Neutronic Study of Two Reactor Cores Cooled with Light and Heavy Water using Computation Method

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***Abstract*—**Most HWRs currently use natural uranium fuel. Using enriched uranium fuel results in a significant improvement in fuel cycle costs and uranium utilization. On the other hand, reactivity changes of HWRs over the full range of operating conditions from cold shutdown to full power are small. This reduces the required reactivity worth of control devices and minimizes local flux distribution perturbations, minimizing potential problems due to transient local overheating of fuel. Analyzing heavy water effectiveness on neutronic parameters such as enrichment requirements, peaking factor and reactivity is important and should pay attention as primary concepts of a HWR core designing. Two nuclear nuclear reactors of CANDU-type and hexagonal-type reactor cores of 33 fuel assemblies and 19 assemblies in 1.04 P/D have been respectively simulated using MCNP-4C code. Using heavy water and light water as moderator have been compared for achieving less reactivity insertion and enrichment requirements. Two fuel matrixes of $(^{232}Th/^{235}U)O_2$ and $(^{238}/^{235}U)O_2$ have been compared to achieve more economical and safe design. Heavy water not only decreased enrichment needs, but it concluded in negative reactivity insertions during moderator density variations. Thorium oxide fuel assemblies of 2.3% enrichment loaded into the core of heavy water moderator resulted in 0.751 fission to absorption ratio and peaking factor of 1.7 using. Heavy water not only provides negative reactivity insertion during temperature raises which changes moderator density but concluded in 2 to 10 kg reduction of enrichment requirements, depend on geometry type.

***Keywords*—**MCNP-4C, Reactor core, Multiplication factor, Reactivity, Peaking factor.

I. Introduction

SMALLER and simpler reactors are attractive; they can meet safety and security standards as well as non-proliferation issues. Hence, in the present study, two 33-fuel and 19-fuel assembly cores have been considered.

In heavy water reactors both the coolant and moderator are heavy water (D2O). A great disadvantage of this type comes from this fact: heavy water is one of the most expensive liquids. However, it is worth its price: this is the best moderator. Therefore, the fuel of HWRs can be slightly (1 % to 2 %) enriched or even natural uranium.

So, heavy water advantages has been planned to be discussed in the proposed thermal reactor cores [1, 2].

The design of nuclear power reactors aims at two main objectives: safety requirements and as economic as possible operation of the reactor. For several decades reactor design is supported by computer simulations. Like all computer simulations, nuclear reactor calculations can only be approximations of the reality. This fact is respected by safety margins in nuclear engineering as well as in all other engineering fields [3]. MCNP-4C nuclear code has been aimed to calculate neutronic parameters of the subjected cores.

Decades ago, many countries abandoned the idea of using thorium as a replacement for uranium. But long-term proponents have always believed 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 (U-233), which is fissile (and long-lived) [4]. Therefore, thorium oxide fuel behavior in a HWR has been planned for comparing HWR having uranium oxide fuel assemblies.

II. Data and Method

The reactor core calculations have been carried out using the MCNP-4C Monte Carlo code. The MCNP code was developed by the Los Almos National Laboratory. It is a general purpose Monte Carlo code [5], 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 neutron, 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 [6].

The ENDF/B-VI nuclear data library has been used to apply neutron induced cross-sections at 294°K. Thermal correction in the phonon band requires separate cross section evaluation, the so called $S(\alpha,\beta)$ cross sections that

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are available for heavy water at a temperature of 294K has been used in the present calculations.

All simulations have been carried out using a KCODE card of 5000 neutron with 250 active cycles and 50 inactive cycles. Core materials have been selected as Table I.

Fuel density changes on different enrichments have been calculated as follow:

$$\frac{1}{\rho}=\frac{w_1}{\rho_1}+\frac{w_2}{\rho_2}+\cdots$$

In which w is weight fraction of an element in the fuel mixture and ρ is its density [7].

TABLE I
CORE MATERIAL COMPOSITIONS

MAT	Composition	Thickness (cm)
Fuel	Th/U, U/U, 1.8-2.7% En.	2
Cladding	Sn: 1.4%, Fe:0.23%, Cr:0.1%, Zr	0.04
Cover Plate	Fe:69.5%, Cr:19.0%, Ni:9.5%, Mn:2.0%	0.2
Reflector	Be:36%, O:64%	2

Two 33-assembly and 19-assembliy cores have been simulated in 1.04 P/D between fuel assemblies and 1.25 P/D between the fuel pins in any assembly (Fig. 1).

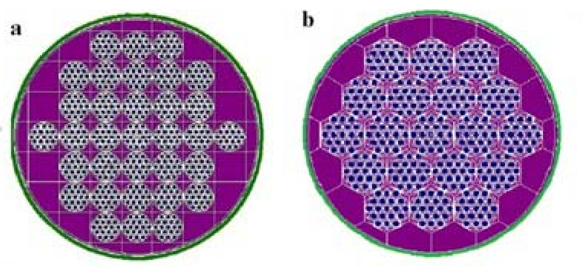

Fig. 1 Core configuration consist of fuel pins of 100 cm height and 2 cm diameter, 4 mm zircaloy clad for any fuel pins, a 2cm thick BeO reflector around the cores, fuel to moderator volume $(M/F)_V$: 5.29 a) 33 assemblies, 627 pins, b) 19 assemblies, 361 pins

Light water (0.9982 g/cm) and heavy water (1.1056 g/cm^3) moderators have been studied in the assumed structures for both $(^{232}Th/^{235}U)O_2$ and $(^{235/238}U)O_2$ fuel mixtures respectively. Effective multiplication factor (k_{eff}) has been determined in several enrichments. The MCNP-4C calculations have been carried out using 1.8-2.1% enrichments for uranium oxide fuel and 2-2.7% enrichments for thorium oxide fuel.

The power peaking factor is an important parameter used in the safety analysis studies. This factor is calculated by the ratio of the fuel element power to the average core power. The optimal design of the fuel element must be achieve lower value of the power peaking factor and maximum effective multiplication factor to extract the maximum energy [8].

Whereas the power is directly related to neutron flux, peaking factor (ϕ_{max}/ϕ_{ave}) has been calculated using f4 tally via maximum to average flux ratio of the cores. Fission to absorption ratio has been determined in some enrichment applications.

A tally is a specification of what should be included in the problem output, for example the neutrons flux through a certain area or the number of neutrons in a particular energy interval. In MCNPX it is possible to calculate integrals of the form

$$C\int \varphi(E)dE \qquad (1)$$

where C is a multiplication constant, φ is the neutron flux. In this way, reaction rates with different materials can be determined.

Moreover, in MCNP4-C the F7 energy deposition tally is the following track length estimates and it is possible to calculate integrals of the form

$$F7=\rho_a/\rho_g\int H(E)\varphi(E)dE \qquad (2)$$

where ρ_a is an atom density, ρ_g is a gram density and H(E) is the heating response (summed over nuclides in a material) [5]. The two mentioned tally have been used to calculate peaking factor and radial power deposition respectively.

Reactivity variations in result of moderator density fluctuations has been studied via assumption of volume percentage of void added into the moderator. Void formation has been considered between 5-30% volume void insertions.

The new density of moderator in any MCNP-4C runs has been determined by means of the $\rho=\rho_0$ (1-void %) equation. To decrease the standard deviation of the data achieved the code, perturbation card has been used.

III. RESULT AND DISCUSSION

According to the simulations, maximum k_{eff} is achievable using $^{235/238}UO_2$ as fuel and heavy water as moderator. $(^{232}Th/^{235}U)O_2$ mixture concludes in the least k_{eff} using the same enrichments and loading light water into the core (Fig. 2).

As it is seen in the Fig. 2, thorium oxide fuel increases enrichment requirements about 1% in comparison of uranium oxide using heavy water. It seems both 19 and 33-assembly cores have similar behavior in the mentioned case. Both the evaluated cores show the same characteristic for two fuel mixtures by means of light water as well.

However two considered cores have identical P/Ds, enrichment requirements for hexagonal-type core and one kind of the fuels is less using light water whereas it is inversed in case of heavy water. So, it seems in CANDU-type simulated core neutron absorption by the moderator or resonances of fuel is dominant because of its more free spaces between assemblies which don't allow achieving higher multiplication factors respect to identical enrichments which is used in hexagonal-type reactor.

Hence, the output data suggests heavy water as more efficient moderator for CANDU-type simulated core.

Hexagonal-type simulated core has more compact assemblies and it seems heavy water have less effects on enrichment reduction than CANDU-type simulated core.

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33-assembly structure concluded in an average discrepancy of 6982.95 pcm of K_{eff} using heavy water instead of light water for uranium oxide fuel assemblies. K_{eff} have an average enhancement of 4587.8 pcm in case of thorium oxide in heavy water moderator. This value was 5785.375 pcm loading heavy water moderators for uranium oxide assemblies in hexagonal core and 5530 pcm enhancements will occur for thorium oxide.

Sharply, heavy water makes possibility of less enrichment applications.

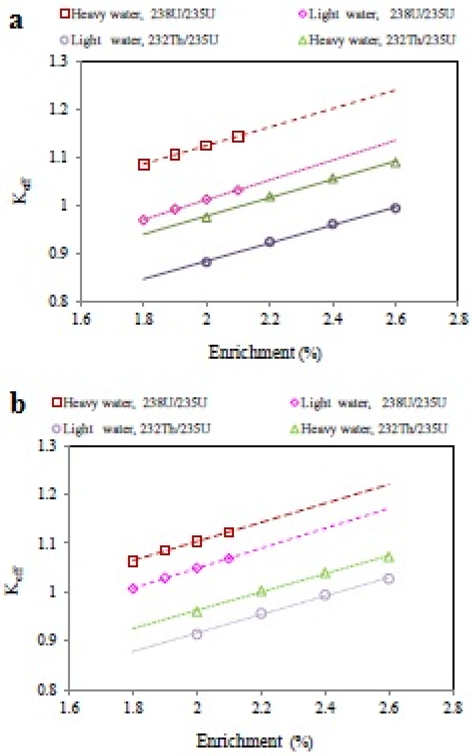

Fig. 2 Comparison of k_{eff} on enrichment percentage, a) 33 assemblies, and 627 pins b) 19 assemblies, 361 pins

The data acquired MCNP-4C code shows that picking factor (PK) of 19 assemblies core is approximately identical for two different fuel mixtures either light water or heavy water moderator except thorium oxide fuel in light water; in which case it has a 5.8% relative enhancement.

The core having 33-assembly configuration concluded in bigger PKs especially in the case of light water moderator. Light water application for both fuel matrixes of 33-assembly core shows a 11% relative enhancement in PK than thorium oxide fuel of 19-assembly configuration. The mentioned discrepancy between 19 and 33-assembly was about 2.6% using fuel matrixes in heavy water. Overall heavy water appliance can be concluded in less PKs for both 19-assembly and 33-assembly cores (Fig. 3).

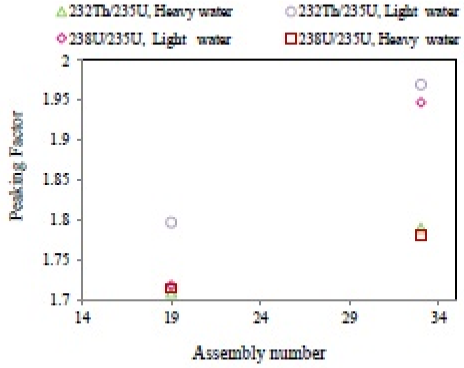

Fig. 3 Comparison of PK on enrichment percentage, a) 33 assemblies, and 627 pins b) 19 assemblies, 361 pins

Two fuel mixture has been compared in $1.029<k_{eff}<1.038$ in view of their fission/absorption and pecking factor. The results indicated maximum fission/absorption for thorium oxide in heavy water moderator of 33&19-assembly cores as well as uranium oxide in light water of 33-assembly configuration.

Minimum PK was occurred for thorium oxide in heavy water moderator of 33&19-assembly cores as well as uranium oxide in light water of 33-assembly configuration (Fig. 4).

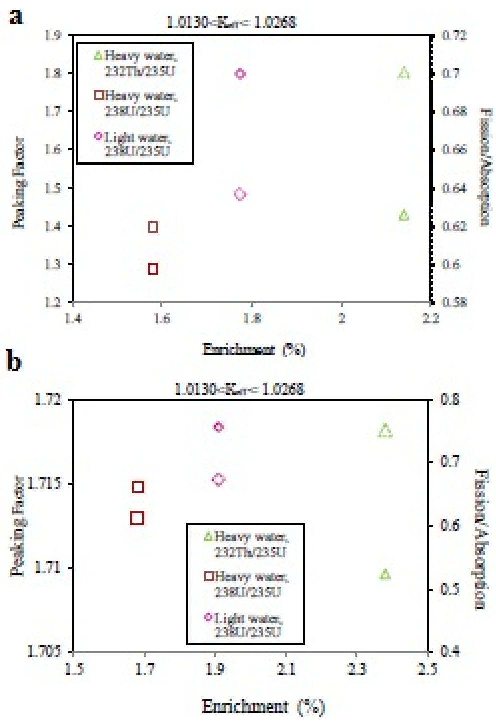

Fig. 4 Comparison of PK and f/a ratio versus enrichment percentage for different fuel matrixes a) 33 assemblies, and 627 pins b) 19 assemblies, 361 pins

Peaking factor is not related to enrichment variations in a constant geometry, but it depends on moderator type, fuel type and geometry variations.

Heavy water appliance concludes in less reactivity formation via moderator density variations or bulb formation for both fuel mixtures than light water in $1.029<k_{eff}<1.038$ domain (Figs. 5, 6).

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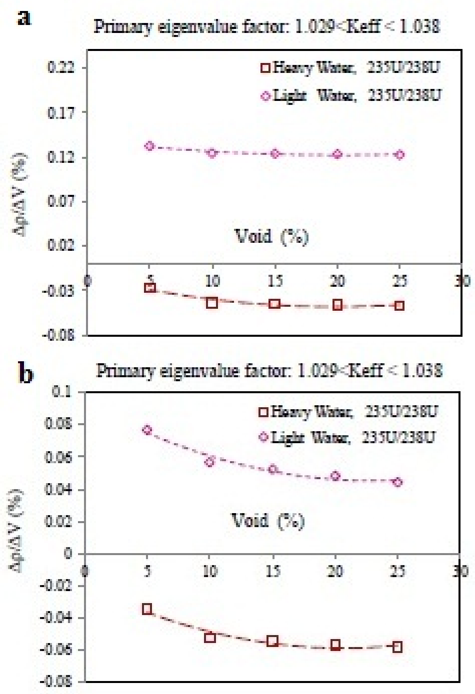


Fig. 5 Comparison of reactivity coefficients on void volume percentage, a) 33 assemblies, and 627 pins b) 19 assemblies, 361 pins

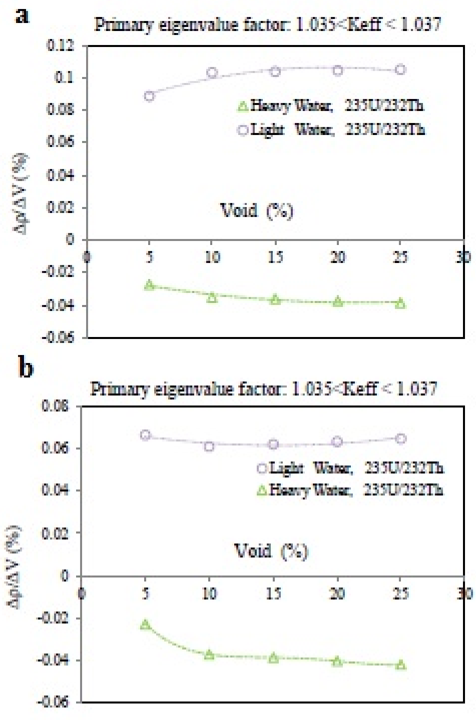


Fig. 6 Comparison of reactivity coefficients on void volume percentage, a) 33 assemblies, and 627 pins b) 19 assemblies, 361 pins

However light water moderator seems to be more favorable respect to fuel temperature reactivity, it causes more variations in reactivity of fuel because of higher slope of the reactivity curve as it depicted in Fig. 7.

Light water concludes in positive void reactivity cofficientes for both the studied cores. As it seen in Fig. 7, fuel reactivity cofficients will be negative for both cores respect to reactivity reduction as a result of fuel tempreature enhancement. Generally, heavy water contains both negative reactivity cofficients of fuel and moderator. This advantage makes a inherentt safety for a reactor.

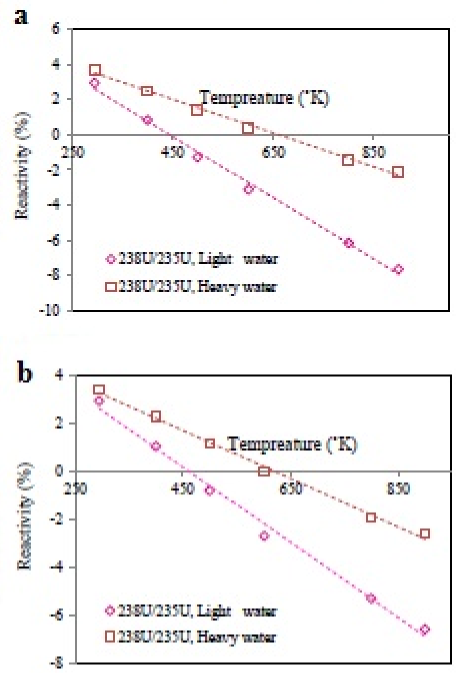
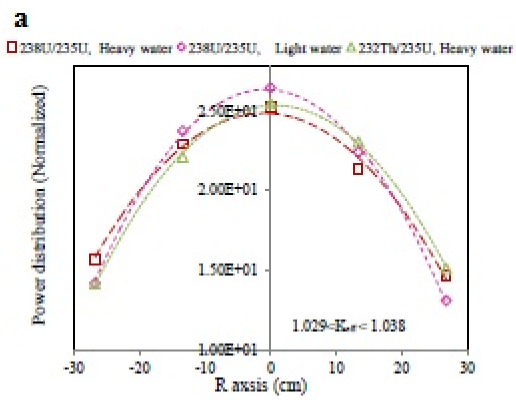


Fig. 7 Comparison of reactivity coefficients on fuel temperature, a) 33 assemblies, and 627 pins b) 19 assemblies, 361 pins

The reactivity curves have been resulted of 1.6% ^{235}U in uranium mixture for heavy water, 2.1% ^{235}U in uranium mixture for light water and 2.3% ^{235}U in thorium mixture for heavy water. Deposited power was compared for tow fuel mixtures in the multiplication of $1.029<k_{eff}<1.038$. According to the MCNP-4C output, their radial powers have overlap with each other approximately (Fig. 8).



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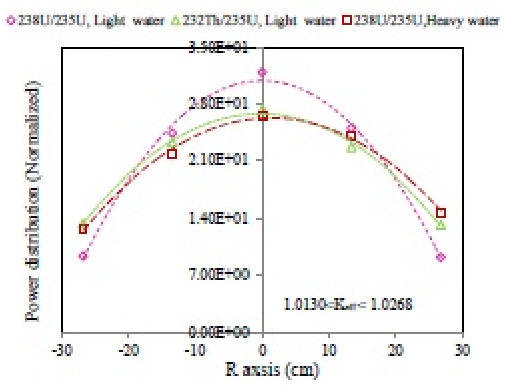

Fig. 8 Comparison of radial power distribution for different fuel matrixes, a) 33 assemblies, and 627 pins b) 19 assemblies, 361 pins

Overall, thorium fuel matrix and heavy water moderator seems to be more preferable in regard that it results in less enrichment in comparison of its loading in light water.

Thorium matrix in heavy water competes with uranium matrix in view of less reactivity accidents during moderator density variations. However the suggested fuel matrix enhances enrichment requirements, but it can be more desirable in regard to its low long-lived waste production [7].

As it is depicted in Tables III, IV, hexagonal type core conclude in less enrichment requirements than CANDU type core because of its more compactable ability.

TABLE II
HEXAGONAL TYPE CORE DYNAMIC PARAMETERS $1.028<K_{EFF}<1.038$, σ=23 pcm

Fuel type/^{235}U (kg)	β (pcm)	β_{eff} (pcm)	ν
HU/13.707	573.0964	666.2161	2.426652
HTh/21.264	792.5399	858.5761	2.418829
LTh/23.408	702.4605	718.7911	2.418287
LU/15.583	677.7590	679.6851	2.425446

TABLE III
CANDU-TYPE CORE DYNAMIC PARAMETERS $1.028<K_{EFF}<1.038$, σ=23 pcm

Fuel type/^{235}U (kg)	β (pcm)	β_{eff} (pcm)	ν
HU/33.138	698.1962	720.1864	2.434124
HTh/52.164	700.3989	740.5624	2.424612
LTh/63.504	699.0084	665.2079	2.420488
LU/43.494	704.0614	705.0244	2.429873

All relative errors of the calculation were less than 0.55% in average.

IV. CONCLUSION

Two 33-assembly and 19-assembly thermal cores have been simulated using MCNP-4C code. Thorium oxide fuel of 2.3% ^{235}U resulted in the most fission/absorption (0.751) and the least peaking factor. Heavy water in the simulated core concluded in less void reactivity insertion with average differences of about -100 mk and -150 mk than light water for 19 and 33-assembly cores respectively. Hence, thorium oxide fuel and heavy water moderator is suggested to achieve optimum economical condition in management of a thermal reactor. Hydrogen absorbs neutrons easily, and therefore takes neutrons out of circulation. The fission chain reaction cannot be self-sustaining with a light-water moderator: the fuel must be enriched in the fissile isotope ^{235}U.

Deuterium (as in heavy water) is very effective as a moderator. In addition, deuterium does not absorb neutrons readily. This is a great advantage as far as perpetuating the chain reaction. Hence, the heavy water moderator promotes excellent neutron economy [9].

Power distributions, flux flatting and burnup calculations are important parameters to complete such calculations which should be paid attention in further studies.

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