

# Optimum Heavy Water Percentage in Moderator for a Th-Pu-U Fueled Nuclear Reactor

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**Abstract-** A Monte-Carlo parametric study was carried out to investigate the nuclear properties of Th-Pu-U fueled model of the LR-0 reactor when moderated by mixtures of heavy/light water at molecular ratios ranging from 0% up to 100% D<sub>2</sub>O at increments of 10% in D<sub>2</sub>O. The mass of control rods needed to make the reactor critical and the potential reactivity in heavy water were tallied at the 11 heavy water percentage moderators being studied. It was found that the changes in these tallied parameters with heavy water percentage in moderator were not monotonic. Very large negative reactivity was found at 90% heavy water moderator.

**Index Terms-** Mixed water moderator, Nuclear reactor, LR-0, Heavy water

radius = 13.60 cm, divided into 331 hexagonal moderator cells; each of radius = 0.736 cm. Each fuel assembly contains 312 fuel pin, 18 cluster tube, and 1 central instrumentation tube. The 18 cluster tubes were arranged according to the standard LR-0 reactor fuel assembly (Kyncl et al., 2005).

## I. INTRODUCTION

Earlier published papers on using mixed water moderator viz.; The spectral shift control reactor “SSCR” reactor physics programs reports (Wehmeyer et al., 1962, and Barrett et al., 1962), The mixed moderator PWR “MPWR” report of Mitsubishi heavy industries, ltd. (Tochihara et al., 1998), and neutronic behavior of LR-0 when being moderated by mixtures of light and heavy water (M. Nagy et al., 2014), concluded that neutron spectrum is non-monotonically hardened on addition of heavy water to originally light water moderated reactor at all heavy water percentages.

This suggested that using mixed-water moderator for Thorium fueled reactors, may improve the conversion factor. However, since the neutronic behavior of a reactor depends strongly on heavy water percentage in moderator, the optimum heavy water percentage had to be investigated for. This work was dedicated to answer this question for an LR-0 reactor fueled by Th-Pu-U.

The current work is an MCNP5 study of the neutronic behavior of hypothetically Th-Pu-U fueled LR-0 reactor when moderated by mixtures of heavy/light water at molecular ratios ranging from 0% up to 100% D<sub>2</sub>O at molecular ratio increment of 10% in D<sub>2</sub>O. Total mass of control rods needed to make the reactor critical and the potential reactivity in heavy water were tallied for each of the 11 heavy water percentage moderators.

## II. MATERIAL

### 2.1. LR-0 Model

13 standard LR-0 reactor fuel assemblies were assembled in an MCNP5 model. Each assembly is hexagonal in shape of

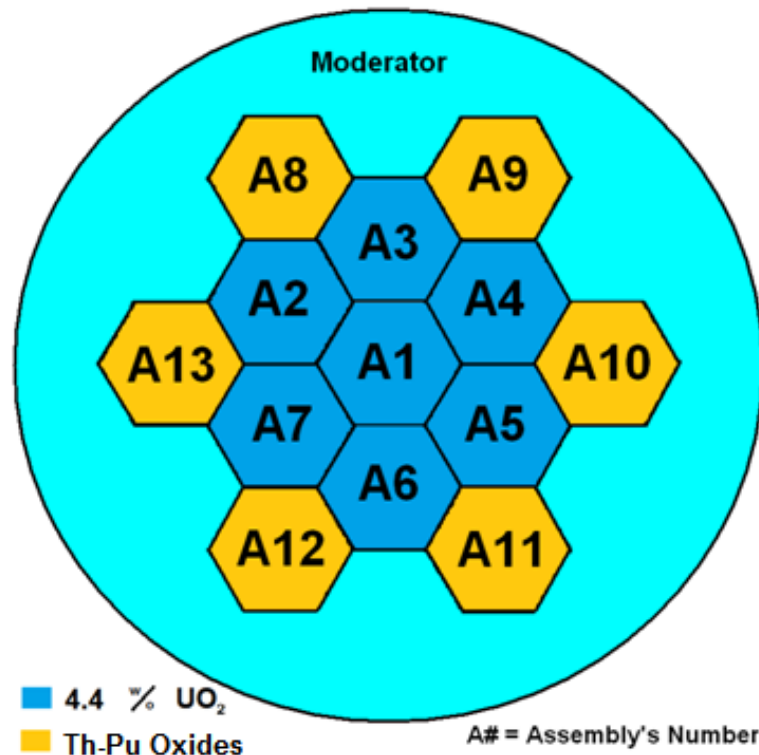


Fig.1. Fuel assemblies numbering, core configuration and fuel distribution.

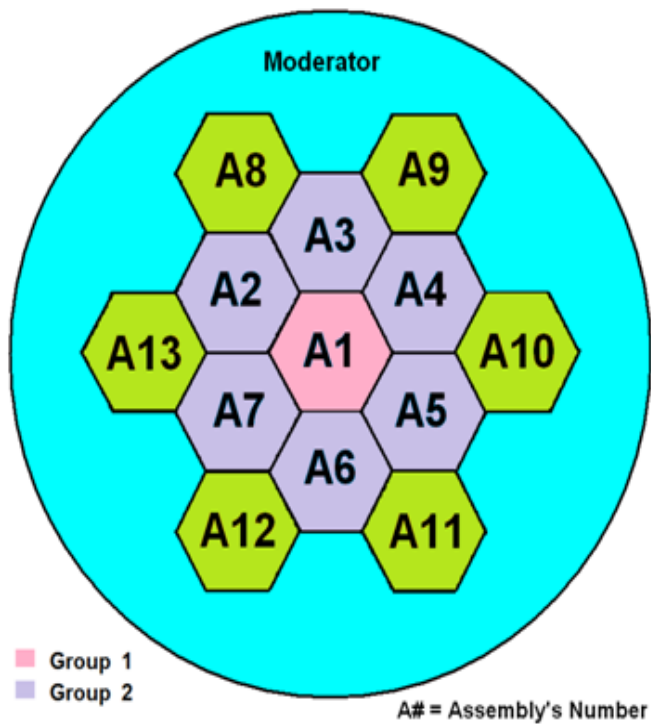


Fig. 2. Control rods groups.

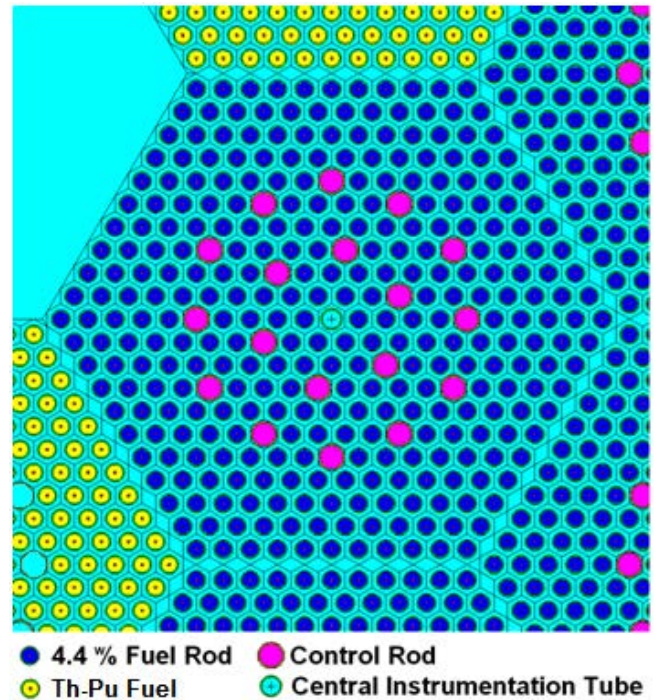


Fig. 4. Structure of fuel assembly

2.2. Fuel pins

Each fuel pin is a hollow cylinder, 125 cm long, with 1.4 mm inner diameter, and 7.53 cm outer diameter. It is encased inside a ZrNbHf alloy clad tube 0.735 mm thick. The axial hollow space is filled with helium gas. The gap between the fuel and the clad is neglected in the model. The 7 central fuel assemblies number had Uranium Oxide fuel at enrichment = 4.4 %<sup>w</sup>, and density = 10.08 g/cm<sup>3</sup>. The outer 6 fuel assemblies had Thorium-Plutonium fuel at density= 9.24 g/cm<sup>3</sup>, its atomic composition was as in table A.2. The clad material is ZrNbHf alloy at density = 6.45 g/cm<sup>3</sup>.

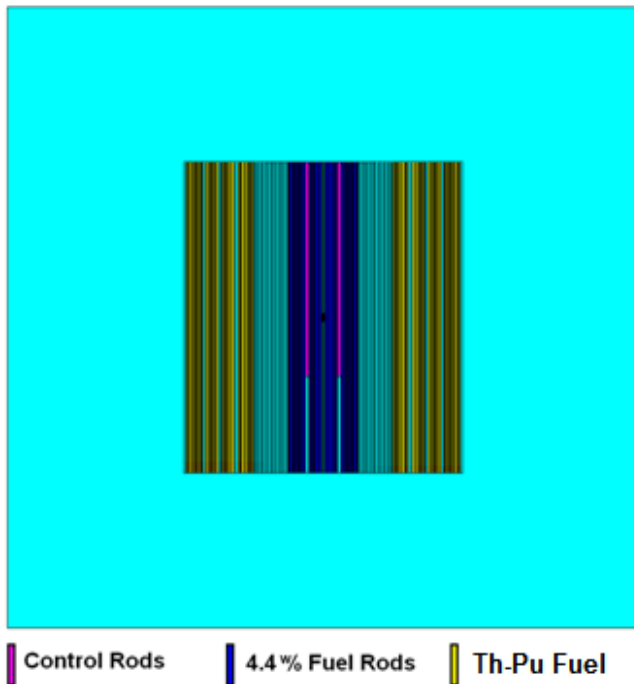


Fig. 3. Longitudinal section of the model.

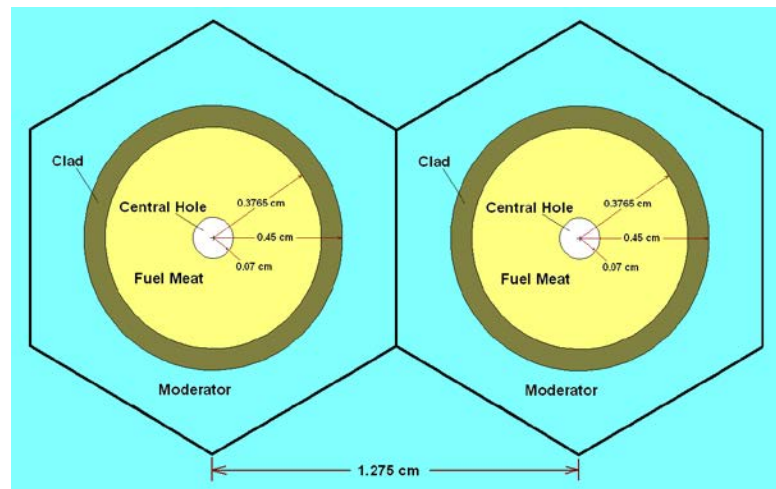


Fig. 5. Fuel Pins & lattice cells geometry.

2.3. Cluster tubes

Cluster tubes are made of stainless steel, with inner diameter of 11 mm, and outer diameter 12.6 mm. They contain the control rods.

### 2.4. Control rods

Control rods are made of B<sub>4</sub>C, 11 mm in diameter. The control rods were grouped into 2 groups; first group in central fuel assembly, second group in fuel assemblies number 2-7. Each group of control rods are moved together. For changing reactor reactivity; the control rods were not (as in real reactors) withdrawn out off core, rather they are shortened or lengthened in the model. This was meant not to disturb the neutronic properties of the moderator in the upper plenum. All boron was B-10, as its very high neutron absorption cross section allowed small changes in control rods lengths to change significantly the criticality of the reactor. Thus it was possible to keep the model critical with the control rods partially inserted in all study steps.

### 2.5. Central instrumentation tube

The central instrumentation tube is made of ZrNbHf alloy, with inner diameter of 8.8 mm, and outer diameter of 10.25 mm. They are filled with moderator.

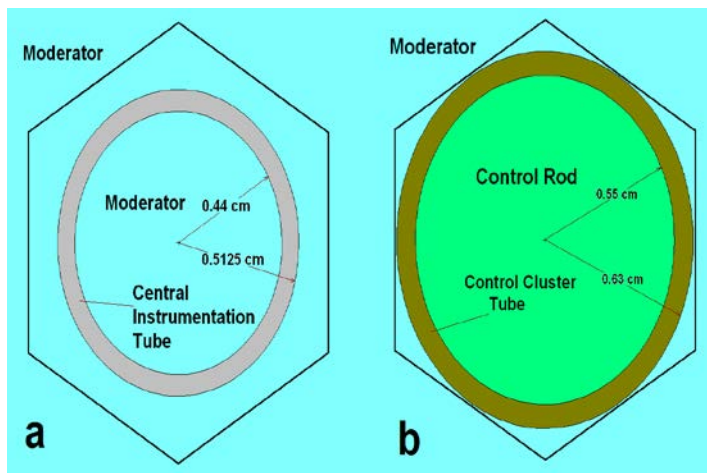


Fig. 7. (a) central instrumentation tube, (b) control cluster tube & rod.

### 2.6. Moderator

The moderators were mixtures of light and heavy water at different molecular ratios. 11 molecular percentages of heavy water in light water were used in the study viz. 0%, 10%, 20%, ..., 100%. The moderator filled all the model spaces and its outer shape was a square cylinder with 2500 mm in diameter and height, symmetrically surrounding the reactor core.

Structural components of the reactor e.g. assembly spacing grids and bottom structures were neglected in the model to simplify modeling and since their neutronic contribution is unwanted for comparing the nuclear properties of moderators having different molecular ratios of heavy water in light water.

## III. METHOD

### 3.1. Code

MCNP5 using cross section library (ENDF/B-VII.1) was used to model the LR-0 reactor and carry out the study. The reactor was assumed to be at room temperature and atmospheric pressure, the real operation conditions of the LR-0 reactor.

### 3.2. Tallies

The tallies included;

- 1) sum of masses of control rods required to set the reactor critical.
- 2) potential reactivity in heavy water were tallied for each of the 11 heavy water percentage moderators.

The study was carried out at 11 steps at different heavy water molecular percentage in moderator; viz. 0%, 10%, 20%, ..., 100%. To keep the reactor critical ( $k_{eff} \approx 1.00000$ , with tolerance of  $+0.00065$ ), lengths of the B<sub>4</sub>C control rods were changed at each step enough to resume criticality.

Because of the probabilistic nature of MCNP code, it was impractical to try achieving  $k_{eff}$  of exactly 1.00000. Rather;  $k_{eff} \approx 1.00000$  with tolerance of  $\sim (+/-) 0.00065$  was accepted at standard deviation (S.D.) not exceeding 0.00020; as shown in table 1.

Table 1.  $k_{eff}$  and relevant statistical data for the 11 studied LR-0 models.

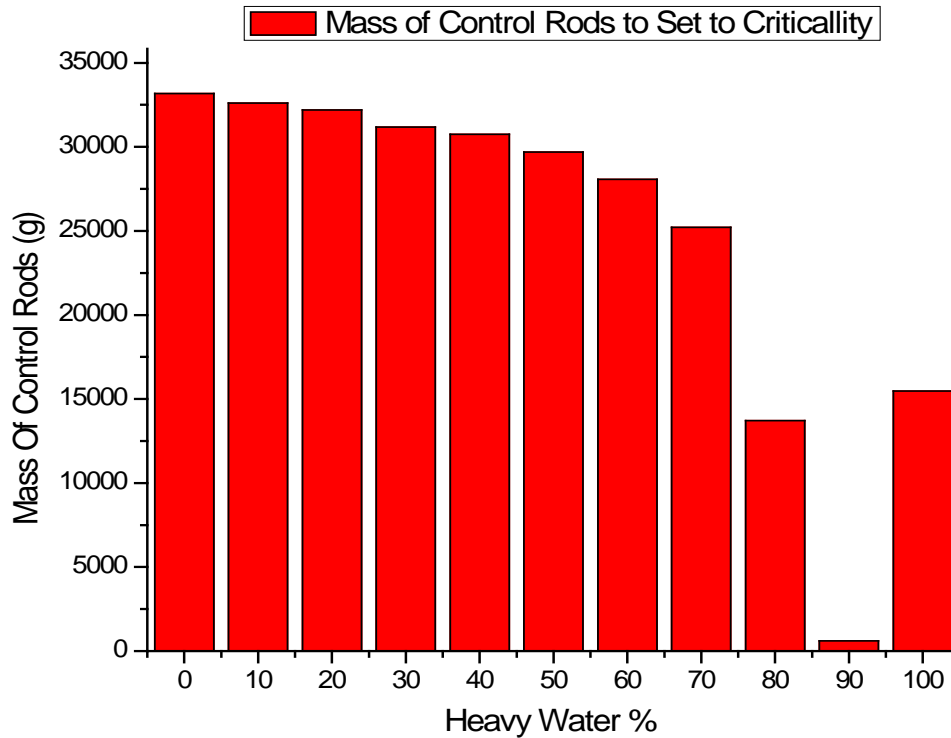
D	0	10	20	30	40	50	60	70	80	90	100
$k_{eff}$	1.00042	1.00044	1.00011	1.00010	1.00007	1.00000	1.00002	1.00005	1.00007	1.00003	1.00001
S.D.	0.00002	0.00002	0.00002	0.00002	0.00002	0.00003	0.00003	0.00002	0.00002	0.00002	0.00009

Therefore; all of the 11 models could be considered exactly **critical**.

## IV. RESULTS & DISCUSSION

### 4.1. Total Mass of Control Rods

Lengths of the control rods were reset for each of the 11 studied cases of heavy water percentage. It was noted that the total mass of the control rods needed to attain criticality for each case was slightly decreasing with increase of heavy water percentage, till 70%. Marked decrease in control rods mass was noted at 80% heavy water. At 90% heavy water, the necessary control rods mass was almost zero. The necessary control rods volume increased again at 100% heavy water percentage. See figure 9.



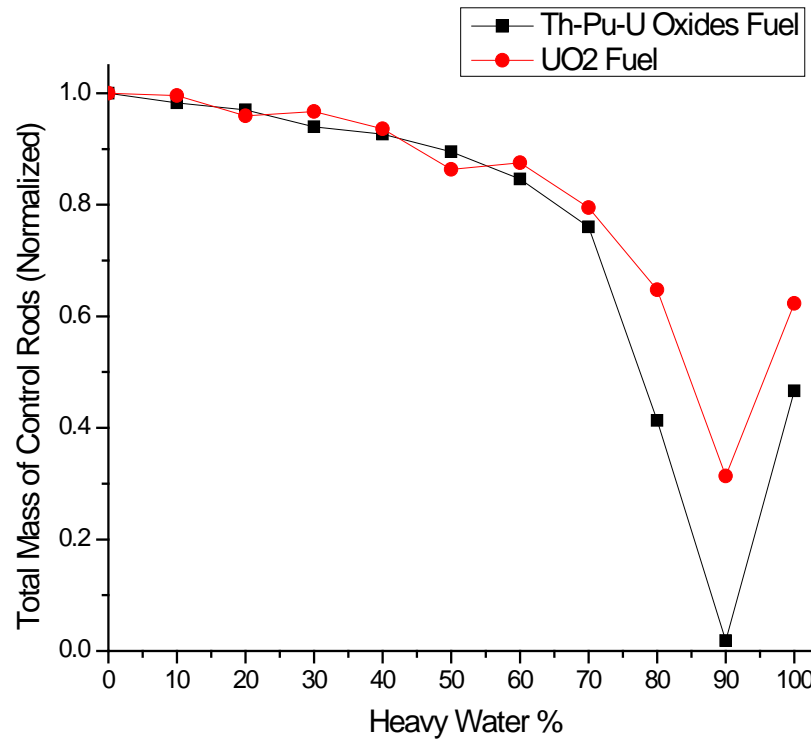
**Fig. 9. Total mass of control material vs. D<sub>2</sub>O%.**

The overall trend of decrease of the total mass of the control rods needed to attain criticality vs. heavy water percentage is simply explained by the reduction in moderation efficiency of the moderator with decrease in available Hydrogen nuclei in moderator with decrease of light water percentages.

The abrupt drop of total mass of the control rods needed to attain criticality at 80 & 90% heavy water percentage might be explained by the fact that at such low light water (Hydrogen nuclei) content in moderator, neutron moderation capability of the moderator is much lowered, hence the reactivity of the system is lowered which necessitates reducing the control rods mass. At

100% heavy water, the total absence of the greedy neutron absorber Hydrogen atoms necessitates the addition of compensatory amounts of neutron poisons.

When compared with results of Nagy et al, 2014, where the fuel was all UO<sub>2</sub>, both results had same trend. The two curves of normalized of control rods mass vs. heavy water percentage for the present study and the referred to study were analogous between 0% - 70% heavy water in moderator. However, beyond 70% heavy water, the decrease in needed control rods mass was more marked with Th-Pu-U fuel than with UO<sub>2</sub> only fuel. See figure 10.



**Fig. 10. Mass of control rods vs. D<sub>2</sub>O%, with Th-Pu-U fuel compared to UO<sub>2</sub> fuel.**

### 3.2. Reactivity Induced by Replacing Moderator by Heavy Water

Reactivity induced by replacing the moderator by mixture of heavy water/light water, while the control rods lengths were the same as in case of 100% light water case was calculated. It was found that adding heavy water induces negative reactivity, which increased with increase of the added heavy water percentage till 80% heavy water. Slight reduction in negative induced reactivity

was noted with 90% heavy water, and marked reduction was noted at 100% heavy water, as seen in figure 11.

When compared with results of Nagy et al, 2014, both results had same trend. Maximum negative reactivity induced by replacing the moderator by mixture of heavy water/light water was noted at 80% heavy water with Th-Pu-U fuel of the present study, while it was noted at 90% heavy water in the study of Nagy et al with UO<sub>2</sub> fuel. See figure 12.

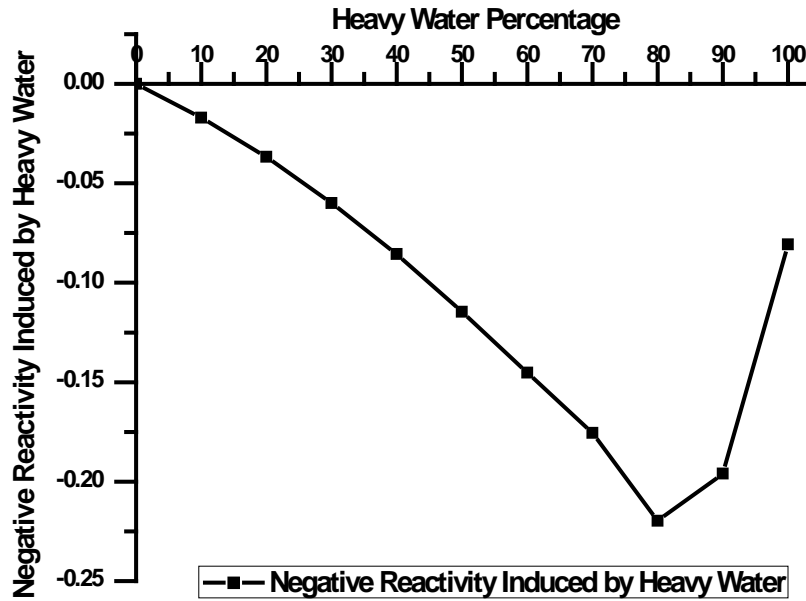


Fig. 11. Reactivity induced by replacing moderator by mixed heavy/light water.

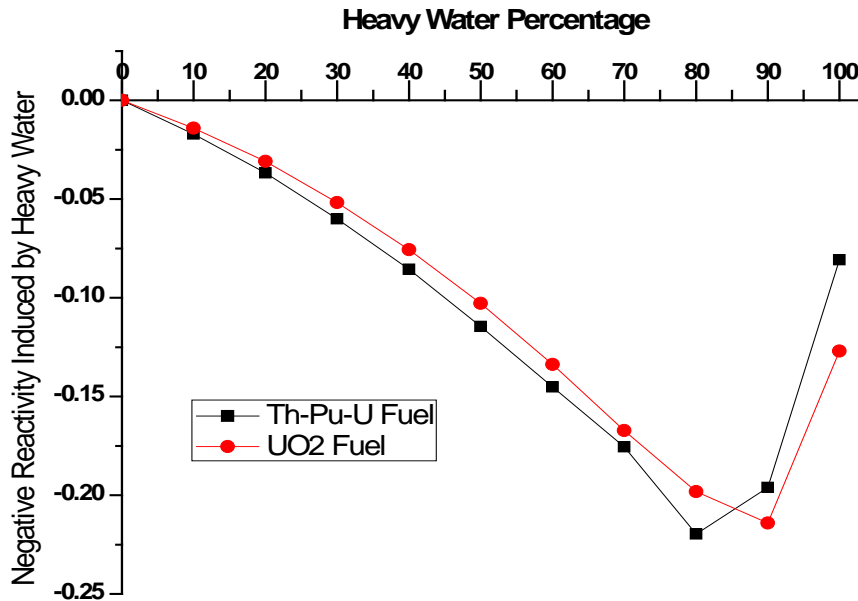


Fig. 12. Induced reactivity vs. D<sub>2</sub>O%, with Th-Pu-U fuel compared to UO<sub>2</sub> fuel.

### V. CONCLUSIONS

A Monte-Carlo parametric study using MCNP5 was carried on a modified model of the light water zero power experimental reactor (LR-0) to examine its nuclear properties if it is moderated by a mixed water moderator; that is a mixture of light and heavy

water at molecular ratios ranging from 0% up to 100% D<sub>2</sub>O with increment of 10% in D<sub>2</sub>O. Lengths of the control rods were reset for each of the 11 studied cases of heavy water percentage. Total mass of the control rods needed to attain criticality slightly decreased with increase of heavy water percentage, till 70% followed by marked decrease at 80% heavy water. At 90% heavy

water, the necessary control rods mass was almost zero. The necessary control rods volume increased again at 100% heavy water percentage. Negative reactivity induced by replacing the moderator by mixture of heavy water/light water increased with increase of the added heavy water percentage till 80% heavy water. Slight reduction in negative induced reactivity was noted with 90% heavy water, and marked reduction was noted at 100% heavy water.

Appendix

Materials specifications

A.1. Fuel

Table A.1

Uranium Oxide fuel material specifications  
Enrichment = 4.4 w/o, density= 10.08 g/cm<sup>3</sup>.

Element	Atom Density (Atom/barn.cm)
U-235	9.93059E-4
U-238	2.13038E-2
O-16	4.45937E-2

Table A.2

Thorium-Plutonium Oxides fuel material specifications

Element	Atom Density (Atom/barn.cm)
Th-232	212.7772712
Pu-238	0.4976955
Pu-239	10.7959799
Pu-240	4.74067
Pu-241	2.50976655
O-16	31.9988

A.2. ZrNbHf alloy for clad & central instrumentation tube

Density = 6.45 g/cm<sup>3</sup>

Table A.3

Clad element composition

Element	Atom Density (Atom/barn.cm)
Zr	4.2141E-02
Nb	4.1808E-04
Hf	6.5285E-06

A.3. Control rods

Boron carbide B<sub>4</sub>C, Density = 2.52 g/cm<sup>3</sup>

Table A.4

Control rod's boron carbide element composition

Nuclide	Atom fraction
Boron-10	4
Carbon	1

A.4. Stainless steel for cluster tubes

Type (GOST 08CH18N10T) stainless steel, density = 7.9 g/cm<sup>3</sup>

Table A.5

Cluster tubes' stainless steel element composition

Element	Atom Density (Atom/cm.barn)
Fe	5.9063E-02
Ni	8.9167E-03
Cr	1.6469E-02
Si	6.7757E-04
Mn	8.6597E-04
C	1.5844E-04
Ti	1.9872E-04

P	2.6879E-05
S	1.4835E-05

A.5. Helium

Helium gas at S.T.P. density = 0.0001785 g/cm<sup>3</sup>

A.6. Moderator

11 mixtures were used.

Table A.6

Moderator specifications

D <sub>2</sub> O %	Density (g/cm <sup>3</sup> )	Atom fraction		
		H	D	O
0	1.0000	20	0	10
10	1.0104	18	2	10
20	1.0208	16	4	10
30	1.0312	14	6	10
40	1.0416	12	8	10
50	1.0520	10	10	10
60	1.0624	8	12	10
70	1.0728	6	14	10
80	1.0832	4	16	10
90	1.0936	2	18	10
100	1.1040	0	20	10

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**نسبة الماء الثقيل المثالية في مهدئ النيوترونات في مفاعل يعمل بوقود ثوريوم – بلوتونيوم – يورانيوم**  
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**الملخص العربي:**

تم إجراء دراسة بارامترية بطريقة مونت كارلو لبحث الخصائص النووية لنموذج لمفاعل LR-0 يعمل على وقود ثوريوم-بلوتونيوم-يورانيوم عند تهندته بواسطة خليط من الماء الثقيل و الخفيف بنسب جزيئية بين 0% و حتى 100% من الماء الثقيل، بزيادة 10% ماء ثقيل فى كل مرة. و قد تم حساب الكتلة الكلية لقضبان الوقود اللازمة لجعل المفاعل حرجاً، و التفاعلية الكامنة فى الماء الثقيل عند الإحدى عشر نسبة من الماء الثقيل فى المهدئ النيوترونى قيد الدراسة. و قد تبين أن التغيرات فى تلك القيم المحسوبة مع التغير فى نسبة الماء الثقيل فى المهدئ النيوترونى كانت غير تناسبية. و قد وجدت تفاعلية سالبة كبيرة جداً عند 90% ماء ثقيل فى المهدئ النيوترونى.



