

# Comparison of (Th-<sup>233</sup>U) O<sub>2</sub> and (Th-<sup>235</sup>U) O<sub>2</sub> fuel burn up into a thermal research reactor using MCNPX 2.6 code

S.A.H. Fegghi<sup>1</sup>, Z. Gholamzadeh<sup>2\*</sup>, L. Soltani<sup>3</sup>, C. Tenreiro<sup>2, 4</sup>

<sup>1</sup>Department of Rays Applications, Nuclear Engineering Faculty, Shahid Beheshti University, Tehran, Iran

<sup>2</sup> Department of Physics, Talca University, Chile

<sup>3</sup> Nuclear Science & Technology Research Institute, AEOL, Tehran, Iran

<sup>4</sup>Department of Energy Science, Sungkyunkwan University, 300 Cheoncheon-dong, Suwon, Korea

## ABSTRACT

### ► Original article

**\* Corresponding author:**

Mrs. Zohreh Gholamzadeh,

Fax: +98 21 29902546

E-mail: [Cadmium\\_109@yahoo.com](mailto:Cadmium_109@yahoo.com)

Received: Nov. 2012

Accepted: Dec. 2012

*Int. J. Radiat. Res., January 2013;*  
*11(1): 29-33*

**Background:** Decrease of economically accessible uranium resources motivates consideration of breeding of fertile elements such as thorium. **Material and Method:** Thorium oxide fuel burn up calculation of a simulated research reactor cooled heavy water has been proposed in the present work using MCNPX 2.6 code. Two <sup>233</sup>U and <sup>235</sup>U isotopes have been used as fissile element of thorium oxide fuel. <sup>135</sup>Xe and <sup>149</sup>Sm reactivity variations has been studied in the core loaded (Th-<sup>233</sup>U)O<sub>2</sub> or (Th-<sup>235</sup>U)O<sub>2</sub> fuel matrixes during 3 months burn up process. **Results:** Thorium oxide having 4% <sup>233</sup>U burned 1 MW power results in less <sup>149</sup>Sm reactivity than thorium oxide having 4% <sup>235</sup>U burned in 0.5 MW power. <sup>135</sup>Xe reactivity has an overestimated shift by 15 days in the core operated in 0.5 MW than the other, after 15 days both the cores behave similarly. 480 g of <sup>233</sup>U burns into the core using 0.5 MW power and 364 g of <sup>233</sup>U invents after 3 months. Burn up calculation of the modeled core of (Th-<sup>233</sup>U)O<sub>2</sub> fuel shows a fissile mass reduction by 60 days while the consumed fissile mass reaches to its initial value after 120 days. The core flux is constant during 3 months for both modeled cores. A considerable negative reactivity occurs up to 15 days in both cores which can be refer to xenon inventory during this time and then neutron multiplication factor is steadier up 3 months. **Conclusion:** Breeder thorium fuel enriched <sup>233</sup>U make several advantages of good neutronic economy, <sup>233</sup>U inventory and less inventory of long-lived alpha emitter wastes.

**Keywords:** Thorium oxide fuel, neutronic parameters, fuel burn up, <sup>233</sup>U fissile material, <sup>233</sup>U fissile material.

## INTRODUCTION

Thorium is three times more abundant in nature compared to uranium and occurs mainly as 'fertile' <sup>232</sup>Th isotope. From the inception of nuclear power program, the immense potential

of <sup>232</sup>Th for breeding human-made 'fissile' isotope <sup>233</sup>U efficiently in a thermal neutron reactor has been recognized. Several experimental and prototype power reactors were successfully operated during the mid-1950s to the mid-1970s using (Th, U)O<sub>2</sub> and (Th, U)C<sub>2</sub> fuels in high temperature gas cooled reactors (HTGR), (Th, U)O<sub>2</sub> fuel in light water reactors (LWR) and

LiF/BeF<sub>2</sub>/ThF<sub>4</sub>/UF<sub>4</sub> fuel in molten salt breeder reactor (MSBR) (1).

Thorium can sustain a thermal breeding cycle using external fissile materials like uranium-235, plutonium or an accelerator driven neutron source.

Some reactors has been designed to burn thorium oxide fuel; the Indian advanced heavy water reactor (AHWR) is designed and developed to achieve large-scale use of thorium for the generation of commercial nuclear power. This reactor will produce most of its power from thorium, with no external input of uranium-233, in the equilibrium cycle. AHWR is a 300 MWe, vertical, pressure-tube type, boiling light water cooled, and heavy water moderated reactor (2).

MCNPX depletion provides a vital modeling framework, within a well established, supported reactor safeguards radiation transport code, for high-fidelity depletion calculations to assist in the development of technologies requiring ample intricate detail in the depletion solution such as the reactor safeguards calculations.

MCNPX will be used to calculate steady-state reaction rates and normalization parameters while CINDER90 will be used to calculate the time-dependent isotope buildup/depletion (3, 4).

Hence, burn up process consideration of thorium oxide fuel enriched by <sup>233</sup>U or <sup>235</sup>U fissile elements has been proposed in the present work using Monte Carol-based transport computational method.

## MATERIALS AND METHODS

Heavy water has been used as coolant and moderator for this reactor. A 3D neutronic model was set up using MCNPX2.6 code in cold zero power situations by means of ENDF/B-VI continuous-energy cross section. The temperature fuel and heavy water was assumed to be 20°C. The cross sections S (α,β) has been used for BeO reflector material and heavy water.

KCODE with 15000 initial neutrons, 250 effective cycles and 50 ineffective cycles has

been used for the parameter calculations.

A 37-assembly core of 35 cm radius and 70 cm height has been modeled as the mentioned dimensions and materials in table 1.

As it is seen in figure 1, fuel pins have been placed in hexagonal array and 19 pins has been used in any assembly. 1 fuel pin has been removed from 6 central assemblies to allow control rods be loaded.

Thorium oxide fuel consists of two isotopes of 232-thorium and 235-uranium/233-uranium (4%). The fuel assemblies have 19 fuel pins of 50 cm height, 5mm He gap and 4 mm zirconium alloy cover which has been placed in pitch to diameter (P/D) ratio of 1.61 in any assembly. P/D ratio of the assemblies has been selected as 1.000011.

Fuel burn up of both structures has been calculated in 363°K temperature. 1MW power has been used for (Th+<sup>233</sup>U) O<sub>2</sub> burning and 0.5 MW has been used for (Th+<sup>233</sup>U)O<sub>2</sub>.

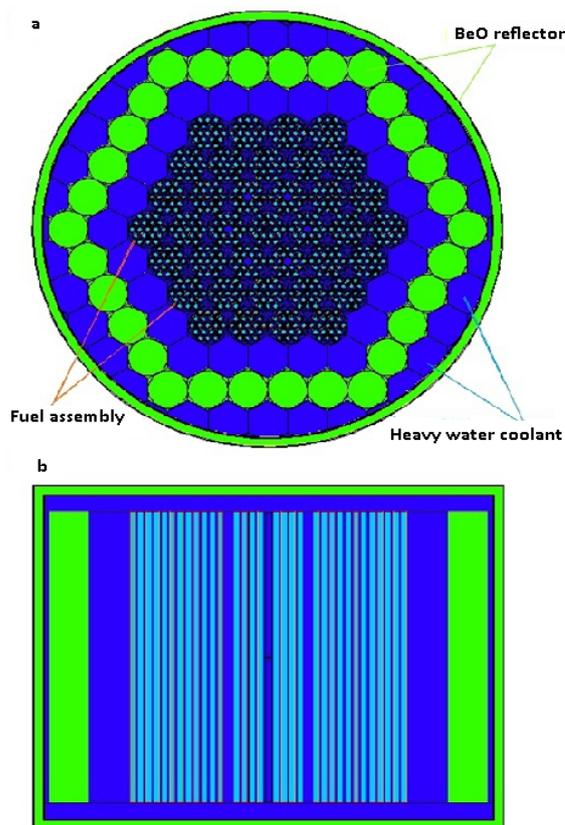


Figure 1. Schematic view of the modeled core, a) cross-sectional b) axial.

Table 1. The used materials in the reactor core.

MAT.	Compounds (wt %)	Density (g/cm <sup>3</sup> )	Thickness (cm)
Fuel	<sup>235/233</sup> U: 4, <sup>232</sup> Th: 96, O:2.09E-06	11.64	1.10
Cover of fuel	Zircaloy-4( Sn:1.4, Fe:0.23, Cr:0.1., Zr: 98.27 )	6.50	0.04
Gap	He	0.000411	0.05
Cover plate	SS-304 ( Fe:69.5,Cr:19.0, Ni: 9.5, Mn: 2.0)	7.92	0.2
Reflector	Be:36, O:64	3.00	2.00

## RESULTS AND DISCUSSION

Reactivity can be calculated using the following formula:

$$\rho = \frac{K_{eff} - 1}{K_{eff}} \quad (1)$$

The reactivity defined in the previous section is often measured in fractions of the effective delayed neutron fraction. One unit of  $\rho/\beta_{eff}$  is called a *dollar* (5). Where  $\beta_{eff}$  is the effective delayed neutron fraction,  $\beta_{eff}$ , defined as the number of fissions induced by delayed neutrons,  $N_d$ , compared to the total number of fissions induced in the same system,  $N_{Tot}$

$$\beta_{eff} = \frac{N_d}{N_{Tot}} \quad (2)$$

By using TOTNU in KCODE card, fraction of delay neutrons can be calculated. Insertion of (Th-<sup>235</sup>U)O<sub>2</sub> assemblies into the simulated core resulted in  $\beta=635$  pcm and  $\beta_{eff}= 711$  pcm while the obtained parameters for (Th-<sup>233</sup>U)O<sub>2</sub> assemblies are  $\beta=252$  pcm and  $\beta_{eff}= 373$  pcm.

As it is seen in figure 2, up 30 days the core reactivity is negative in case of both modeled cores. After 30 days, the reactivity starts to be positive by 3 months.

The F4 tally is used to calculate neutron flux and the code outputs could be normalized by following equation (6).

$$\frac{dN_i}{dt} = \sum_j \gamma_{ij} \sigma_{f,j} N_j \varphi + \sum_k \sigma_{c,k \rightarrow i} N_k \varphi + \sum_l \lambda_{l \rightarrow i} N_l - (\sigma_{f,i} N_i \varphi + \sigma_{a,i} N_i \varphi + \lambda_i N_i)$$

If a particle of weight  $W$  and energy  $E$  makes a track-length (segment)  $T$  within a specified cell of volume  $V$ . This segment makes a contribution  $WT/V$  to the flux (fluence) in the cell. The sum of the contributions is reported as the F4 tally in

$$F4 = \frac{1}{V} \int_V dV \int_E dE \int_{4\pi} d\Omega \Phi(r, E, \Omega) \quad (3)$$

the MCNP output. Technically, if  $\Phi(r, E, \Omega)$  were the energy and angular distribution of the fluence as a function of position, the F4 tallies would measure (7):

Neutron flux is steady during the three months burnup process for both the evaluated cores. The flux value is completely suitable for research goals (figure 3).

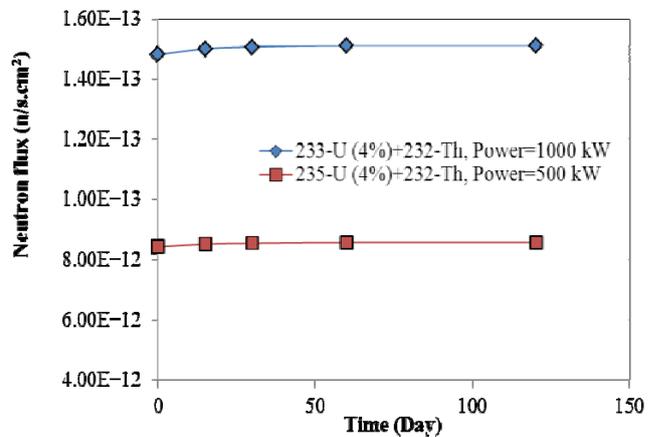


Figure 3. Neutron flux on operation time.

Mathematically, the material balance process can be described at any time by the following depletion equation:

Where  $\frac{dN_i}{dt}$  = time rate of change in concentration of isotope i,  $\sum_j \gamma_{ij} \sigma_{fj} N_j \phi$  = production rate per unit volume of isotope i from fission of all fissionable nuclides,  $\sum_k \sigma_{c,k \rightarrow i} N_k \phi$  = production rate per unit volume of isotope i from neutron transmutation of all isotopes including (n, $\gamma$ ), (n,2n), etc.,  $\sum_l \lambda_{l \rightarrow i} N_l$  = production rate per unit volume of isotope i from decay of all isotopes including  $\beta^-$ ,  $\beta^+$ ,  $\alpha$ ,  $\gamma$ , etc.,  $\sigma_{fi} N_i \phi$  = removal rate per unit volume of isotope i by fission,  $\sigma_{a,i} N_i \phi$  = removal rate per unit volume of isotope i by neutron absorption (excluding fission),  $\lambda_i N_i$  = removal rate per unit of isotope i by decay, the computation code follows the equation calculation to present time rate of change in concentration of any isotope (8).

Fuel burn up calculations showed 480 g of  $^{235}\text{U}$  will burn during 3 months burn up process in 500 kW power in case of (Th+ $^{235}\text{U}$ )O<sub>2</sub> fuel loaded into the core. In the modeled core of (Th+ $^{233}\text{U}$ )O<sub>2</sub> fuel, 100 g of  $^{233}\text{U}$  decreases up 60 days then  $^{233}\text{U}$  mass starts to enhancement and the enhanced mass value reaches to 100 g at 120<sup>th</sup> day (figure 4).

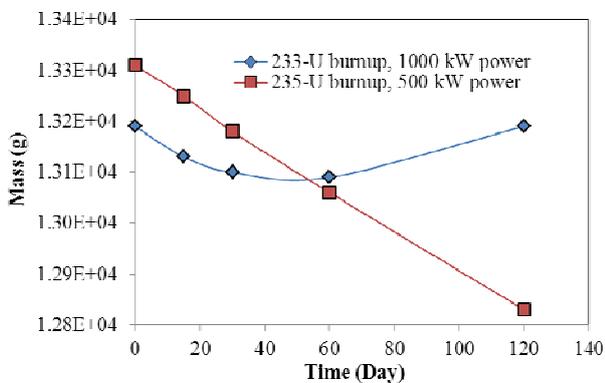


Figure 4 . Fissile mass burnup loaded into the core on operation time.

364 g of  $^{233}\text{U}$  will be produced during the fuel burn up in 500 kW power as well that it can efficiently compensate the fissile missing during the core operation. In the modeled core of (Th+ $^{233}\text{U}$ ) O<sub>2</sub> fuel operated in 1000 kW power, 0.45 g  $^{235}\text{U}$  will be produced after 3 months (figure 5).

$^{149}\text{Sm}$  reactivity inventory is higher for the core of  $^{235}\text{U}$  enrichment while the reactivity is

less in case of the core of  $^{233}\text{U}$  enrichment (figure 6).

$^{135}\text{Xe}$  reactivity inventory is higher for the core of  $^{235}\text{U}$  enrichment up 15 days. While the reactivity is similar with the core of  $^{233}\text{U}$  enrichment after 15 days (figure 7)

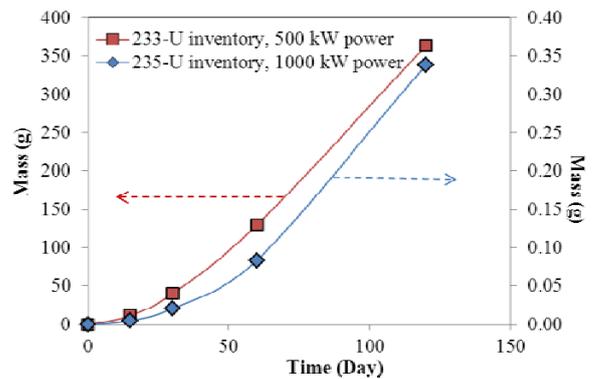


Figure 5. Fissile mass inventory into the core on operation time.

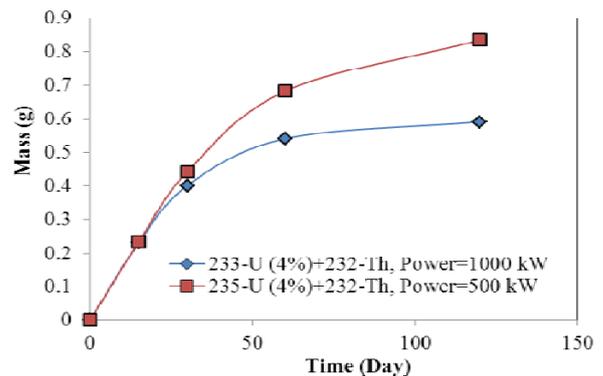


Figure 6.  $^{149}\text{Sm}$  inventory into the core on operation time.

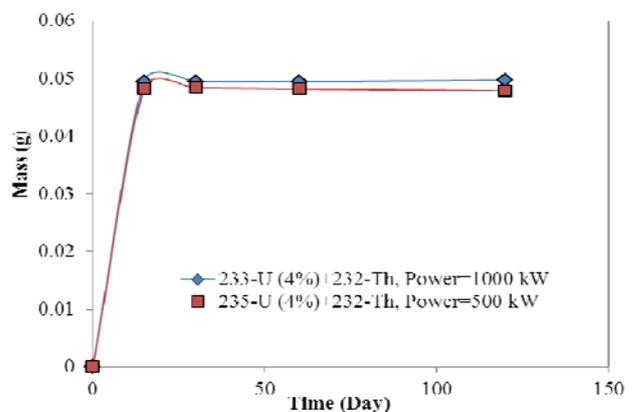


Figure 7.  $^{135}\text{Xe}$  inventory into the core on operation time.

## CONCLUSION

Uranium-233 is a long-lived fissile isotope produced in reactors by single-neutron capture in fertile isotope of  $^{232}\text{Th}$ . One reason for interest in U-233 as a reactor fuel is the superior conversion ratios CR that can be achieved with it in slow-neutron reactors. In fact, the Th-232/U-233 fuel cycle can have  $\text{CR} > 1$  that means it can be a net “breeder” of fissile material in thermal-neutron.  $^{233}\text{U}$  created in the core fed  $(\text{Th}+^{235}\text{U})\text{O}_2$  fuel can be supplied into the research core designed to burn  $(\text{Th}+^{233}\text{U})\text{O}_2$  fuel.

## REFERENCES

1. (IAEA-TECDOC-1450) (2005) Thorium fuel cycle — Potential benefits and challenges, IAEA report.
2. BARC HIGHLIGHTS Reactor Technology & Engineering.
3. Pelowitz DB (2008) MCNPX2.6.0. (LANL, LA-CP-07-1473)
4. Fensin M L (2008) *Development of the MCNPX depletion capability: A monte carlo depletion method that automates the Coupling between MCNPX and CINDER90 for high fidelity burn up calculations* (Florida university) .
5. Persson CM (2005) Reactivity Determination and Monte Carlo Simulation of the Subcritical Reactor Experiment – “Yalina”, Department of Nuclear and Reactor Physics Royal Institute of Technology Stockholm. 16.
6. Snoj L and Ravnik M (2006) Calculation of Power Density with MCNP in TRIGA Reactor, Nuclear Energy for New Europe 2006, International Conference, 109.1.
7. Shultis JK and Faw RE (copyright 2004-2010) An MCNP primer. Dept. of Mechanical and Nuclear Engineering Kansas State University.
8. Bakkari BEI, Bardouni TEI, Merroun O, Younoussi ChEI, Boulaich Y, Chakir E (2009) Development of an MCNP-tally based burnup code and validation through PWR benchmark exercises. *J Annal Nucl Energ*, **36**: 626-633.

