Neutronic calculations for CANDU thorium systems using Monte Carlo techniques

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Abstract: In this paper, we have investigated the prospects of exploiting the rich world thorium reserves using Canada Deuterium Uranium (CANDU) reactors. The analysis is performed using the Monte Carlo MCNP code in order to understand how much time the reactor is in criticality conduction. Four different fuel compositions have been selected for analysis. We have obtained the infinite multiplication factor, k_∞, under full power operation of the reactor over 8 years. The neutronic flux distribution in the full core reactor has already been investigated.

Key words: CANDU reactors, thorium oxide, plutonium oxide, MCNP code

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1 Introduction

Alternative fuels can open new dimensions for conventional nuclear reactors with well established technology and long operational experiences. One of the primary interests is to reduce plutonium inventories, because of the serious public and political concern in the world about misuse of plutonium and about accidental release of highly radiotoxic material into the environment [1]. In that respect, various studies have been performed for Canada Deuterium Uranium (CANDU) reactors. Previous work has investigated extensively and in detail the incineration of plutonium in CANDU reactors in combination with thorium [1–3]. As thorium, by itself, is not a nuclear fuel, we need fissile material such as plutonium-239 as a source of neutrons in the early stages of the cycle Eq. (1), [4, 5]. We can use uranium as a booster fissile fuel material but in Eq. (1) it is obvious it can produce more plutonium [5].

$$\begin{aligned}
&\mathrm{U238}\xrightarrow{(n,\gamma)}\mathrm{U239}\xrightarrow{\beta}\mathrm{Np239}\xrightarrow{\beta}\mathrm{Pu239}\xrightarrow{(n,f)}\mathrm{Fission{-}Products},\\
&\mathrm{Th232}\xrightarrow{(n,\gamma)}\mathrm{Th233}\xrightarrow{\beta}\mathrm{Pa233}\xrightarrow{\beta}\mathrm{U233}\xrightarrow{(n,f)}\mathrm{Fission{-}Products}.
\end{aligned}\tag{1}$$

There has been about 40 years' study on thorium fuel cycles. Basic research and development has been conducted in the USA, Germany, India, Russia, Japan and the UK. Several test reactors have been partially or completely loaded with thorium fuel [6]. Whole core demonstration of thorium fuels were explored in the 1960s and 1970s in two types of arrangement. First, thorium dioxide was mixed with highly enriched uranium dioxide in a uniform lattice e.g. the BORAX-Ⅳ, Indian Point Ⅰ, and Elk River BWR Power Stations. Second, a heterogeneous arrangement of seed and blanket regions was used, where the blanket has less uranium and is responsible for most of the in-core fissile production e.g. the high water breeder core of the Sipping-port Reactor Plant [7].

In the past few years, a second round of evaluations was initiated, driven mainly by the goals of reducing plutonium production and perhaps also long-term radioactivity of waste. The USA is conducting four projects involving use of the thorium fuel cycle. All four projects are based on once-through, proliferation resistant, high burn up, long refueling cycle use of thorium in a light water reactor. Three of these projects are part of the Nuclear Energy Research Initiative (NERI) program. In the Russian Federation, research work on the thorium fuel cycle began at nearly the same time as on the uranium based cycle. Atomic Energy of Canada Ltd (AECL) has a very comprehensive program of work on thorium fuel cycles underway. AECL has investigated many techniques for thorium fuel fabrication and has fabricated hundreds of thorium-based fuel elements. A number of full-sized thorium CANDU fuel bundles (uranium-thorium, plutonium-thorium and pure thorium) have

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been irradiated at full power for years in the AECL National Research Universal (NRU) research reactor. High quality thorium fuel bundles have been produced and the program of fuel production is continuing [8]. A typical CANDU reactor core has 380 fuel bundles. The fuel channels have a radius of 23.243 cm and height of 594 cm and contain D_2O moderator at low temperature (<71 ℃) and at ~100 kPa pressure. In the fuel channels there are two tubes with 12.90 and 10.3378 cm radius and 2.794 and 8.686 mm width, made of zircalloy-2 and 97.5%Zr–2.5%Nb, respectively. These two tubes are separated through a gap in order to ensure an effective heat barrier between the low-temperature D_2O moderator and high-temperature D_2O coolant. The gap is filled with CO_2 gas. In smaller tubes, pressure tubes, D_2O coolant and fuel rods are used. Coolant enters the tubes at 266 ℃ and leaves at 310 ℃ at a pressure of ~10 MPa. In the CANDU reactor, each fuel channel contains 37 fuel rods in the fuel bundle zone. The cladding of the rod is made of zircalloy-4 with width 0.874 mm. Each fuel rod has a radius of 1.2243 cm [2]. The full core model has been outlined in Ref. [9].

Calculation of neutron flux in the core is very important and necessary for several areas such as power, neutron activation analysis, radiation damage, neutron dosimetry, and thermal neutron physics [10].

Since the MCNP code [11] results are normalized to one source neutron, the result has to be properly scaled in order to get absolute comparison to the measured quantities (flux, reaction rate, fission density, etc). When one wants to scale the calculated F4 tally "average volume flux", Φ_{F4}, one must use the following equation:

$$\Phi\left[\frac{\text{neutron}}{\text{cm}^2\text{s}}\right] = \frac{P[\text{W}]\bar{\nu}\left[\frac{\text{neutron}}{\text{fission}}\right]}{\left[1.6022\times10^{-13}\frac{\text{J}}{\text{MeV}}\right]w_{\mathrm{f}}\left[\frac{\text{MeV}}{\text{fission}}\right]} \times\frac{1}{K_{\mathrm{eff}}}\Phi_{\mathrm{F4}}\left[\frac{1}{\text{cm}^2}\right], \tag{2}$$

where Φ denotes the actual total neutron flux in the system [12]. In our previous work, we have indicated that how we can calculate k_∞ and neutron flux for the same reactors [13, 14].

In the present work, the neutronic analysis is presented for a CANDU reactor fueled with thorium and 4% reactor grade plutonium or with 3% weapons grade plutonium. Furthermore, for enhanced inherent safeguarding purposes, 5% natural uranium has been added to the mixed fuels. We have selected reactor grade plutonium and weapons grade plutonium to investigate whether or not this type of fuel is useful to reduce plutonium inventories and nuclear warheads. Finally, 5%U-235 is used

Table 1. Composition and atomic density of the reactor fuels.

Fuel name	material	element	weight fraction
Fuel 1	96% ThO_2+4% PuO_2	^{16}O	0.059347653
		^{232}Th	0.905365854
		^{239}Pu	0.021983485
		^{240}Pu	0.008574618
		^{241}Pu	0.002893492
		^{242}Pu	0.001834898
Fuel 2	91% ThO_2 +5%UO_2+4% PuO_2	^{16}O	0.062428518
		^{232}Th	0.858211382
		^{235}U	0.000308515
		^{238}U	0.043765092
		^{239}Pu	0.021983485
		^{240}Pu	0.008574618
		^{241}Pu	0.002893492
		^{242}Pu	0.001834898
Fuel 3	97% ThO_2+3% PuO_2	^{16}O	0.058744906
		^{232}Th	0.914796748
		^{239}Pu	0.024870845
		^{240}Pu	0.001587501
Fuel 4	92% ThO_2+5% UO_2+3% PuO_2	^{16}O	0.061825771
		^{232}Th	0.867642276
		^{235}U	0.000308515
		^{238}U	0.043765092
		^{239}Pu	0.024870845
		^{240}Pu	0.001587501

for the purpose of denaturing the new U-233 fuel with U-238. We will use in the MCNP code the inputs from Table 1, which shows the composition and weight fraction of the different reactor fuels.

2 Calculations

The calculations in this paper are performed using the MCNP code [11]. Fig. 1 shows a cross-sectional view of the fuel cell of a CANDU reactor as described in Section 1.

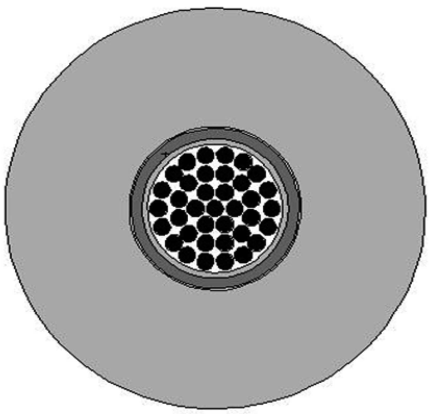

Fig. 1. Cross-sectional view of the fuel cell.

We have applied a reflecting boundary condition in the centre and a white boundary condition at the outer periphery of the cylinderized moderator region. In large CANDU reactors, the k_∞ value of a macro lattice is very close to the $k_{\rm eff}$ of the entire reactor. Criticality of the fuel channel with a white boundary condition at the periphery can represent the reactor core. One of the limitations in MCNP code is that it can't calculate parameters in terms of time. So, to solve this problem, we used the graphs from Refs. [2, 3] and obtained density variations of the fissile and fissionable isotopes in the bundle. Fig. 2 shows one of these graphs and Table 2 shows the values obtained from Fig. 2. We then use these values in code entry and calculate multiplication factor in terms of time.

Figure 3 shows the temporal behavior of reactor criticality k_∞ in terms of operation period.

Figures 4 and 5 show the results from our calculated k_∞ compared with Refs. [2, 3]. The broken lines show the results from Refs. [2, 3] and the solid lines are our calculations. At startup, the composition of fuel in all the rods is uniform and independent of its position in the bundle. During the reactor operation, however, the uniformity of the fuel composition will be lost in the heterogeneous bundle. Hence, fuel burn up and breeding and all other nuclear transformations proceed at the periphery faster than in the center. The middle fuel rod and the next six rods are the central row and the other fuel rods are the peripheral row.

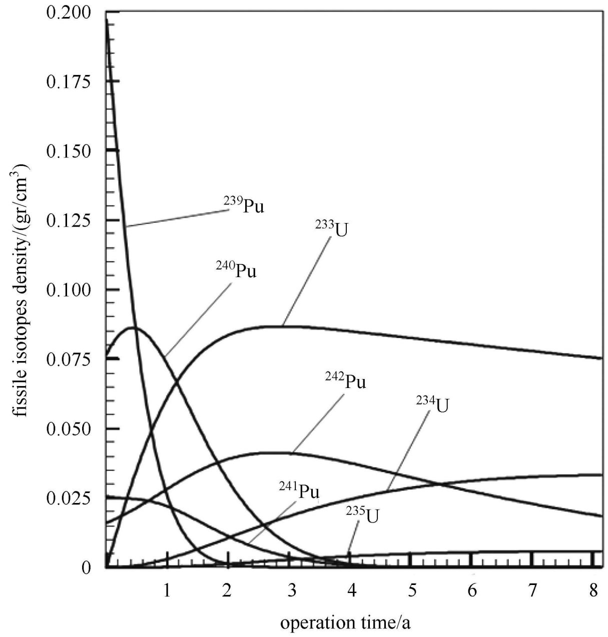

Fig. 2. (color online) Density variations of the main fissionable isotopes in the central fuel row of the bundle with Fuel 1.

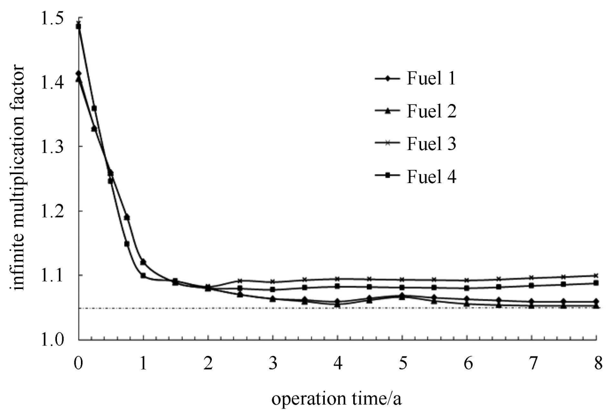

Fig. 3. (color online) Infinite multiplication factor as function of operation time for five different fuel assemblies.

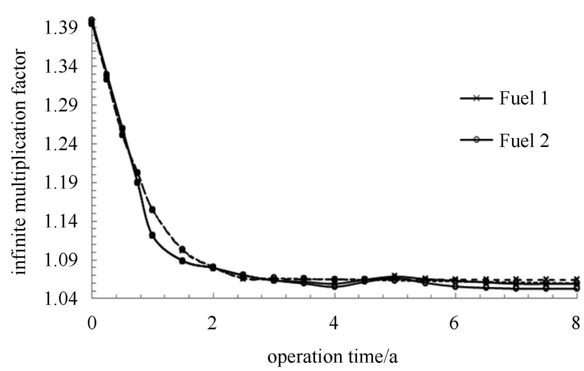

Fig. 4. (color online) Infinite multiplication factor as function of operation time (broken lines: Ref. [2]; solid lines: our work).

Table 2. Density variations of the main fissionable isotopes in the peripheral fuel row of the bundle with Fuel 1.

time/a	density/(g/cm^3)							
	Th-232	U-233	U-234	U-235	Pu-239	Pu-240	Pu-241	Pu242
0	6.629	0	0	0	0.1975	0.0765	0.0252	0.0160
0.25	6.614	0.0176	0.0002	0	0.1405	0.0812	0.0251	0.0186
0.5	6.585	0.0352	0.0005	0	0.0835	0.086	0.0245	0.0212
0.75	6.571	0.0481	0.0019	0	0.0547	0.0795	0.0233	0.0247
1	6.520	0.0610	0.0034	0	0.0260	0.0725	0.0221	0.0282
1.5	6.455	0.0760	0.0070	0	0.0068	0.0515	0.0170	0.0350
2	6.400	0.880	0.0115	0.0001	0.0010	0.0316	0.0112	0.0391
2.5	6.320	0.0879	0.0147	0.0020	0	0.0175	0.0075	0.0409
3	6.280	0.0875	0.0182	0.0030	0	0.0080	0.0040	0.0409
3.5	6.180	0.0865	0.0220	0.0040	0	0.0042	0.0015	0.0396
4	6.107	0.0850	0.0243	0.0044	0	0.0017	0	0.0370
4.5	6.010	0.0840	0.0268	0.0047	0	0.0005	0	0.0350
5	5.920	0.0831	0.0287	0.0050	0	0	0	0.0324
5.5	5.840	0.0815	0.0300	0.0054	0	0	0	0.0297
6	5.783	0.0800	0.0314	0.0055	0	0	0	0.0273
6.5	5.705	0.0785	0.0324	0.0056	0	0	0	0.0250
7	5.600	0.0770	0.0330	0.0056	0	0	0	0.0228
7.5	5.506	0.0750	0.0334	0.0057	0	0	0	0.0204
8	5.440	0.0740	0.0338	0.0057	0	0	0	0.0190

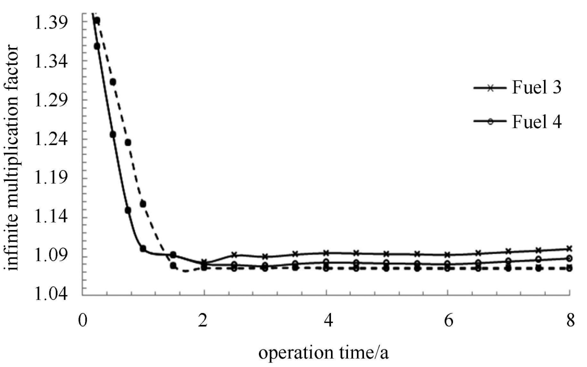

Fig. 5. Infinite multiplication factor as function of operation time (broken lines: Ref. [3]; solid lines: our work).

2.1 Criticality for fuel compositions

Figure 3 shows the infinite lattice criticality k_∞ as a function of the plant operation period by full power for the four different fuel compositions of Section 1. It starts with k_∞=1.413 and 1.405 for reactor grade plutonium (Fuel 1 and Fuel 2, respectively) and with k_∞=1.491 and 1.485 for weapons grade plutonium (Fuel 3 and Fuel 4, respectively). One can observe a steady decrease of the criticality in the first two years. A fuel bundle can be reshuffled in the core until the discharge reactivity $k_{\text{end}}$is attained. The k_{end} is typically 1.06–1.08 considering the leakage from the core and the parasitic absorption in the core.

2.2 Neutron flux calculations

For a continuous source of fission neutrons present in a reactor, we divided the neutron flux into three different energy distributions. The first is thermal neutrons, which have an energy spectrum with a Maxwellian distribution for energy below 0.625 eV. The second is epithermal neutrons, with an energy spectrum characterized by a $1/E^{\alpha+1}$ distribution, where α is the shape parameter, for energy 0.625 eV< E <0.550 MeV. The third is fast neutrons, with an energy range of E>0.550 MeV. Figs. 6 and 7 show the normalized axial and radial thermal, epithermal, fast and total neutron flux over a surface for Fuel 4 for the full core reactor as describes in Section 1. As can be seen from these figures, the thermal neutrons are a significant portion of the flux in the core, and the core is fairly thermalized.

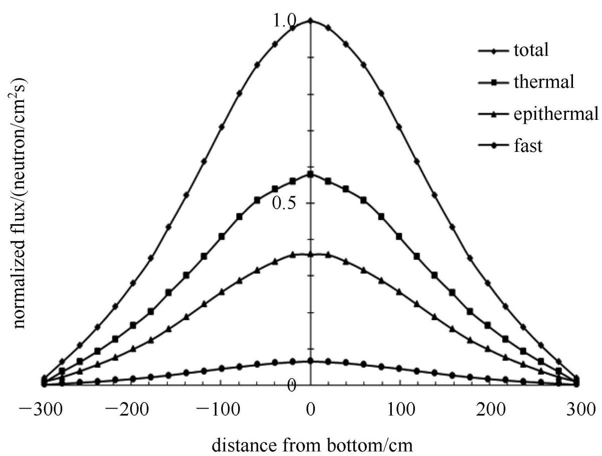

Fig. 6. Comparing normalized axial thermal, epithermal, and fast neutron flux with total normalized axial neutron flux.

With Eq. (2) we can calculate $\Phi_{\max}$ and Φ_{av} of the core to be equal to 4.9×10^{14} and $1.4\times10^{14}\dfrac{\text{neutron}}{\text{cm}^2\text{s}}$, respectively. Dividing the maximum thermal flux by its average value gives

$$\Omega = \frac{\phi_{\mathrm{max}}}{\phi_{\mathrm{av}}} = 3.25. \quad (3)$$

This is a measure of the overall variation of the flux within a reactor and is an indication of the extent to which the power density at the center of the system exceeds the average power density.

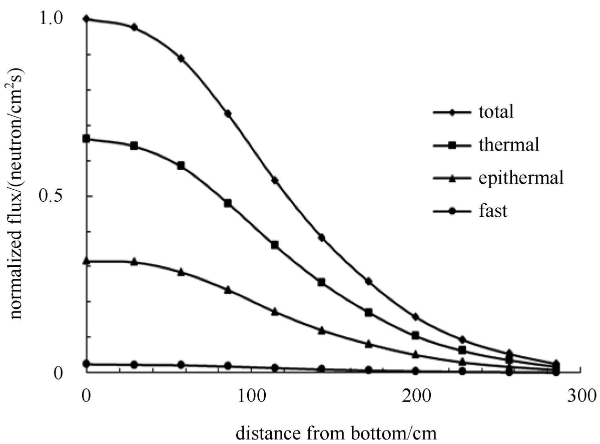

Fig. 7. Comparing normalized radial thermal, epithermal, and fast neutron flux with total normalized radial neutron flux.

In Ref. [15], Ω has been calculated numerically for a bare finite homogeneous cylinder reactor and a value 3.64 obtained. We calculated the volume flux distribution for the full core model, as shown in the Fig. 8. The colors indicate flux intensity. Each colored block represents a single fuel assembly. The power production has a maximum at the center of the reactor core and decreases as the fuel assemblies are further away.

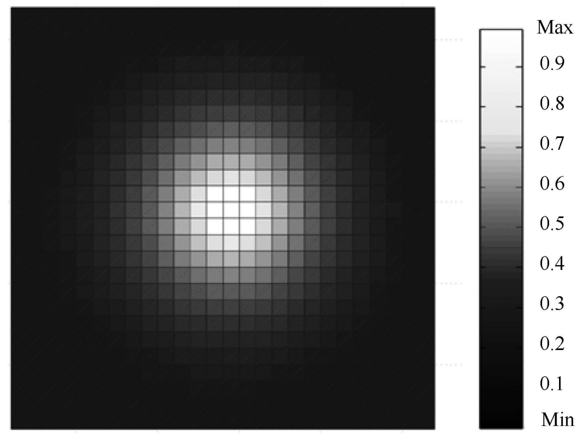

Fig. 8. Normalized flux distribution of neutrons in the core reactor.

3 Conclusions

We can conclude that PuO_2 mixed with thoria would make it possible to run a CANDU reactor over unprecedentedly long operation periods without the need for fuel renewal. At startup, the criticality is quite high with $k_\infty \sim 1.40$. In the first $\sim$2 years, it will drop towards an asymptote well with $k_\infty \sim 1.06$ for operation at full plant power. A criticality value of $k_\infty \sim 1.06$ for the CANDU fuel lattice is considered to be sufficient for a continuous reactor operation.

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References

1 Şahin S, Şahin H M, Acir A. Nuclear Engineering and Design, 2010, **240**: 2066–2074
2 Şahin S, Acir A. Energy Conversion and Management, 2006, **47**: 1661–1675
3 Şahin S, Yildiz K, Şahin H M, Şahin N, Acir A. Nuclear Engineering and Design, 2006, **236**(17): 178–179
4 Busse M. Optimization Of Thorium-Based Seed-Blanket Fuel Cycles For Nuclear Power Plants. M.S., Nuclear Engineering Instituto Balseiro, University of Cuyo, Argentina, 1995
5 Canerl M, Dugan E T. Annals of Nuclear Energy, 2000, **27**: 759–770
6 Chanyun L. Design and Neutronic Evaluation of Thorium Fuel in Pressurized Water Reactors. Master of Science Thesis Reactor Physics Department Royal Institute of Technology, Stockholm, Sweden, 2008
7 LONG Y. Modeling the Performance of High Burn-up Thoria and Urania PWR Fuel. Department of Nuclear Engineering, B.S., Tsinghua University, Beijing, China, 1995
8 IAEA. Thorium Based Fuel Options for the Generation of Electricity: Development in the 1990s, IAEA-TECDOC-1155, 2000
9 Margeanuand C A, Rizoiu A C. Thorium-Based Fuels Preliminary Lattice Cell Studies For CANDU Reactors. Proceedings of the 7$^{\mathrm{th}}$ Conference on Nuclear and Particle Physics. Sharm El-Sheikh, Egypt, 2009
10 Moosakhani A, Nasrabadi M N, Timuri B. Nuclear Engineering and Design, 2011, **241**: 1459–1462
11 Oak Ridge National Laboratory, Monte Carlo N-Particle Transport Code System. Los Alamos National Laboratory, Los Alamos, New-Mexico, 2000. "MCNP4C manual"
12 Snoj L, Ravnik M. Calculation of Power Density with MCNP in TRIGA Reactor. Nuclear Energy for New Europe, International Conference, Portorož, Slovenia, 2006
13 Eshghi Yaraziz M, Shayesteh M. Golobal J. P& A Sci. and Tech., 2011, **v01**: 65–72
14 Eshghi M, Shayesteh M. Archives Des Sciences, 2012, **65**(4): 1
15 Lamarsh J R. Introduction to Nuclear Engineering. Second ed. Addison-Wesley Publishing Co., USA, 1983