Evaluation of subcritical multiplication parameters in MYRRHA-FASTEF accelerator driven system reactor

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Abstract. In the present study, the fast spectrum transmutation experimental facility (FASTEF) core that considered for the MYRRHA reactor is modelled using Monte Carlo MCNPX code. The effect of changing the type of material and radius of the cylindrical target source as well as the energy of the proton beam on the final production of neutrons and the subcritical multiplication of the system are evaluated. Subcritical models of the investigated reactor have been numerically investigated as well. Six target materials; uranium (U), lead-bismuth eutectic (LBE), tungsten (W), lead (Pb), bismuth (Bi), and copper (Cu) are used with varying target radii from 3.5 to 20 cm. The beam energy is varied from 0.2 to 2.0 GeV. The present study depends on numerical calculations of the subcritical multiplication factors and the efficiency of the external source using MCNPX code. The obtained results revealed that the favourable target material, radius, and beam energy can be precisely determined.

1. Introduction
The accelerator-driven subcritical reactor represents an interesting and promising system, not only for transmutation of large half-life heavy elements but also for its capability to produce energy, reduce the stock of radioactive materials. The ADS concept consists basically of a proton accelerator coupled to a subcritical core by a spallation target [1-3].

The FP7 CDT Project took the XT-ADS design as a starting point, which has evolved into the last official version known as MYRRHA-FASTEF [4]. MYRRHA (Multi-purpose Hybrìd Research Reactor for High-tech Applications) is a flexible experimental Accelerator-Driven System currently under development at SCK-CEN [5-7]. MYRRHA is designed to help fuel improvements for creative reactor frameworks, radioisotope production for therapeutic modern applications, and other purposes. Since 2009, it is development under the FP7 EC Project Central Design Team (CDT) where the reactor is designed as FASTEF [6]. Great efforts have been devoted to optimize the cooling and safety purposes of the reactor using suitable codes and the available benchmarked data [8-10].

The aim of the present work is to study the effect of radius and target material of the external neutron source in addition to the proton beam energy on the final production of neutrons and the subcritical system multiplication of MYRRHA-FASTEF reactor. Six different targets were used, namely, uranium,
lead-bismuth eutectic, lead, bismuth, tungsten, and copper with varying the target radii from 3.5 to 20cm, and the beam energy from 0.2 to 2 GeV. The MCNPX 2.6 code was used for the purpose of the numerical evaluation of the different subcritical parameters and the related neutron production values.

2. Subcritical multiplication parameters.
The neutron multiplication $M$ and the subcritical multiplication factor $k_s$ [11-14] at a steady state conditions for subcritical system with an external source can be explained in the following forms:

$$M = \frac{F + S}{S}$$  \hspace{1cm} (1)

$$k_s = \frac{F}{F + S}$$  \hspace{1cm} (2)

$$F = \int_V \int_0^\infty \nu \sum_i (r, E)\phi_i (r, E)dE d^3r$$  \hspace{1cm} (3)

$$S = \int_V \int_0^\infty s(r, E)dE d^3r$$  \hspace{1cm} (4)

where, $\phi_i (r, E)$ is the neutron flux value in the position $r (x, y, z)$ at energy $E$, $s(r, E)$ is the external neutron source, $F$ is the total production of neutrons by fission and $S$ is the total production of neutrons by the external source, $\nu$, per unit time. $V$ represents the system volume, $\nu$ is the average number of fission neutrons per fission reaction and $\Sigma_f (r, E)$ is the cross-section of the fission.

The external source efficiency $\varphi^*$ is defined as the ratio of the average external source importance to the average fission importance that can be defined by means of the well-known effective multiplication factor $k_{eff}$ and $k_s$ applying the following form:

$$\varphi^* = \frac{1 - 1/k_{eff}}{1 - 1/k_s}$$  \hspace{1cm} (5)

3. Subcritical core.
During the FP7 CDT project the FASTEF core, Fuel Assembly (FA), and the first associated system was established. The core at Beginning of Life (BoL) that means fresh fuel core lattice consists of 151 assembly positions can be taken by 58 fuel assemblie s, 6 control rods, a spallation target, 38 dummy that are LBE filled, 42 reflector are filled by Yttrium Zirconium Oxide (YZrO) pellets, and 6 in-pile test sections (IPS). The central position contains the spallation target. The FA design is hexagonal closed with a triangular lattice having 127 pins where one of them is empty located in the middle and six rows of 126 fuel pins. Each pin has 60 cm fissile length. The fuel is Mixed Oxide (MOX) with the 30wt. % Pu mass content and the rest part is natural U. Pu and Am are derived from PWR spent fuel of 45 GWe/t burn up (feed with 4.5% of $^{233}$U) and a cooling time of fifty years. The decay of nuclides undergoing fission, as $^{241}$Pu, is considered by introducing the 1.65 wt. % Am in Pu content. The LBE coolant operation lies between 200 and 400 $^\circ$C to avoid corrosion risks and freezing). The coolant velocity is kept less than 2 m/s. Most of the primary structures of the system in MYRRHA are AISI 316L stainless steel. The fuel assembly, the core support plate, in-guide tub of the pile, and the shutdown facilities are constructed from T91 ferritic-martensitic steel, because it has higher stresses, lower swelling under the effect of irradiation and higher creep resistance values than AISI 316L. Austenitic 15-15Ti stainless steel (15Ni-15Cr stainless steel stabilized by Ti) was chosen as a material for the fuel cladding for its high resistance to embrittlement.
The design of the sub-critical core was performed at a desired subcriticality level where $k_{eff} \sim 0.95$ was the chosen value at the end of any irradiation sub-cycle [15]. The $k_{eff}$ at beginning of cycle results in $\sim 0.965$ for the $\sim 1500$ pcm sub-cycle swing in 90 Equivalent Full Power Days (EFPDs). Based on the previously studies [16], with such $k_{eff}$ levels, the core will remain at sustainable sub-critical conditions until turning off the accelerator.

3.1. MCNPX Model.
MCNPX model for MYRRHA-FASTEF is shown in figure 1. The core layout at BoL has been considered to have 58 fuel assemblies according to the previous description in section 2. To obtain $k_{eff}$, MCNPX with ENDF/B-VII was used in the calculations related to the subcritical core and eigenvalues. The active cycle of histories was $15 \times 10^6$ with uncertainty 0.00018 in $1\sigma$, and the value of the power can be kept at 81 MW in the first 90 EFPDs sub-cycle. Figure 2 depicts vertical view of the sub-critical core.

![Figure 1. Horizontal view of MCNPX model of MYRRHA-FASTEF configuration.](image-url)
The target also has been modeled independently without the core. Its cylindrical LBE target has radius and length equal 5 cm and 40 cm respectively. A horizontal and vertical schematic view of the MCNPX target model is shown in figure 3.

**Figure 2.** Vertical view of MCNPX model of MYRRHA-FASTEF configuration.

**Figure 3.** Horizontal and vertical view of the test model with MCNPX.
4. Results and discussion.

4.1. Target investigation.

In the first part of the target investigation, we have calculated the neutrons multiplicity as a function of beam energy to validate our target model. The neutron multiplicity is the neutrons number produced per one beam particle (n/p). The change of n/p according to change of protons beam energy has been investigated. In this case, the calculations are done for proton beam energies in the range of 0.2-4 GeV and the cylindrical target has 5 cm fixed radius. The results are compared with reference [17] referring to an overall agreement with the previous calculations as shown in figure 4.

![Graph showing the dependence of neutron yield on proton beam energy](image)

**Figure 4.** Dependence of the neutron yield on the incident proton energy compared with previous data.

The neutron production from the different target materials with different radii at 600 MeV proton incident energy has been calculated where six materials have been used; Uranium, Lead, Lead-bismuth Eutectic, Tungsten, Bismuth, and Cupper. At the same time, the radii of the targets are varied from 3.5 to 20 cm. The results are illustrated in figure 5, where one can observe that the variation of the spallation neutrons (total escape neutrons from the target) is proportional to the atomic mass number of target elements, for instance one U nucleus produces a number of neutrons more than one W nucleus as well as the atomic number for U is more than W. On the other hand, the atomic density of the target affects the neutron production so that W spallation reaction rate is higher than that of Pb; therefore, a relatively large number is produced in W target.

The production of neutrons is linearly dependent on the target radius because high energy particles have more chances to execute neutron production reaction before they escape from the target. From figure 5, one can observe also that the produced neutrons increased dramatically in case of uranium target while the increasing is small for other target material specifically after 15 cm radius, this leads us to conclude that when the dimension of the target increases the neutrons leakage from the target decreases. For materials other than uranium, n/p shows saturation after certain r.
In the present work, the neutron yield of the target having a cylindrical shape at different energies from 0.2 to 2.0 GeV fixing the radius at 5 cm and length at 40 cm has been calculated. As shown in figure 6, all target materials U, LBE, Pb, Bi, W, and Cu produced neutrons proportional linearly with the beam energy. Of course, there is a difference in the value of linear slope related to the type of material, but the results showed the effect of energy increase on the neutron production for varies material with different atomic numbers.

Figure 5. Dependence of the neutron yield per proton on the target radius for U, LBE, Pb, Bi, W, and Cu targets.

Figure 6. Neutron yield per proton as a function of Proton beam energy for U, LBE, Pb, Bi, W, and Cu targets.

The neutron spectrum of the source neutrons produced from the six target materials has been calculated and the results are shown in figure 7. The incident proton beam energy was fixed at 600 MeV where the
target radius and length were 5 cm and 40 cm respectively for the six materials. It is clear from figure 7 that the spectrum is hard for all types of materials with a small shift in the maximum peak of the neutron flux. The uranium produced relatively more neutrons within a wide range of fast neutron than the other considered material (W and Pb). Those fast neutrons are very important and useful for minor actinide transmutation inside the ADS reactor core. Therefore, these results for neutron spectra give a primary indication for the best material that provides a higher number of fast neutrons.

![Figure 7. Comparison between calculated neutron spectra for U, LBE, Pb, Bi, W, and Cu targets.](image)

4.2. Numerical calculations of $k_s$ and $\phi^*$. Before the evaluation of the results of the source efficiency and the source multiplication, the whole core model has been verified against published results [4]. The comparisons of the $k_{eff}$ values are presented in Table 1. The present obtained results were calculated at The FASTEF core (58FA-81 MW subcritical core layout at BoL) with a 600 MeV proton beam injected onto the LBE target. Good agreement was obtained except a slight variation was reached around 536 pcm related to the differences between the library data [18] and MCNPX version used in the calculations of the present and previous analogous studies.

| calculation         | $k_{eff}$ (std. dev.) | MCNP | Library        |
|---------------------|-----------------------|------|----------------|
| Present Work        | 0.95944 (0.00018)     | MCNP2.6 | ENDF/B-VII    |
| Reference[4]        | 0.96480 (0.00016)     | MCNPX | JEFF-3.1.     |

The calculations set up to investigate $k_s$ and $\phi^*$ parameters (defined in Section 1) for MYRRHA-FASTEF (58FA-81 MW sub-critical) core at BoL were executed also with the use of the MCNPX code,
in combination with nuclear data library ENDF/B-VII. The core is coupled with a 600 MeV proton LINAC (designed for 4 mA as maximum current), and used to drive the core in a subcritical configuration. The target is located at the central thimble as shown in figures 1 and 2. The target in the center will take into consideration the highest possible heat generation and mostly is relevant to the proposed ADS operation. The sub-criticality was fixed at 0.95944 in $k_{\text{eff}}$ the proton beam entered the target from the top. The MCNPX was utilized to evaluate the total fission and source neutrons rates, $F$ and $S$, respectively, for the aforementioned core design. $k_s$ and $\varphi^*$ has been obtained for six materials, uranium, lead-bismuth, lead, bismuth, tungsten, and copper targets at the described position, as shown in Table 2. The results showed that there is no significant difference in neutron efficiency between the materials used as targets except in case of cupper where the efficiency was ~1.8, this actually because of its low source neutrons compared to the fission neutrons which mean increase in $k_s$ and $\varphi^*$ values. Although of this relatively high neutron source efficiency for cupper target, unfortunately cupper has a low thermal property to use as target in ADS reactor.

Table 2. $k_s$ and $\varphi^*$ for different target material.

| 1. Target Materials         | 2. $k_{\text{eff}} = 0.95944$ | 3. $k_s$ $^a$ | 4. $\varphi^*$ $^b$ |
|----------------------------|-------------------------------|---------------|---------------------|
| 5. Uranium                 |                               | 6. 0.94220    | 7. 0.68909          |
| 8. Lead-Bismuth Eutectic   |                               | 9. 0.96526    | 10. 1.17453         |
| 11. Lead                   |                               | 12. 0.96460   | 13. 1.15193         |
| 14. Bismuth                |                               | 15. 0.96523   | 16. 1.17345         |
| 17. Tungsten               |                               | 18. 0.94792   | 19. 0.76946         |
| 20. Copper                 |                               | 36. 0.97689   | 37. 1.78661         |

$a$ Statistical error in $k_s$ is less than 0.0017.

$b$ Statistical error in $\varphi^*$ is less than 0.06.

5. Conclusions
In the present work, MCNPX stochastic code is successfully used to evaluate the neutronic behavior of different spallation targets. So, numerical investigation of the effects of changing the external neutron source cylindrical target material, radius, and the proton beam energy on the final neutron production and the external source efficiency of the subcritical system of MYRRHA-FASTEF core reactor was performed.

The study illustrates that the neutrons production depends on the atomic number and density for the studied target materials. So, the highest neutrons yield achieved when we used U target for all proposed radii, also the results showed the linear dependence of the neutron production on the incident proton beam energies at all material cases. The source efficiencies $\varphi^*$ for U, LBE, Pb, Bi, W, and Cu targets were obtained. The Cu target produced relatively high source efficiency, where it has a low source neutrons production. From the present calculations, LBE target still has the superiority among the other targets in MYRRHA-FASTEF subcritical ADS reactor as it gives a high efficiency and has good thermal properties.
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