

# EVALUATIONS OF TH-BASED CANDU 6 FUEL BUNDLE PERFORMANCE USING MONTE CARLO AND COLLISION PROBABILITY METHODS

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## ABSTRACT

The present study represents a brief analysis of the neutronic parameters (infinite multiplication factor and power distribution) in the CANDU 6 reactor estimated by both Monte Carlo and Collision Probability methods. The simulations were performed using the Continuous-energy Monte Carlo Reactor Physics Burn-up Calculation Code SERPENT 2 along with JEFF-3.1.1 library and the Open-Source Deterministic Transport Code DRAGON 5 with the IAEA 69 energy groups library.

The fuel composition chosen for this study has different fissile concentration placed in the bundle rings. The central element contains only ThO<sub>2</sub>, while the inner and intermediate rings contain 60% ThO<sub>2</sub>, and the outer ring 80% ThO<sub>2</sub>. Different bundle fuel charges were investigated by varying the <sup>235</sup>U enrichment in radial direction and keeping constant the Th/U ratio.

The results highlight that using of (Th,U)O<sub>2</sub> in CANDU 6 reactors is both technically feasible and economically useful.

**Key words: Thorium, CANDU, Monte Carlo, Collision Probability**

## Introduction

The CANDU reactors have the capability to operate with various types of fuels, such as DUPIC (Direct Use of spent PWR fuel In CANDU reactor) fuel, NUE (Natural Uranium Equivalent) fuel, and thorium-based fuel [1]. The versatility of the CANDU system comes from the on-power refuelling and using of the heavy water moderator which provides superior neutron economy characteristics.

The interest for thorium-based fuel in CANDU reactors was renewed by inherent advantages: in nature, thorium is three to four times more abundant than uranium [2]; ThO<sub>2</sub>, has superior physical-chemical properties than UO<sub>2</sub> [3]; the fissionable isotope of thorium fuel cycle, <sup>233</sup>U, has the highest average reproduction factor in a thermal spectrum from among the four practical fissionable isotopes (<sup>233,235</sup>U, <sup>239,241</sup>Pu); the use of thorium-based fuels produces substantially less amounts of minor actinides and plutonium than the uranium-based fuels [4].

## Roadmap Study

The complexity of a nuclear reactor analysis requires a simplified model, with penalties in results precision [5]. The aim of this study is to perform a comparison between probabilistic Monte Carlo (MC) and deterministic Collision Probability (CP) methods used for CANDU 6 lattice cell calculation. In the present study, the Continuous-energy Monte Carlo Reactor Physics Burn-up Calculation Code SERPENT 2, version 2.1.30 [6] has been used. SERPENT 2 calculations were performed using ACE format cross section library based on JEFF-3.1.1 [7]. To perform the deterministic calculations, the open-source deterministic transport code DRAGON 5 [8] along with the IAEA 69 energy groups library [9] were used.

The simulated geometry consists in a 3D lattice cell model which is representative for the average CANDU 6 core. The radial section for this fuel bundle model is shown in Fig. 1. This simple approximation offers relevant indications for the use of thorium in CANDU 6. The reflective boundary conditions are used to simulate an infinite lattice of elementary cells. Burn-up calculations were performed at an average bundle power of 700 kW (mean value obtained considering ~80% of the fuel bundles in the core) [3]. Model characteristics, material and geometry data for CANDU 6 fuel bundle are according to a test problem presented in Ref. [10]. The materials used for the calandria tube and the pressure tube were Zircaloy-2 and Zr-Nb, respectively. The annular gas between the pressure tube and the calandria tube is the carbon dioxide. The heavy water coolant and moderator have different D<sub>2</sub>O purity, namely: 92.22 % (coolant) and 99.91 % (moderator). The coolant is located inside the pressure tube and the moderator is outside the calandria tube. The best matching temperature in the libraries, for nominal conditions, are 1000 K for the fuel, 600 K for the D<sub>2</sub>O coolant, Zircalloy-4 fuel clads and Zr-Nb pressure tubes, and 300 K for the Zircaloy-2 calandria tubes, CO<sub>2</sub> annular gas and D<sub>2</sub>O moderator, respectively.

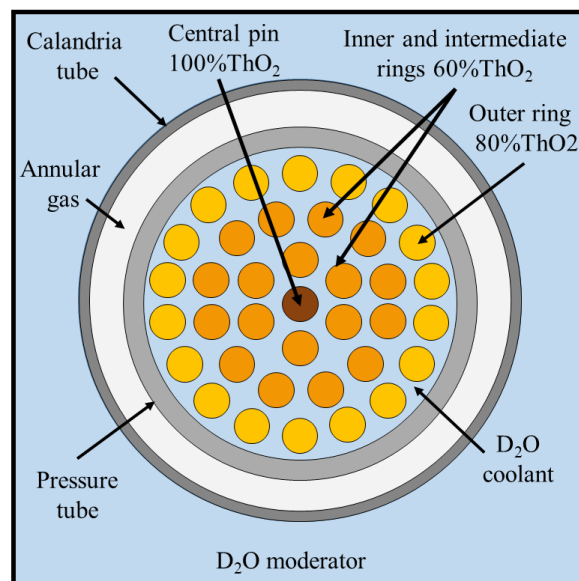


Fig. 1. Radial section of the lattice cell for CANDU 6.

Since some fissile material is needed to maintain the chain reaction in Th-based fuel systems, the objective of the study was to define a fuel composition based on Low Enriched Uranium (LEU) and Thorium mixed oxide (Th,U)O<sub>2</sub> for the CANDU 37 elements bundle, thus obtaining an advanced fuel bundle, hereafter named T37.

Based on previous preparatory work, the bundle rings were considered to contain different fissile concentration in the fuel pellets. The central element contains only ThO<sub>2</sub>, with the pellet density of 9 g/cm<sup>3</sup>, while the inner and intermediate rings contain 60% ThO<sub>2</sub>, and the outer ring 80% ThO<sub>2</sub>, the pellet density being considered 9.6 g/cm<sup>3</sup>. The pellet densities were lower than the usual CANDU one

(10.7 g/cm<sup>3</sup>), given the ThO<sub>2</sub> synthesising technology limits. Different bundle fuel charges were investigated by varying the <sup>235</sup>U enrichment in radial direction. The neutronic performance results of different ThO<sub>2</sub>/UO<sub>2</sub> fuels in CANDU were compared with the standard CANDU 6 fuel bundle (U<sub>nat</sub>) results.

## Results and discussions

### SERPENT criticality evaluations

The model validation has been performed by simulating a U<sub>nat</sub> bundle. Once the model has been validated for U<sub>nat</sub> bundle, the fuel was replaced by thorium–uranium mixed oxide (Th,U)O<sub>2</sub>. To obtain the best results for criticality along with extended burn-up and power flattening, different tests have been conducted by varying the <sup>235</sup>U enrichment in the radial direction. The SERPENT results for the evolution of criticality are given in Fig. 2 for the five preliminary Th-U "best fit" bundle variants, as follows:

- T37\_666 contains 6% <sup>235</sup>U in the inner, intermediate and outer rings;
- T37\_667 contains 6% <sup>235</sup>U in the inner and intermediate rings, and 7% <sup>235</sup>U in the outer ring;
- T37\_668 contains 6% <sup>235</sup>U in the inner and intermediate rings, and 8% <sup>235</sup>U in the outer ring;
- T37\_776 contains 7% <sup>235</sup>U in the inner and intermediate rings, and 6% <sup>235</sup>U in the outer ring;
- T37\_777 contains 7% <sup>235</sup>U in the inner, intermediate and outer rings.

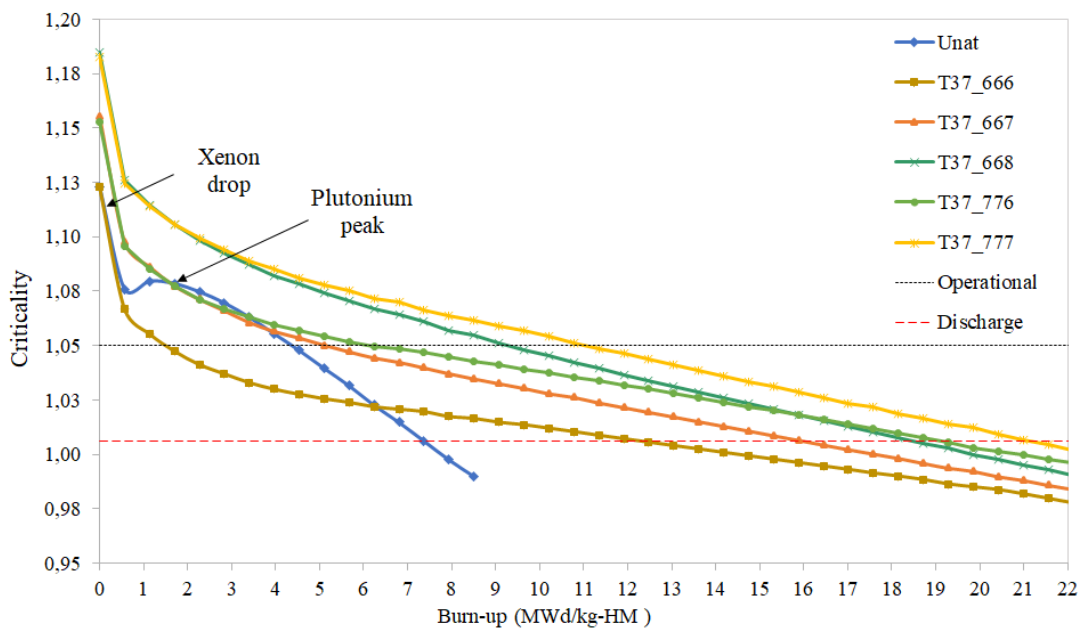


Fig. 2. Evolution of criticality for different T37 fuel bundle cases and the U<sub>nat</sub> bundle.

The initial value of the infinite lattice multiplication factor ( $k_{\infty}$ ) depends on the fissile and fertile material content in the fuel bundle. As it can be seen in Fig. 2, the initial  $k_{\infty}$  is higher for the cases with higher initial fissile material contents. The evolution of criticality with burn-up for the five preliminary cases shows that only T37\_667 and T37\_776 variants are both technically feasible and economically useful.

The first  $k_{\infty}$  drop observed both in T37 and U<sub>nat</sub> cases occurs due to the formation of absorbing <sup>135</sup>Xe while the second effect, called the “plutonium peak” appears only in the case of U<sub>nat</sub> bundle being explained by the important concentration of <sup>238</sup>U that produces the fissionable <sup>239</sup>Pu isotope.

*Criticality and burn-up*

The criticality results for the depletion curves of the two T37 bundles cases are shown in Fig. 3 in comparison with those obtained for the reference  $U_{nat}$  bundle. The figure shows relatively large discrepancies between the results obtained with SERPENT 2 and DRAGON 5 codes. In the case of  $U_{nat}$ , SERPENT 2 gives higher values for  $k_{\infty}$  along with burn-up, while in the T37 cases it gives lower values than DRAGON 5. This behaviour can be explained by the different methods and different cross section libraries used by the two codes. Therefore, an additional evaluation has been performed by means of the deterministic WIMS-D5 [11] using the IAEA 69 energy groups library [9]. As it can be observed, excepting the “plutonium peak”, the results obtained with WIMS-D5 are in good agreement with the SERPENT 2 results for  $U_{nat}$  and with the DRAGON 5 results for T37 cases.

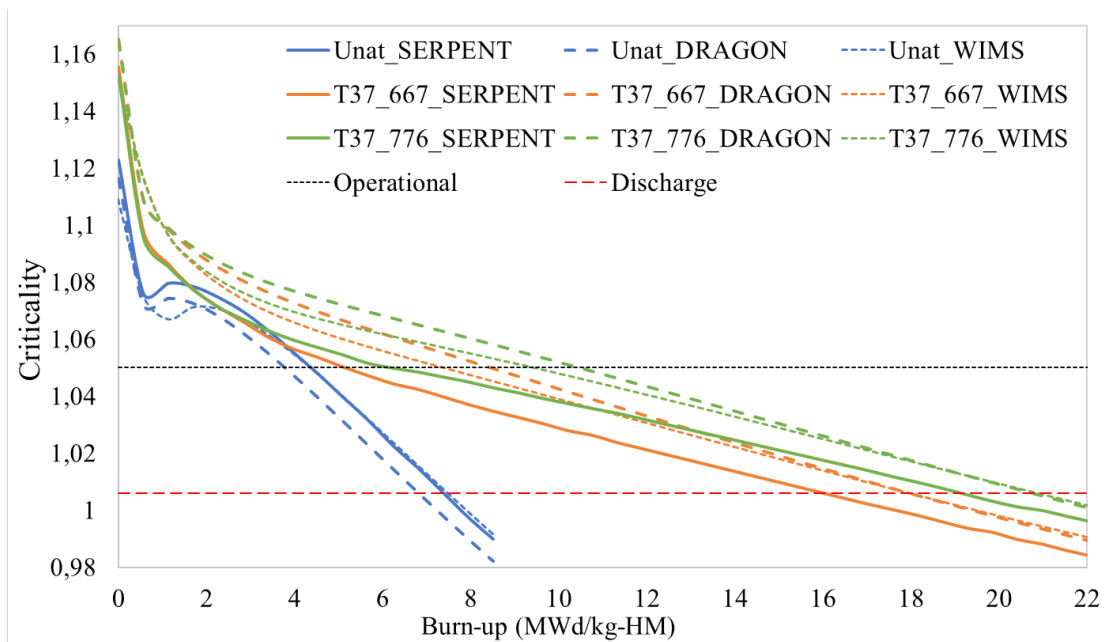


Fig. 3. SERPENT vs. DRAGON and WIMS evolutions of criticality for T37 and  $U_{nat}$  bundles.

The discharge burn-up (expressed in MWd/kg of Heavy Metal, HM) results obtained in SERPENT 2/DRAGON 5/WIMS-D5 calculations for T37 and  $U_{nat}$  bundles are given in Table 2.

Table 2. SERPENT vs. DRAGON and WIMS discharge burn-up of the T37 and  $U_{nat}$  bundles.

	Discharge burn-up[MWd/kg-HM]		
	SERPENT	DRAGON	WIMPS
$U_{nat}$	7,4	6,8	7,4
T37_667	15,9	17,6	17,6
T37_776	18,7	20,4	20,4

Based on the obtained results, the following observations can be made:

- the discrepancies between SERPENT 2 and WIMS-D5 results are caused only by using of different nuclear data libraries, regardless the transport equation solving methods implemented in the two codes;
- when the same IAEA 69 nuclear data library was used, the discrepancies between WIMS-D5 and DRAGON 5 results rely only on the different solving methods.

Let us note that the differences between the SERPENT 2 and DRAGON 5 results mainly rely on the different methods (MC and CP) used by each code.

*Bundle power distribution*

The bundle power distribution plays an important role in safety analyses and also in estimating the fuel cost effectiveness. The variation of the Th/U ratio along with different fissionable material has been introduced to obtain the flattening of the bundle power distribution. As compared with the  $U_{nat}$  bundle, the T37 bundles induce a balanced radial power distribution by increasing the power corresponding to the central pin, inner and intermediate ring elements and decreasing the power on the outer ring [3]. The radial pin power factors (PF) obtained with SERPENT 2 code at the Beginning-Of-Cycle (BOC) and at End-Of-Cycle (EOC) for the considered T37 bundles as compared to the reference  $U_{nat}$  case are shown in Figs. 4 and 5. The "ideal situation" (PF=1) is represented with black dotted line.

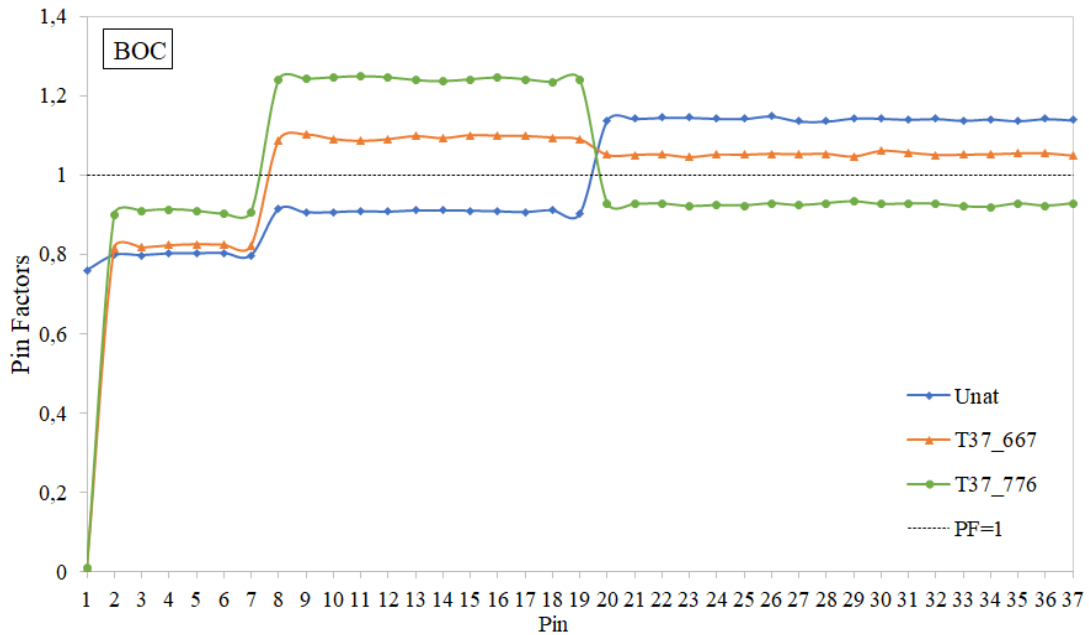


Fig. 4. SERPENT pin power (normalised to the mean power) at BOC.

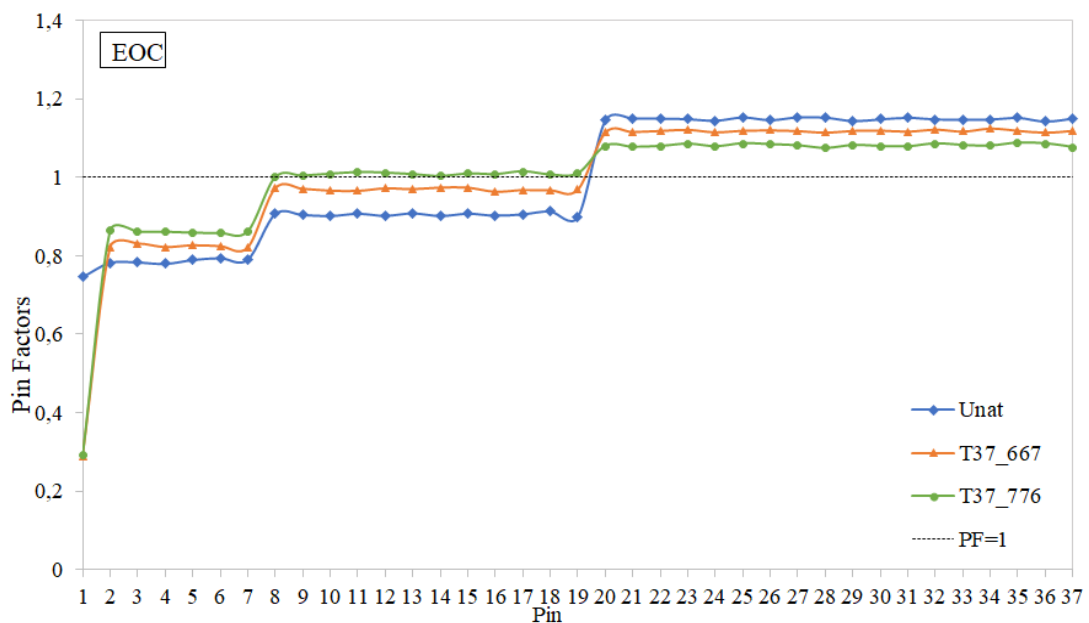


Fig. 5. SERPENT pin power (normalised to the mean power) at EOC.

As observed, both at BOC and EOC, the T37 configurations improve the power flattening leading to a better utilization of the fuel. It is useful to note that the lack of the fissionable material in the central pin leads to lower values of the corresponding PF. The radial decreasing of the enrichment on the outer ring (case T37\_776) leads to a more balanced power distribution with burn-up than the radial increasing of the enrichment (case T37\_667).

The radial power distributions at BOC and EOC obtained with SERPENT 2 and DRAGON 5 codes expressed by PFs are shown in Table 2 and Table 3, respectively. Although the two codes use different methods, the results are close.

Table 2. SERPENT and DRAGON pin power factors of the T37 and  $U_{nat}$  bundles at BOC.

		$U_{nat}$	T37_667	T37_766
PF_1	SERPENT	0.76	0.01	0.01
	DRAGON	0.78	0.01	0.01
PF_2	SERPENT	0.80	0.82	0.91
	DRAGON	0.81	0.86	0.95
PF_3	SERPENT	0.91	1.09	1.24
	DRAGON	0.92	1.11	1.26
PF_4	SERPENT	1.14	1.05	0.93
	DRAGON	1.13	1.03	0.90

Table 2. SERPENT and DRAGON pin power factors of the T37 and  $U_{nat}$  bundles at EOC.

		$U_{nat}$	T37_667	T37_766
PF_1	SERPENT	0.75	0.29	0.29
	DRAGON	0.81	0.33	0.35
PF_2	SERPENT	0.79	0.82	0.86
	DRAGON	0.84	0.85	0.88
PF_3	SERPENT	0.91	0.97	1.01
	DRAGON	0.93	0.98	1.00
PF_4	SERPENT	1.15	1.12	1.08
	DRAGON	1.11	1.10	1.08

## Conclusions

- C1. The present study represents a brief analysis of the neutronic performance for LEU and thorium mixed oxide fuel in CANDU 6 using SERPENT 2 and DRAGON 5 codes. The analysis using different types of codes, based on MC and CP methods, has been performed by comparing the evolution of criticality with burn-up and evaluating the pin power factors at BOC and EOC, respectively.
- C2. The CP method used in DRAGON 5 code estimates lower values of  $k_{\infty}$  than the MC method implemented in SERPENT 2 code. The higher values given by DRAGON 5 code for T37 cases are due to using of the IAEA 69 nuclear data library. Based on the results obtained for  $U_{nat}$ , the expected  $k_{\infty}$  results given by SERPENT 2/ DRAGON 5 codes with the same nuclear data library should be lower for DRAGON 5.
- C3. The T37 configurations improve the power flattening leading to a better utilization of the fuel. For the T37\_776 bundle, the radial decreasing of the enrichment leads to a more balanced power distribution with burn-up than the case T37\_667.
- C4. The SERPENT 2 and DRAGON 5 codes provide similar radial pin power factors both at BOC and EOC.

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