere will be a water reflector. The water used here will be heavy Water. The third Sphere is filled with a Thorium-232 (Th-232)-Uranium-232 fuel mixture. The fourth sphere is filled with the Heavy Water which acts as the reflector, similar to the second sphere. In both the second and fourth sphere, the heavy water acts as the reflector to focus the neutrons in the thorium-Uranium region.



Simplified view of the Reactor core

Core design has been constructed using the MCNP4C Student Version and the MCNP Visual Editor Version 19L, the construction of the fuel card can be constructed.

The construction of the reactor core which was discussed in the previous sub-topic (3.3.8. Constructing the reactor core). The third sphere is where the thorium fuel is assembled and the fourth sphere is where the uranium-233 element is located. For an ideal state, the core was designed such that the entire third sphere was to be the location of all the thorium fuel. For this design, the difference between the third and fourth sphere will always be 9cm in radius. This means the difference in the diameters was 9cm. The third and fourth sphere will change according to the sphere formula (equation below).

$$\boldsymbol{A = \left(\frac{\pi}{4} * 30cm^2\right) - \left(\frac{\pi}{4} * rcm^2\right)}$$

where A= Effective area of thorium

R= radius of the third (thorium) sphere.

The dimensions of the third and fourth sphere is tabulated below:

Percentage of thorium to effective area of thorium

Thorium Percentage (%)	**Radius (cm)**	**Effective area (thorium) [cm^2]**
100	21.00	360.498
90	21.90	330.174
80	22.80	298.577
70	23.70	265.708
60	24.60	231.567
50	25.50	196.153
40	26.40	159.467
30	27.30	121.509
20	28.20	82.278
10	29.10	41.775

From the table above, it can be seen that as the radius of the third sphere, thorium filled sphere, decreases with respect to the percentage of thorium in the sphere itself, and the effective area also decreases. Inversely, as the effective area of the thorium decreases, the effective area of the uranium will gradually increase.

```
Sample coding (100% Thorium dioxide).
Thorium criticality
c ============================ cells =====================
10      1 4.84101E-02      -1       imp:n=1       $ critical compound
20      2 1.00343E-01      1  -2    imp:n=1       $ water reflector
30      3 0.878809         2  -3    imp:n=1       $ Thorium
40      2 1.00343E-01      3  -4    imp:n=1       $ water reflector
99      0                        4       imp:n=0       $ outside world

c ============================ surfaces ==================
1 SPH 0 0 0   6
2 SPH 0 0 0  21
3 SPH 0 0 0  30
4 sph 0 0 0  35
```

coordinates of the thorium fuel

diameters of the spheres

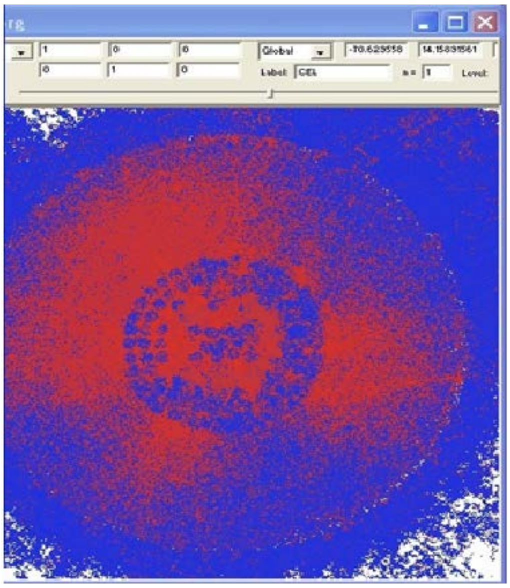
Example of fuel and reactor core script.

In order to manipulate the thorium-uranium content in the third and fourth sphere respectively, the basic script needs to be manipulated to meet the size requirements based on the values in previous table. The sphere 2 and sphere 3 is 21 cm and 30 cm respectively. The absence of a fifth sphere is because in this situation of 100% thorium filled sphere, the 3rd sphere is 9cm (in radius) filled with thorium. This translates to the core having 360.498 cm^{2}of thorium. As the thorium percentage decreases, so does the effective area of thorium. The effective area ranges from 360.498cm^{2}at 100% thorium-0% Uranium and 41.775cm^2 at 10% thorium-90% Uranium.

In order to determine the most suitable nuclear reactor design and thorium-uranium fuel configuration, a study on the particle distribution needs to be conducted first. In order to conduct this study via simulation, the MCNP4C and MCNP Visual Editor Version 19L needs to be done.

The reason the particle distribution was done prior to real simulation was to ensure that there would be enough energy throughout the configured reactor core designed during the fission process [2]. The particle display simulation works in a where will track then display the number of neutron collisions, along with the neutron source that occurred in the reactor. The tracking of the neutrons was to find out how many neutrons would collide with the thorium-uranium mixture.

High amounts of collisions will result in a high amount of energy at that area due to the high concentration of neutrons colliding at that area. Nevertheless, since the MCNP software does not track the amount of neutrons absorbed nor does it detect the amount of neutrons released, the particle display cannot be used as tool to evaluate the criticality of the of the nuclear reactor. Therefore, the sustainability of a nuclear chain reaction cannot be determined just by conducting the particle display simulation.



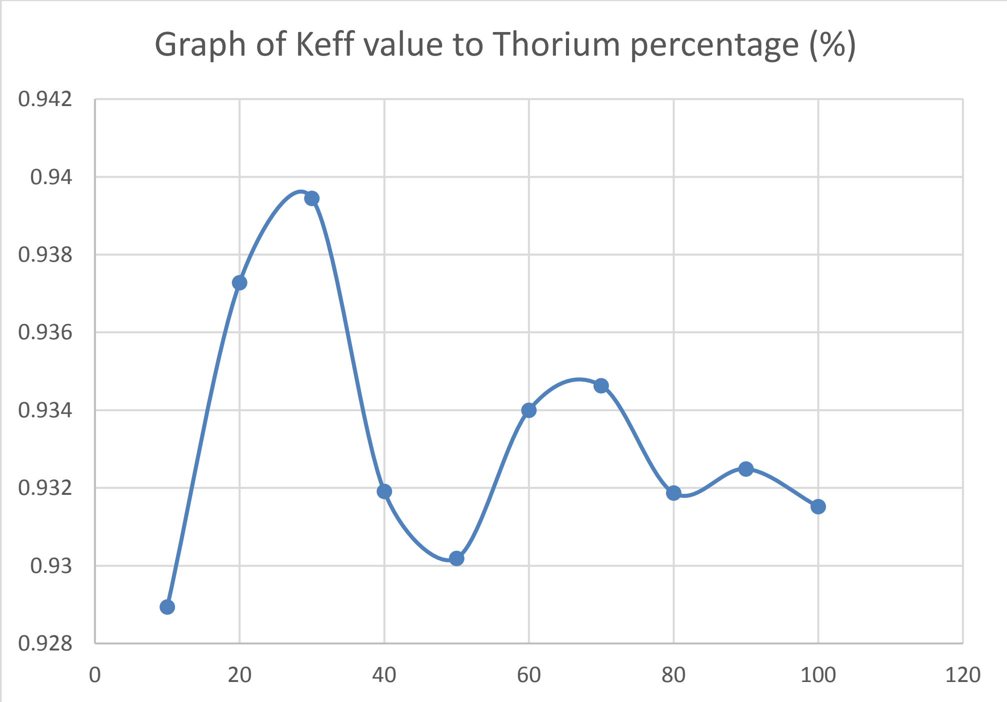
Particle display of designed

Based on the studied design, it can be seen that most of the neutrons available for bombardment with the thorium-uranium fuel is located just outside the centre of the reactor core (red particles) whereas it is seen less in the outer region (blue region). This is because due to the water reflectors on sphere two and sphere five are reflecting the neutrons back into that said area. This makes it a suitable location to place the thorium-uranium fuel mixture.

From the experiment conducted using the MCNP4C Student Version and MCNP Visual Editor Version 19L software, the k_{eff} results were obtained with respect to the difference in the thorium content in the reactor core. The results of the simulation have been tabulated in the following table.

Percentage of thorium to effective area of thorium

Thorium Percentage (%)	Thorium-232 weightage	k_{eff}
100	0.8788090	0.93152
90	0.7909281	0.93249
80	0.7030472	0.93187
70	0.6151663	0.93463
60	0.5272854	0.93400
50	0.4394045	0.93019
40	0.3515236	0.93191
30	0.2636427	0.93945
20	0.1757618	0.93728
10	0.0878809	0.92894



k_{eff} values to Thorium percentages (%)

Based on the Graph of k_{eff} value to Thorium percentage (%), it is seen that as the percentage of the thorium increases, the k_{eff} value gradually fluctuates in a sinusoidal manner between 0.94 to 0.93 until it approaches the k_{eff} value of 0.932.

The simulation using the MCNP4C Student Version and MCNP Visual Editor Version 19L software, conducted also was used to obtain the data of Standard Deviation related to the k_{eff}value. The results of the simulation have been tabulated in the following table.

k_{eff} values to Standard Deviation		
Thorium Percentage	**Thorium-232 weightage**	**Standard Deviation**
100	0.878809	0.00305
90	0.7909281	0.00282
80	0.7030472	0.00252
70	0.6151663	0.003313
60	0.5272854	0.00331
50	0.4394045	0.00288
40	0.3515236	0.0033
30	0.2636427	0.00259
20	0.1757618	0.00312
10	0.0878809	0.00288

Based on the Graph of standard deviation to k_{eff} value, it is seen that the values of Standard deviation fluctuate between the values of 0.0035 to 0.0025 in a very inconsistent manner. For all k_{eff} values, it is seen that the standard deviation did not exceed more than 0.0035. This means the variation of all k_{eff} values obtained from the 60 cycles simulated did not vary much from each other [15].

As an overall conclusion, it can be said the neutronic behaviour of the neutrons of the thorium-uranium fuel acting in the designed nuclear reactor was not suitable. This is because a self-sustaining nuclear chain reaction could not be obtained. Even the most suitable configuration, a 30% thorium fuel configuration, could not meet the requirements for a self-sustaining nuclear chain reaction which is k_{eff} must equals to 1.

Therefore, in order to achieve a self-sustaining nuclear chain reaction, there are several procedure that can be done in order to design an appropriate configuration. One of it is to construct a more fissile nuclear fuel. Since the configured fuel produced a subcritical result, a more fissile nuclear element could be used and tested using the MCNP software since conducting a hands-on experiment could prove to be costly and too time consuming.

Another way to improve the configuration to become a more self-sustaining nuclear chain reaction, the design of the nuclear reactor needs to be improved. Even though the current nuclear reactor design is said to be the most ideal, it can further be improved. A better nuclear reflector may be used in order to reflect more neutrons back to the centre core. By doing so, this can boost up the k_{eff}values and in turn may allow a self-sustaining nuclear chain reaction to be obtained.

Thus, it can be concluded that, the thesis aim has been achieved. The neutronic simulation of the thorium-uranium fuel mixture has been observed. Unfortunately, the fuel configuration and the reactor design has been proven to be unsuitable for energy production use.

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MATERIALS DATA

Table of Properties of Heavy Water

353 Water, Heavy

Formula =	D2O	Molecular weight (g/mole) =	20.02760356
Density (g/cm3) =	1.105340	Total atom density (atoms/b-cm) =	9.971E-02

The above density is estimated to be accurate to 4 significant digits. Uncertainties are not addressed.
The following data was calculated from the input formula.

Element	Neutron ZA	Photon ZA	Weight Fraction	Atom Fraction	Atom Density
H-2	1002	1000	0.201133	0.666667	0.066473
O	8016	8000	0.798867	0.333333	0.033237
Total			1.000000	1.000000	0.099710

MCNP Form	Weight Fractions		Atom Fractions		Atom Densities	
Neutrons	1002	-0.201133	1002	0.666667	1002	0.066473
	8016	-0.798867	8016	0.333333	8016	0.033237
Photons	1000	-0.201133	1000	0.666667	1000	0.066473
	8000	-0.798867	8000	0.333333	8000	0.033237

CEPXS Form:	material	H-2	0.201133
		O	0.798867
	matname	Water, Heavy	
	density	1.105340	

Comments and References

The National Physical Laboratory, which is the national measurement standards laboratory for the United Kingdom, lists the density for D2O for T=0° to 100°C (http://www.kayelaby.npl.co.uk/general_physics/2_2/2_2_1.html). At T=20°C, the density = 1.10534 g/cm3 at 101.325 kPa (1.0 atm) from measurements in 1949, 1951, and 1963.
Density = 1.1054 g/cm3 is from Petrie et al. (2000). Density = 1.1056 g/cm3 at STP (20°C) is listed at http://en.wikipedia.org/wiki/Heavy_water.
Also call deuterium oxide.

Table of Properties of Natural Uranium

347 Uranium, Natural (NU)

Formula =	-	Molecular weight (g/mole) =	-
Density (g/cm3) =	18.950000	Total atom density (atoms/b-cm) =	4.794E-02

The above density is estimated to be accurate to 3 significant digits. Uncertainties are not addressed.
The following data were calculated from the input weight fractions.

Element	Neutron ZA	Photon ZA	Weight Fraction	Atom Fraction	Atom Density
U-234	92234	92000	0.000057	0.000058	0.000003
U-235	92235	92000	0.007204	0.007295	0.000350
U-238	92238	92000	0.992739	0.992647	0.047591
Total			1.000000	1.000000	0.047944

MCNP Form	Weight Fractions		Atom Fractions		Atom Densities	
Neutrons	92234	-0.000057	92234	0.000058	92234	0.000003
	92235	-0.007204	92235	0.007295	92235	0.000350
	92238	-0.992739	92238	0.992647	92238	0.047591
Photons	92000	-0.000057	92000	0.000058	92000	0.000003
	92000	-0.007204	92000	0.007295	92000	0.000350
	92000	-0.992739	92000	0.992647	92000	0.047591

CEPXS Form:	material	U-234	0.000057
		U-235	0.007204
		U-238	0.992739
	matname	Uranium, Natural (NU)	
	density	18.950000	

Comments and References
See pg 286 of Shleien (1992).
Density for natural uranium = 18.95 g/cm3, http://physics.nist.gov/cgi-bin/Star/compos.pl?matno=092 (NIST 1998).

Table of Properties of Thorium

310 Thorium

Formula =	Th	Molecular weight (g/mole) =	232.0381
Density (g/cm3) =	11.720000	Total atom density (atoms/b-cm) =	3.042E-02

The above density is estimated to be accurate to 4 significant digits. Uncertainties are not addressed.

The following data was calculated from the input formula.

Element	Neutron ZA	Photon ZA	Weight Fraction	Atom Fraction	Atom Density
Th	90232	90000	1.000000	1.000000	0.030417
Total			1.000000	1.000000	0.030417

MCNP Form	Weight Fractions		Atom Fractions		Atom Densities	
Neutrons	90232	-1.000000	90232	1.000000	90232	0.030417
Photons	90000	-1.000000	90000	1.000000	90000	0.030417

CEPXS Form:	material	Th	1.000000
	matname	Thorium	
	density	11.720000	

Comments and References

Density from http://physics.nist.gov/cgi-bin/Star/compos.pl?matno=090 (NIST 1998).