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Neutronic simulation of a research reactor core of (^{232}Th, ^{235}U)O_2 fuel using MCNPX2.6 code

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Abstract. The small reactor design for the remote and less developed areas of the user countries should have simple features in view of the lack of infra-structure and resources. Many researchers consider long core life with no on-site refuelling activity as a primary feature for the small reactor design. Long core life can be achieved by enhancing internal conversion rate of fertile to fissile materials. For that purpose, thorium cycle can be adopted because a high fissile production rate of ^{233}U converted from ^{232}Th can be expected in the thermal energy region. A simple nuclear reactor core arranged 19 assemblies in hexagonal structure, using thorium-based fuel and heavy water as coolant and moderator was simulated using MCNPX2.6 code, aiming an optimized critical assembly. Optimized reflector thickness and gap between assemblies were determined to achieve minimum neutron leakage and void reactivity. The result was a more compact core, where assemblies were designed having 19-fuel pins in 1.25 pitch-to-diameter ratio. Optimum reflector thickness of 15 cm resulted in minimal neutron leakage in view of economic limitations. A 0.5 cm gap between assembles achieved more safety and 2.2% enrichment requirements. The present feasibility study suggests a thermal core of acceptable neutronic parameters to achieve a simple and safe core.

Keywords. Critical; MCNPX2.6; reactor core; thorium oxide.

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1. Introduction

In the face of global energy shortage and the search for better technologies, there is a real case for widening the range of potential variations in the design of nuclear power plants. In principle, smaller and simpler reactors are attractive, provided they can meet safety and security standards and non-proliferation issues.

Decades ago, many countries abandoned the idea of using thorium as a replacement for uranium. But long-term proponents have always believed that the thorium fuel cycle could make nuclear energy as safe and sustainable as possible.

Thorium is seen by some as the nuclear fuel of the future. For a start, there is much more thorium than uranium in the Earth's crust, and all the thorium mined can be used in a reactor (compared to below 1% of natural uranium). Thorium fuel cycles also produce much less plutonium and other radioactive transuranic elements than uranium fuel cycles. Although not fissile itself, Th-232 will absorb slow neutrons to produce uranium-233 (^{233}U), which is fissile (and has long life) [1].

Accordingly, the present work describes the tentative design of a small research reactor core fuelled with a (Th,U)O_2 matrix using a general purpose Monte Carlo particle transport code.

1.1 *General considerations for the design of the reactor core*

The number of years in which nuclear reactors based on light water moderator technology have been in operation indicates that the most successful commercial application of fission reactors is the production of electricity. However, heavy water has a moderating coefficient 80 times smaller than light water, reducing therefore the need for higher fuel enrichments. The water both moderates and cools the reactor, and graphite or beryllium is generally used for the reflector, although other materials may also be used [2]. BeO can be a more useful reflector material than the others [3]. For structural materials, the composition of Zircaloy-4 differs from that of Zircaloy-2 in that it does not have nickel and has a slightly greater amount of Fe. Both variations aim at reducing the hydrogen absorption. The corrosive behaviour of Zircaloy-4 is very similar to that of Zircaloy-2, but the hydrogen absorption for Zircaloy-4 is significantly lower, particularly when the metal is exposed to water at 360°C or above. At this temperature, hydrogen absorption for Zircaloy-4 is less than half of Zircaloy-2's. So, Zr-4 can be chosen for cladding [4]. Stainless steel 304 has a high melting point (1390°C), and is used in several sections of the reactors [5,6]. Except for Mn that has neutron cross-sections of about 50 b in thermal and fast region, other SS-304 components do not have neutron cross-sections of more than 20 b [7]. It is known that highly enriched uranium (HEU $>$ 20% ^{235}U) allows more compact cores [8]. (As mentioned before, fuels of thorium fertile which are prominent not only in view of ^{233}U inventory as well as less production rate of Pu long-lived alpha emitter radioisotopes, but it is naturally abundant in most countries and can be studied as a good replacement of ^{238}U fertile material which is being finished.) One of the goals of this work is to aim for the lowest possible enrichment that is compatible with the compact core design fed with thorium oxide fuel instead of low enrichment uranium (LEU). As indicated, in the present simulation, a minimum enrichment was determined, for a compact core and as shown in the figures, below 4% enrichment was achieved.

2. Material and methods

The reactor core calculations were carried out using the MCNPX2.6 Monte Carlo code which was developed by the Los Alamos National Laboratory. It is a general purpose Monte Carlo code [9], which facilitates independent or coupled neutron, photon and electron transport calculations. The code treats an arbitrary three-dimensional configuration of material and geometric cell, and provides a versatile description of the source, the variance reduction techniques, a flexible tally structure, and an extensive collection of cross-section data in continuous energy representation. For neutrons, all reactions given in a particular cross-section data evaluation are accounted for, and cover the energy range between 10^{-5} eV and 20 MeV.

The ENDF/B-VI nuclear data library was used to apply neutron-induced cross-sections at 293 K. Thermal correction in the phonon band requires separate cross-section evaluation, the so-called $S(\alpha, \beta)$ cross-sections that are available for BeO and heavy water at a temperature of 294 K used in the present calculations. The $S(\alpha, \beta)$ thermal scattering treatment is a complete representation of thermal neutron scattering by molecules and crystalline solids. Two processes are allowed: (1) inelastic scattering with cross-section σ_{in} and a coupled energy-angle representation derived from an ENDF/B $S(\alpha, \beta)$ scattering law and (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 elastic scattering treatment is chosen with a probability of $\sigma_{\text{el}}/(\sigma_{\text{el}} + \sigma_{\text{in}})$.

Earlier research showed the acceptable capabilities of MCNPX2.6 calculations. Stamatelatos and Tzika [10] used the code for Greek research reactor simulations. They found very good agreement between the calculated and experimentally determined thermal neutron flux. Khattab and Sulieman [11] used the code for neutron activation analysis using a miniature neutron source Syrian reactor. Their calculation showed a maximum difference between experimental and calculated flux of less than 7%. Both these works used the ENDF/B-VI library in their calculations.

Since the MCNPX2.6 results are normalized to one source neutron (for example, the unit for the F4 tally, which estimates particle flux, is given in n/cm^2. Source particle), the results have to be properly scaled in order to get absolute comparison with the measured quantities (flux, reaction rate, fission density, etc.). Therefore, to normalize an F4 tally to the steady-state thermal power of the system, the following scaling factor in units of fission neutrons per unit time should be used [12]:

$$s = \frac{\bar{\upsilon}\left(\frac{\text{neutron}}{\text{fission}}\right) p\,[W]}{\epsilon\left(\frac{\text{MeV}}{\text{fission}}\right) * 1.602 * 10^{-13}\left(\frac{\text{J}}{\text{MeV}}\right)} \cdot \frac{1}{K_{\text{eff}}} \quad \left(\frac{n}{s}\right), \tag{1}$$

where υ is the neutron/fission number, P is the reactor power and ϵ is the released energy per fission; division of the equation per K_{eff} seems to result in a more precise neutron source because the critical multiplication of the core is not exactly 1.00000 in all conditions.

In the case of the neutron flux, this can be written as:

$$\phi\left(\frac{\text{neutron}}{\text{cm}^2\cdot\text{s}}\right)=s\left[\frac{n}{s}\right]\cdot\phi_{\text{F4}}\left(\frac{1}{\text{cm}^2}\right), \tag{2}$$

where ϕ_{F4} denotes the MCNPX tally output.

All simulations were carried out using a KCODE card of 5000 neutrons with 250 active cycles and 50 inactive cycles. The thermal region was defined in the energy range of $10^{-5} < E < 0.025$ eV. Core materials were selected as in table 1.

The calculations were aimed at achieving a compact core with suitable neutron flux and having lower enrichment. For finding the optimal geometry, an initial set-up was used and then the geometry was optimized.

In the design, core diameter and height were considered as 120 cm and 140 cm, respectively. Core configuration consisted of 19 assemblies with 19 fuel elements of 100 cm height in every assembly. BeO reflector of 5 cm thickness was considered around the core [13]. (Th, U)O_2 fuel elements, having a diameter of 2 cm and 2.2% enrichment of ^{235}U, were used and heavy water was selected as moderator. Gaps of 0.5 cm and 0.5 cm, 1 and 2 cm between the fuel pins and the assemblies, respectively, were selected. 0.2 cm stainless steel covered the BeO reflector.

A way to decrease the neutron leakage is to choose a reflector having proper composition and thickness. If neutrons diffuse far enough into the reflecting medium, there is a significant probability that some will diffuse back into the core. Hence, the reflector was optimized by varying the BeO thickness from 5 cm up to 30 cm.

To avoid criticality accidents, six silver alloy control rods were used [14].

Reactivity was calculated using the following formula:

$$\rho=\frac{K_{\text{eff}}-1}{K_{\text{eff}}}. \tag{3}$$

The reactivity defined in the previous section is often measured in fractions of the effective delayed neutron fraction. One unit of ρ/β_{eff} is called a dollar [15], where β_{eff} is

Table 1. Core material compositions.

Material	Composition (wt%)	Thickness (cm)	Density (g/cm^3)
Fuel	(U,Th)O_2	2.00	10.00
	^{235}U: 2.2, ^{232}Th balance, O		
Cladding	Zircaloy-4	0.04	6.50
	Sn:1.4, Fe:0.23, Cr:0.1, and Zr		
	SS 304		
Cover plate	Fe: 69.5, Cr: 19.0, Ni: 9.5, Mn: 2.0	0.2	7.92
	Side	Variable	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

the effective delayed neutron fraction. β_{eff} is defined as the ratio of fissions induced by delayed neutrons, N_{d}, to the total number of fissions induced in the same system, N_{Tot}. That is,

$$\beta_{\text{eff}} = \frac{N_{\text{d}}}{N_{\text{Tot}}}. \tag{4}$$

By using TOTNU in KCODE card, delayed neutrons were calculated. The fraction of delayed neutrons, β, is expressed as

$$\beta = \frac{\bar{\nu}_{\text{d}}}{\bar{\nu}_{\text{Tot}}}. \tag{5}$$

The voids, pin deformation at 400 K, and temperature reactivity coefficients were calculated by means of the mentioned formulae. To calculate the void reactivity coefficient, some void fraction was introduced homogeneously in the moderator.

The thermal expansion of the fuel elements (including the cladding) occurs during the reactor operation resulting in a reactivity insertion. This deformation was calculated using the thermal expansion coefficients of Zircaloy-4 and that of the fuel matrix at 400 K [16, 17]. The temperature reactivity coefficient was calculated using neutron-induced cross-sections at the same temperature. Burn-up calculations were carried out using the code in 1 MW power to consider the fuel burn-up and waste inventory. Reactivity variations due to moderator, fuel, Xe and Sm were estimated using the code results. Moderator reactivity was calculated using moderator density changes in effect of temperature enhancement and it has been demonstrated on void volume percentage as $\rho = \rho_0(1 - \text{void } \%)$. Fuel reactivity was calculated using different temperatures for the fuel pins.

Maximum reactivity of 149-samarium and 135-Xe has been calculated using the burn-up data as well; the burn-up output data after Xe equilibrium has been loaded instead of the fresh fuel material and K_{eff} has been calculated with and without the presence of Xe in the fuel mixture. Sm reactivity has been calculated in a similar way.

3. Result

Neutronic parameters of a hexagonal 19-assembly core containing $(^{232}\text{Th}, ^{235}\text{U})\text{O}_2$ fuel matrix with 2.2% enrichment was considered and its simulations were carried out as follows:

A maximum K_{eff} of 1.00026 was achieved for a critical core configuration consisting of 19 assemblies with 19 fuel elements each, interspaced by 0.5 cm, and arranged hexagonally in a core of 120 cm diameter surrounded by a 274750 cm^3 heavy water moderator (figure 1). Increasing the gap between the assemblies to 1 and 2 cm resulted in a decrease of K_{eff} to 0.99680 and 0.97491, respectively, using a 5 cm BeO reflector.

Neutron fluence per source particle in the most compact assemblies is larger than the others because thermal neutrons are born in the moderator and travel to the fuel. On the other hand, fast neutrons are born in the fuel and proceed to the moderator. When there is a 2 cm interval between the assemblies, some differences were observed in the neutron spectra at the core compared to the calculation using on 0.5 cm; -1.78% in thermal region, 4.16% in epithermal and 3.94% in fast regions. The calculations showed relative

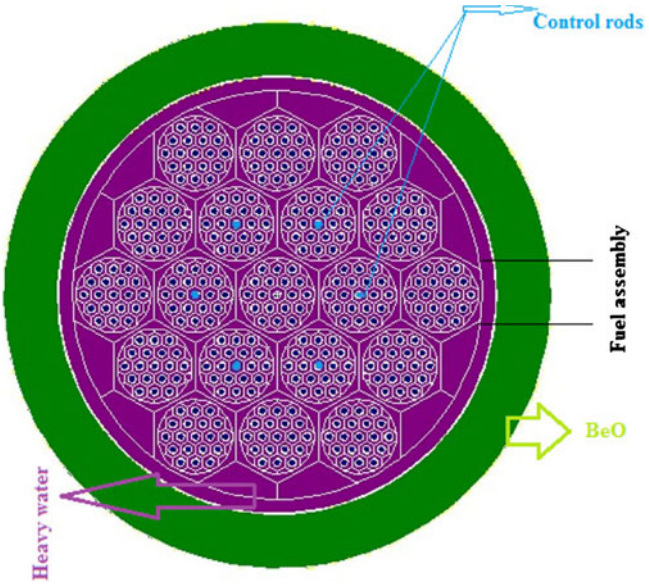

Figure 1. Critical core configuration consisting of 19-assemblies, a 15 cm thick BeO reflector and 2.2% (atom fraction) of ^{235}U; six silver alloy control rods of 2.08 cm diameter, 356 fuel rods of 2.08 cm diameter.

discrepancies of −5.68% in thermal region, 4.82% in epithermal and 4.26% in fast regions using 2 cm fuel assembly gap in comparison with 1 cm gap (figure 2). So, 0.5 cm gap seems to be preferable for its higher thermal neutron percentage than the others.

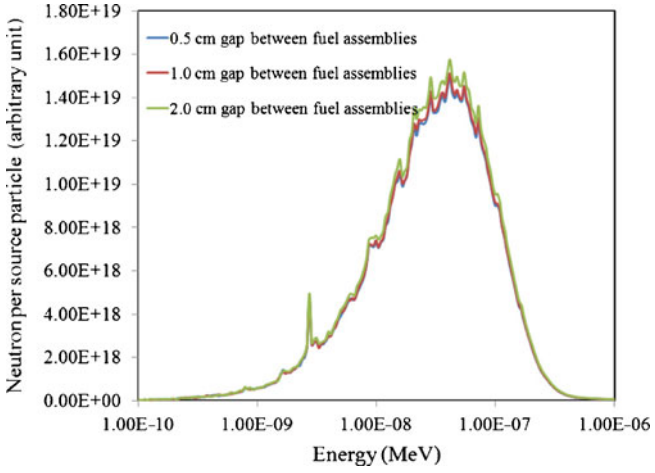

Figure 2. Comparison of core neutron spectra of various gaps between fuel assemblies.

Table 2. Effect of BeO on K_{eff}, ^{235}U enrichment: 2.2%, core diameter: 120 cm, core height: 140 cm, gaps between the assemblies: 2 cm and 0.5 cm, respectively.

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

SD: Standard deviation

The use of BeO of 5–30 cm thickness caused some fluctuations in K_{eff}. The K_{eff} variations were more flat for 2 cm gap between assemblies than for 1 and 0.5 cm gaps (table 2).

Comparison of neutron spectra in the reflector showed that a thickness of 15 cm can reflect more thermal neutrons towards the core (figure 3). As seen in figure 4, when the gap was 0.5 cm, K_{eff} fluctuations were less than the others. In fact, additional water volume can itself act as a reflector and decrease the presence of thermal neutrons in the BeO reflector. However, increase of reflector thickness causes the reflector to act as a shield for neutrons and decreases neutron scattering towards the heart of the core. Hence, other simulations would be a guide to choose the best reflector thickness. Core thermal

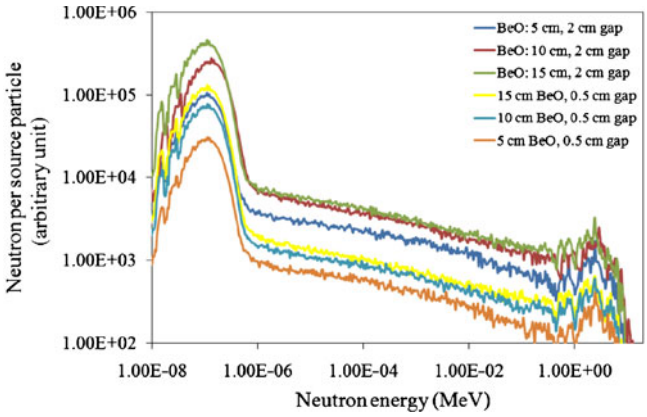

Figure 3. Comparison of reflector neutron spectra with various reflector thicknesses. Gaps between assemblies are 2 cm and 0.5 cm, respectively.

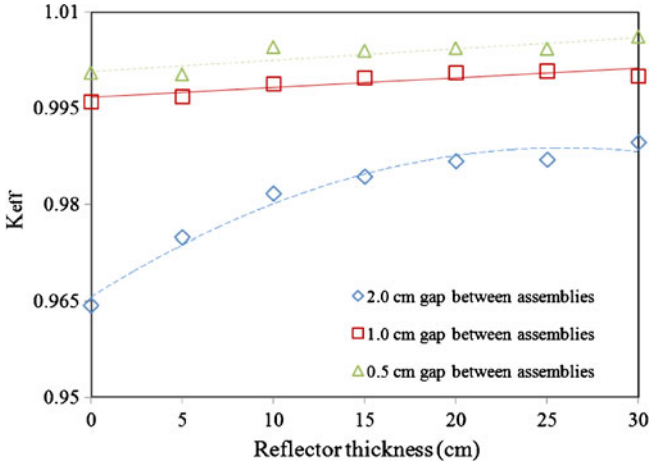

Figure 4. Comparison of K_{eff} with various reflector thicknesses. Gaps between assemblies are 2, 1 and 0.5 cm respectively.

flux fluctuations using BeO of different thicknesses showed that core of 5 cm BeO had about 1.87% enhancement of thermal flux in comparison of 15 cm reflector and a 25 cm reflector caused 9.8% increase in thermal flux (figure 5). Study of leakage percentage indicated an approximate linear decrease after 15 cm thickness of the reflector (figure 6). BeO is expensive but has a compact structure, is safe and economical; hence, 15 cm thickness was chosen as the best for this configuration.

Since maximum resonance absorptions occur in epithermal neutron spectra, design should be managed so that maximum thermal/epithermal flux ratio can be achieved in the fuel assemblies. Calculation showed this ratio is the highest for 0.5 cm assembly intervals compared to the others (table 3).

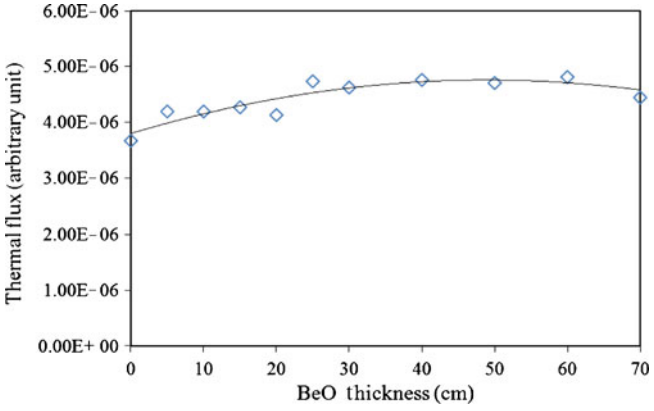

Figure 5. Core thermal flux variations vs. reflector thickness. The gap between assemblies is 0.5 cm.

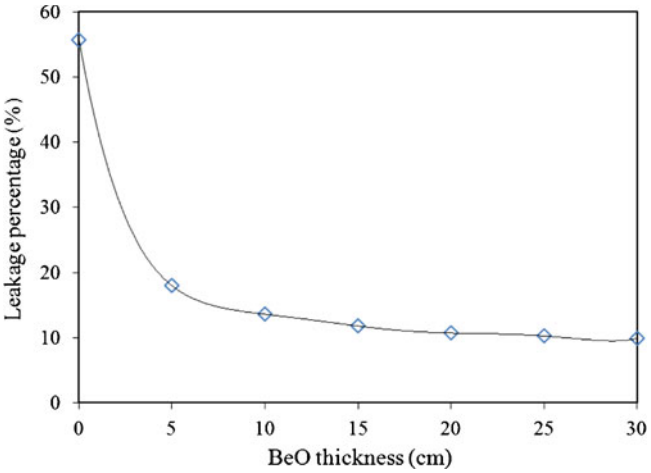

Figure 6. Core thermal neutron leakage percentage vs. reflector thickness variation. The gap between assemblies is 0.5 cm.

According to the simulations, the optimum value for the pitch-to-diameter ratio of the fuel pin (P/D) was 1.25 for the 19-assembly core configuration. In the present study, the P/D ratio for the fuel was not discussed and kept unchanged at 1.25. The optimized core yielded an average of 0.707 fission/capture ratio and 2.437 neutrons per fission. The thermal flux distribution of the reactor was evaluated versus arbitrary unit and ^{235}U fuel mass of 0.0185 ton (figure 7).

For a 0.5 cm gap between the assemblies, peaking factor (Φ_{max}/Φ_{ave}) of 1.21 was achieved; while these values were 1.43 and 1.44 for 1 and 2 cm gaps between the assemblies, respectively. Value of fission/capture ratio is 0.670 for the 1 cm and 0.652 for the 2 cm gap.

To determine the best gap, another important parameter called reactivity was calculated.

Table 3. Epithermal and thermal neutron flux (per source neutron) in the fuel and moderator as a function of the space between the fuel assemblies.

	Epithermal, φ_1	Thermal, φ_2	φ_2/φ_1
	2 cm gap		
Moderator	2.88378E−05	6.18653E−06	21.45
Fuel	1.84729E−05	5.77265E−06	31.24
	1 cm gap		
Moderator	1.67461E−05	4.66808E−06	27.87
Fuel	1.27737E−05	5.83399E−06	45.67
	0.5 cm gap		
Moderator	1.45282E−05	4.02487E−06	27.70
Fuel	1.27621E−05	5.87805E−06	46.05

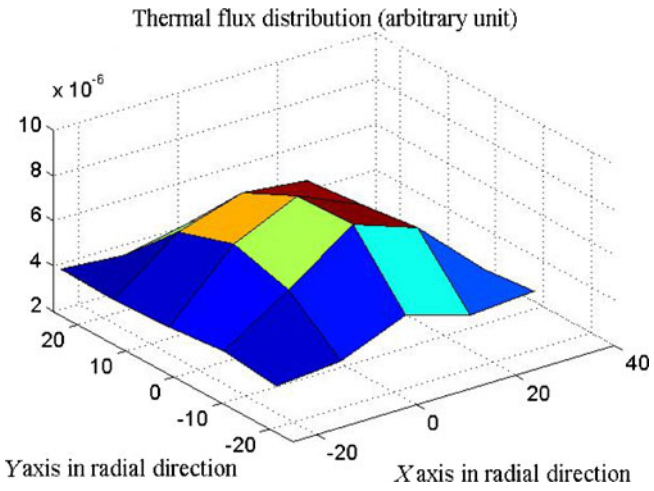

Figure 7. Core thermal neutron distribution vs. assembly position. The gap between assemblies is 0.5 cm.

Using total neutron achieved fission of uranium, prompt neutrons+delay neutrons (TOTNU) card, the delayed neutron fraction, β, and effective delayed neutron fraction, β_{eff}, were estimated to be 0.008 and 0.0074, respectively.

According to the calculations, bubble or gas formation in the moderator will result in a negative reactivity insertion (figure 8). However, this value is more negative for both 1 and 2 cm gaps, 0.5 cm gap is suggested for its lower peaking factor and maximum f/a ratio. Calculations showed that if the circulation system of the moderator is damaged, reactivity insertion will be negative (figure 9).

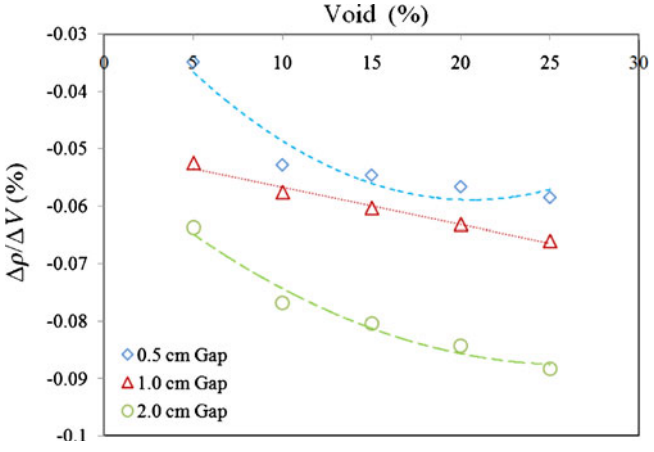

Figure 8. Void reactivity curve as a result of gas formation, BeO: 15 cm, core height: 140 cm, En: 2.2% of ^{235}U.

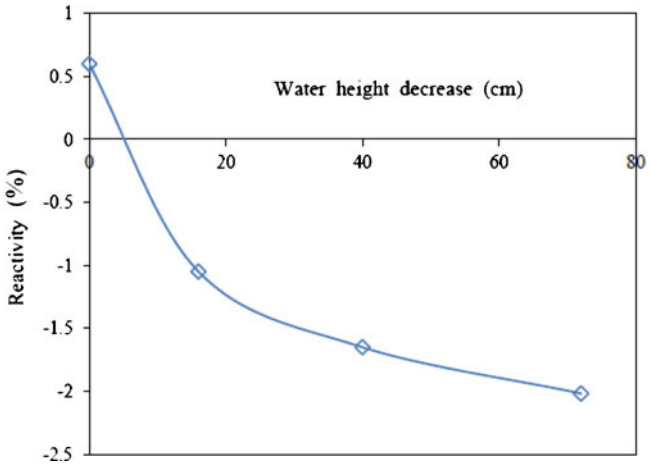

Figure 9. Void reactivity curve as a result of coolant circulation system failure, BeO: 15 cm, core height: 140 cm, En: 2.2% of ^{235}U, gap between the assemblies: 0.5 cm.

Deformation of the fuel pins due to excessive temperature increase causes a 36 μm radial expansion and 2.4 mm axial expansion of the fuel element. Similarly, the thermal expansion of the fuel clad leads to a 14.6 μm radial and 2.5 mm axial linear expansion.

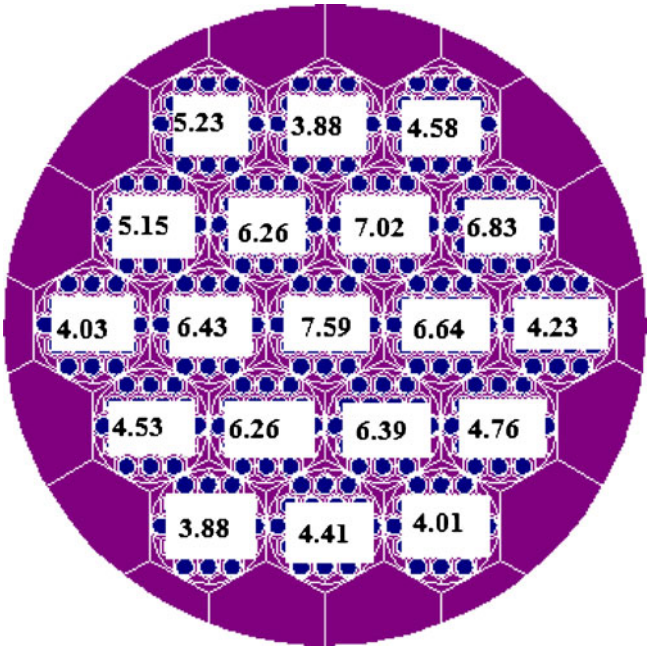

Figure 10. Normalized power distribution vs. arbitrary unit, BeO: 15 cm, core height: 140 cm, En: 2.2% of ^{235}U, gap between the assemblies: 0.5 cm.

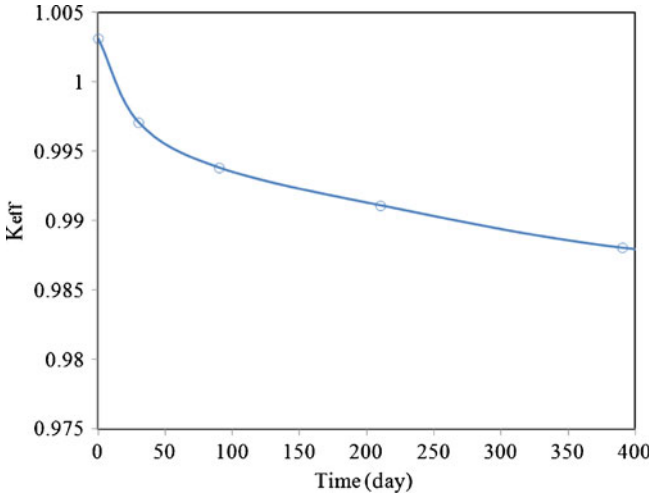

Figure 11. Multiplication on reactor operation time, BeO: 15 cm, core height: 140 cm, En: 2.2% of ^{235}U, gap between the assemblies: 0.5 cm.

Fuel density will decrease to 9.31 g/cm^3 through this expansion. These linear expansions will result in the insertion of -0.33% reactivity coefficient for a 0.5 cm gap. This value is -0.16% for a 2 cm gap.

Inserting six outer control rods concluded in $K_{\text{eff}} = 0.96834$ that causes a -3166 pcm (-31.66 mk) reactivity. Calculation of power distribution using F7 tally resulted in the most intense power on central assembly (figure 10).

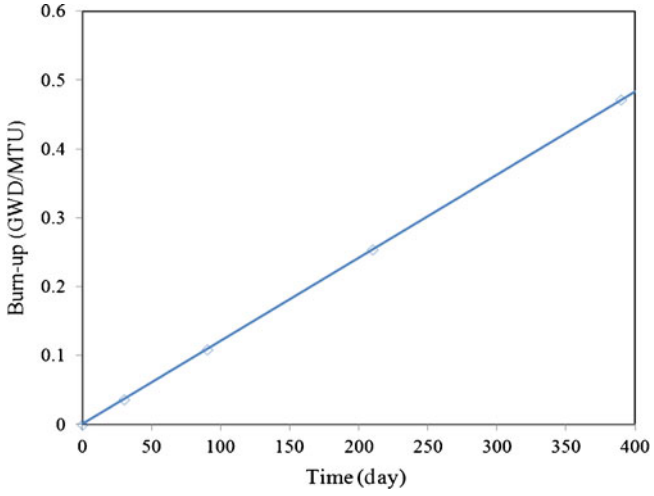

Figure 12. Burn-up, BeO: 15 cm, core height: 140 cm, En: 2.2% of ^{235}U, gap between the assemblies: 0.5 cm.

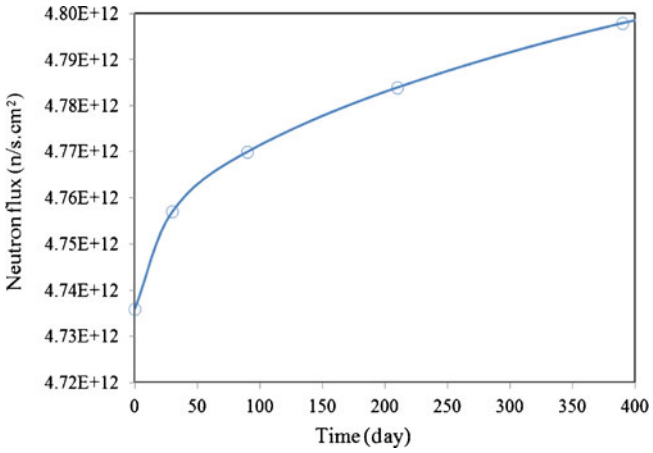

Figure 13. Neutron flux vs. operation time, BeO: 15 cm, core height: 140 cm, En: 2.2% of ^{235}U, gap between the assemblies: 0.5 cm.

Overall, using the interval between assemblies at 0.5 cm implies higher thermal flux through the core and least enrichment needed for criticality. Central channel flux is 8.84×10^{12} (n/s·cm^2), which can be used for radioisotope production or research purposes.

According to burn-up calculations, after 90 days K_{eff} drops to less $1-\beta$. Hence, an assembly management is required after 90 days (figure 11). As seen in figure 12, a 0.109 GWD/MTU burn-up will be achieved after 90 days. Neutron flux has an exponential growth during those 90 days (figure 13). Accumulation of the most important poisons such as ^{135}Xe and ^{149}Sm indicates amounts less than 0.03 and 0.4 g, respectively; ^{135}I has been calculated for ^{135}Xe accumulation along with its direct inventory (figure 14). After

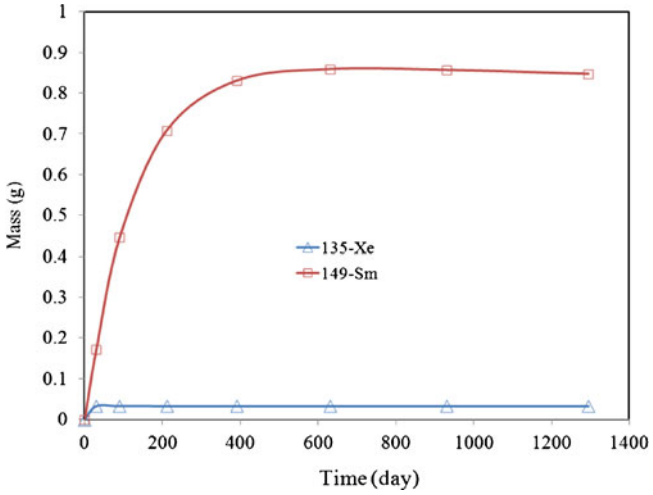

Figure 14. Xe and Sm accumulations vs. reactor operation time, BeO: 15 cm, core height: 140 cm, En: 2.2% of ^{235}U, gap between the assemblies: 0.5 cm.

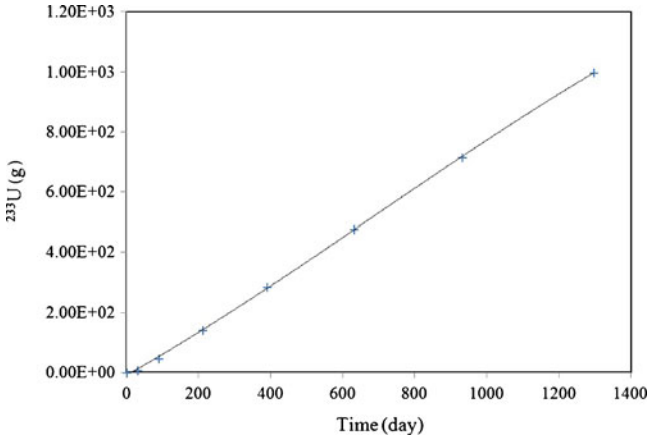

Figure 15. ^{233}U accumulation vs. reactor operation time, BeO: 15 cm, core height: 140 cm, En: 2.2% of ^{235}U, gap between the assemblies: 0.5 cm.

90 days, ^{233}U (44.77 g) is produced during burn-up process (figure 15). Only ^{237}Np is produced after 90 days as long-lived waste (table 4).

According to figures 16 and 17, sum of the fuel and moderator reactivity will be −136.1576 pcm at 100°C. Hence, it can decrease 310 pcm additional reactivity of the first burn-up cycle to 173.8324 pcm (1.738342 mk). Using control rods, positive reactivity can be controlled. Running the core in higher temperatures decreases reactivity to a value lower than the mentioned value because of Doppler broadening phenomena in fuel rods as depicted in figure 16.

Using the core in 1 MW power, which is adequate for research purposes, eliminates high-temperature operations of the core and limits its operation temperature up to a maximum of 100°C.

Table 4. Actinide inventory during burn-up process.

	Mass (g)	Activity (Ci)	Mass (g)	Activity (Ci)	Mass (g)	Activity (Ci)
zaid	30 days		90 days		210 days	
90231	2.36E−03	1.26E+03	2.41E−03	1.28E+03	2.42E−03	1.29E+03
90232	8.10E+05	8.88E−02	8.09E+05	8.88E−02	8.09E+05	8.88E−02
90233	1.83E−02	6.61E+05	1.83E−02	6.61E+05	1.83E−02	6.63E+05
91233	1.71E+01	3.55E+05	2.87E+01	5.95E+05	3.18E+01	6.59E+05
92233	7.41E+00	7.14E−02	4.48E+01	4.31E−01	1.39E+02	1.34E+00
92234	6.68E−03	4.15E−05	4.51E−02	2.80E−04	1.87E−01	1.16E−03
92235	1.84E+04	3.98E−02	1.83E+04	3.96E−02	1.82E+04	3.93E−02
92236	5.88E+00	3.80E−04	1.76E+01	1.14E−03	4.10E+01	2.65E−03
93237	0.00E+00	0.00E+00	2.49E−03	1.76E−06	1.53E−02	1.08E−05

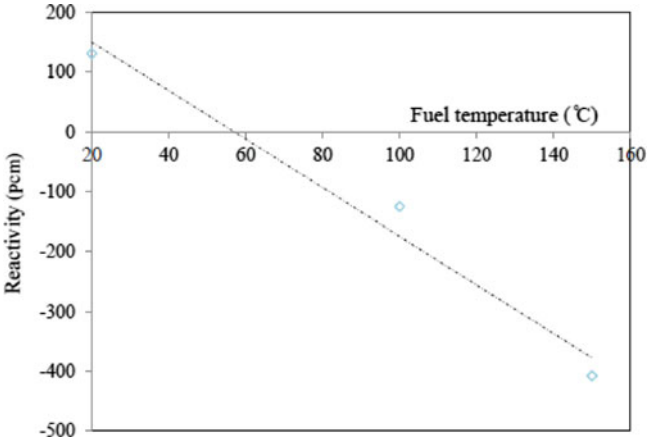

Figure 16. Fuel reactivity variations, BeO: 15 cm, core height: 140 cm, En: 2.2% of ^{235}U, gap between the assemblies: 0.5 cm.

Reactivity of Xe and Sm can be calculated using the computational code as well. Hence, maximum Xe and Sm reactivity achieved is −5.07 mk and −1.5 mk, respectively.

Overall, the discussed parameters provide a safe condition for the operation of a research reactor.

4. Conclusion

19-assemblies compact core with 2.2% ^{235}U enrichment and ^{232}Th were simulated using MCNPX2.6. The designed core resulted in a suitable thermal flux using heavy water

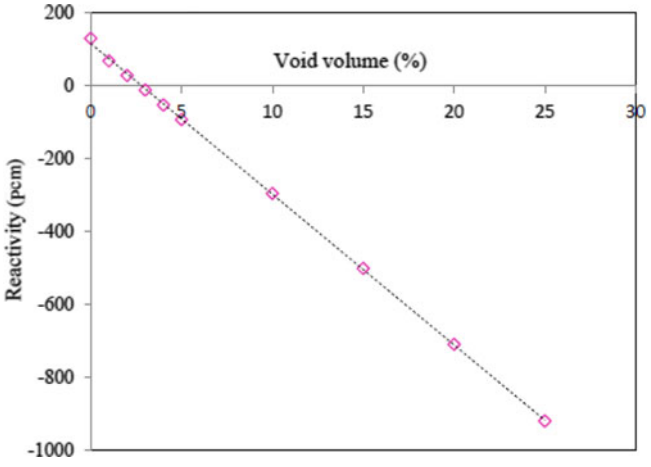

Figure 17. Void reactivity variations, BeO: 15 cm, core height: 140 cm, En: 2.2% of ^{235}U, gap between the assemblies: 0.5 cm.

moderator. The achieved desirable neutron parameters make it operational for training and to the implementation of a nuclear research program. Minimum waste production is one of the most favourable advantage for ^{235}U burning in a research reactor of thorium fertile fuel.

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