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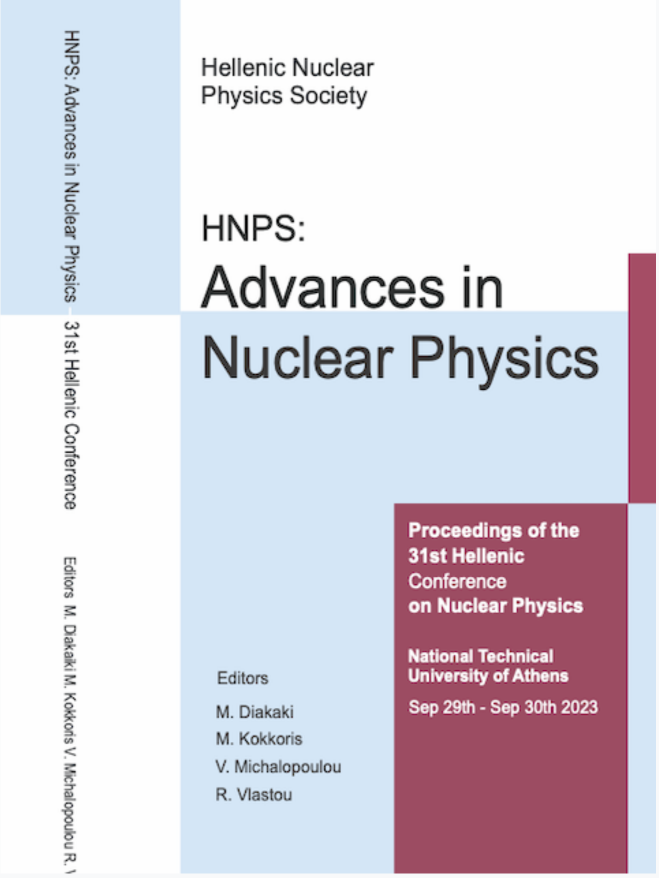

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Cross Section Biasing Technique in ^{3}H(d,n)^{4}He Reaction using the GEANT4 Toolkit

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Abstract Simulations using Monte Carlo GEANT4 [1] toolkit was performed to quantify parasitic neutrons production from the ^{3}H(d,n)^{4}He reaction in the TANDEM [2] accelerator laboratory at N.C.S.R "Demokritos". In this reaction, parasitic neutrons are produced, which contaminate the main neutron beam. For studying parasitic neutrons, the cross section biasing technique has been applied to increase the cross sections of the reactions and to obtain accurate statistical results in a short computational time. However, the implementation of a biasing technique can significantly impact the physical processes simulated. The experimental setup contains the accelerator line and the tritium flange, which consists of molybdenum, tritium and copper. Then, the target materials are purposefully exposed to the neutron beam to conduct cross section measurement experiments. The simulation code aims to understand neutron flux distribution and transport through the targets. Finally, the corresponding results obtained using GEANT4, through the application of biasing techniques, were compared to those resulting from the combined use of the MCNP 6.1 [3] and NeuSDesc [4] codes.

Keywords Monte Carlo, GEANT4, TANDEM accelerator, parasitic neutrons, cross section biasing

INTRODUCTION

This study is based on the need to quantify neutrons produced by the (d,n) reaction in tritium within the neutron energy range of 15–20 MeV. The main purpose is to use the resulting monoenergetic beam for studying cross-sections in various targets. Different simulation methods are conducted to accurately determine this neutron flux. In the context of this work, the Monte Carlo GEANT4 code is used to determine the neutron flux originating from the primary reaction ^{3}H(d,n)^{4}He and, additionally, the parasitic neutrons that contaminate the beam due to the interaction of secondary particles with elements in the experimental setup. The GEANT4 code tracks the secondaries within the target, using libraries with evaluated reaction data for energies below 20 MeV, such as TENDL [5] and ENDF [6]. Due to the relatively low cross section of (d,n) reactions leading to low statistical generation of neutrons, biased sampling techniques (cross-section biasing techniques) were necessary in the Monte Carlo sampling process to reduce computational time for simulations.

ANALYSIS DETAILS

Biasing technique application

In neutron production, a biasing technique is used to modify the cross section of a specific reaction. GEANT4 toolkit uses the mean free path (λ) of a particle to determine the likelihood of a reaction occurring. The mean free path is inversely proportional to the macroscopic cross section (Σ):

$$\lambda = \frac{1}{\Sigma}$$

The macroscopic cross section (Σ) is calculated from the microscopic cross section (σ) using the

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formula:

$$\Sigma(\mathrm{m}^{-1}) = \mathrm{N}\left[\frac{\mathrm{nuclei}}{\mathrm{m}^3}\right] \cdot \sigma[\mathrm{m}^2]$$

here, N is the number of nuclei per cubic meter, and σ is the microscopic cross section for each deuteron – induced reaction.

To implement the biasing technique, the mean free path is multiplied by a biasing factor (f_b). This increases the probability of deuteron–induced interactions, reducing the value of λ accordingly. However, using this technique without careful consideration may lead to unintended differences between biased and unbiased (analog) simulations, affecting the expected physical results.

In simpler terms, the biasing technique adjusts the likelihood of particle interactions by changing the mean free path and using it without proper awareness can result in discrepancies between biased and unbiased simulations. The process is illustrated in Figures 1 and 2, comparing an unbiased case (with $f_b=1$) with a biased case (with $f_b>1$):

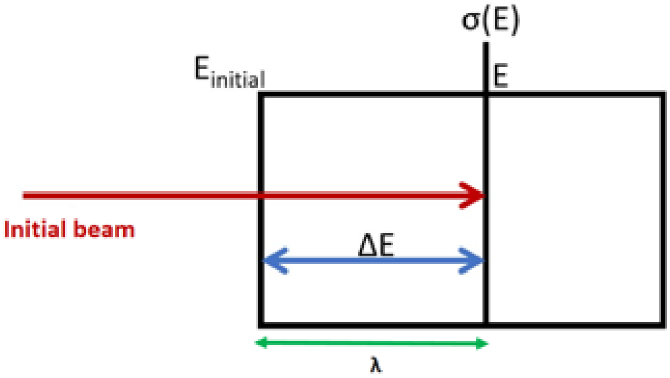

Figure 1. *Illustration of an unbiased (analog) case in a reaction with energy loss of the particle equal to ΔE*

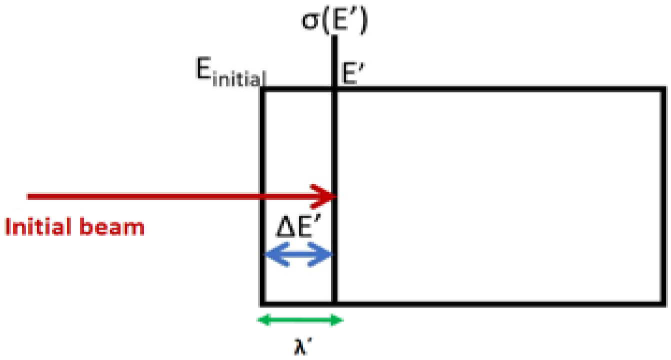

Figure 2. *Illustration of a biased case in a reaction with energy loss of the particle equal to* $\Delta E' < \Delta E$

By applying a specific value of the biasing factor, the energy loss of a particle changes. This can happen because of the increase in the probability of an interaction happening. In Figure 2, the energy loss of the particle is reduced. Therefore, the particle interacts with matter, having a different cross section and energy.

Control Simulations

To determine any discrepancies between biased cases and unbiased cases, control simulations were conducted on special targets. The simulated geometry consists of a deuteron source emitting towards the target axis with an initial energy $E_d = 2–3.45$ MeV, a thick cylindrical target and a cylindrical void detector covering almost a 2π neutron detection angle. A depiction of the simulated geometry is shown in Figure 3.

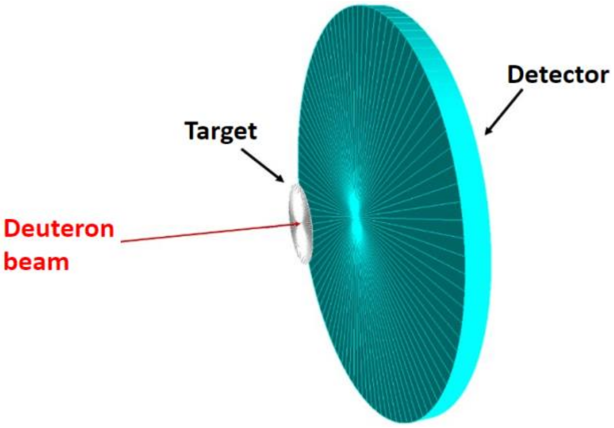

Figure 3. *Simulated geometry for the control simulations of special targets*

The output information of the control simulations is the neutron energy distribution in analog (unbiased – with the number of primaries $N_d = 10^9$ and $f_b = 1$) and biased (with $f_b = 100, 1000, 10000$) case and the number of neutrons as a function of the target depth. In Figures 4 and 5, a comparison is shown between these four cases using a 3.45 MeV deuteron beam and a thick aluminum foil as a target. The deuteron beam deposits all its energy into the aluminum foil. To efficiently determine any discrepancies between the analog case and the biased cases, the product of the number of beam particles (N_d) and the chosen biasing factor (f_b) was kept normalized to the proportional case.

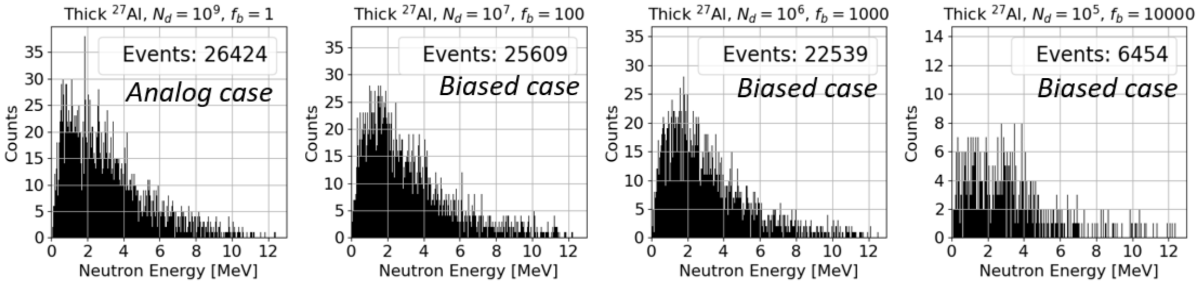

Figure 4. *Neutron energy distribution. Comparison of the biased bases with the analog case*

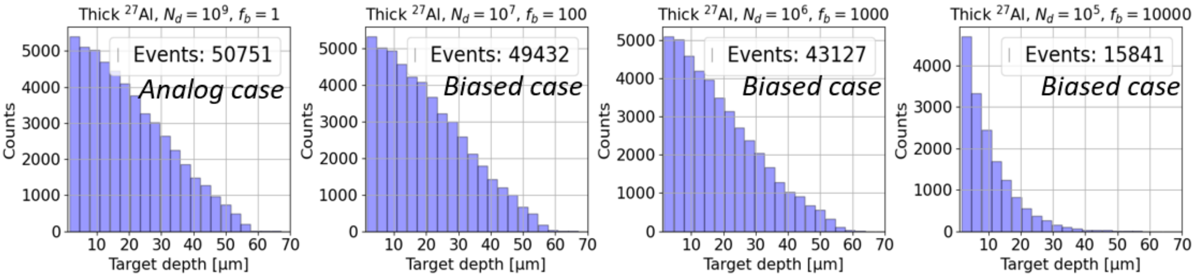

Figure 5. *Neutron production as a function of the target depth. Comparing biased cases with the analog case*

From the above simulations in the aluminum target, statistical results remain accurate as the biasing factor reaches the value of $f_b = 1000$. For $f_b = 10000$, the shape of the distributions and the total number of neutron events have obviously changed because of the impact on the physical processes.

Furthermore, additional control simulations were conducted to effectively determine the proper biasing factor in each foil of the tritium flange in the TANDEM accelerator. Running various simulations on these special targets with different depths and energies, three main criteria should be taken into consideration:

a. The total stopping power of the charged particle into the target relates to the energy spectrum of the neutrons and their final distribution
b. The depth of the target determines the available energies of the primary particles that are about to interact with the target
c. The cross section sharp fluctuations for the reaction of interest can lead to different neutron production distribution when a biasing factor is applied

SIMULATED GEOMETRY AND RESULTS

The GEANT4 simulated geometry is based on the experimental setup of the TANDEM accelerator at N.C.S.R. “Demokritos”. The geometry consists of the accelerator line, the two collimators, the flange and five targets irradiated with the resulting neutron beam from the $^{3}H(d,n)^{4}He$ reaction, as shown in Figure 6.

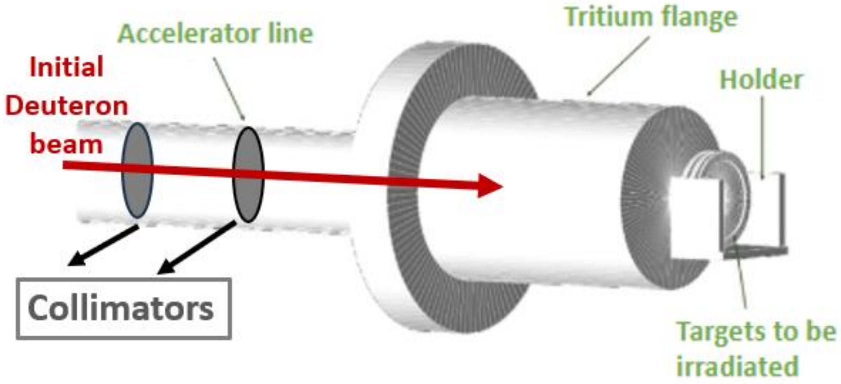

Figure 6. *Visualization of the geometry of the “Demokritos” experimental setup through the GEANT4 code. The initial deuteron beam is shown in red, then you can see the accelerator line, the two collimators, the tritium flange and the targets to be irradiated, which are on a base (holder).*

For every deuteron energy of reference (2.11 MeV, 2.9 MeV and 3.45 MeV), different biasing factors have been applied to the flange foils (Table 1).

Table 1. *Biasing factors f_b for each flange foil for every deuteron energy of reference*

Deuteron Beam Energy [MeV]	Molybdenum foil (f_b)	Tritium foil (f_b)	Copper foil (f_b)
2.11	---	1000	---
2.90	---	1000	---
3.45	1000	1000	100

For the initial deuteron beam energies of 2.11 MeV and 2.9 MeV, the cross section for the (d,n) channel in molybdenum and copper approaches zero. The cross section biasing technique applied to molybdenum and copper did not give improved statistical results for the total neutron energy spectrum. Consequently, the biasing technique was not implemented in these specific cases. The simulation results for each energy level are presented in Figs. 7 and 8 below. Fig. 7 illustrates the distribution of incident neutron energy in the first target for each initial beam energy (for 2.11 and 3.45 MeV the chosen target is Au, while for 2.9 MeV the target is Al). Additionally, Fig. 7 compares the results of GEANT4 simulations with the neutron flux distribution obtained from the MCNP & NeuSDesc codes.

Finally, in Fig. 8, the contribution of neutrons from each volume in GEANT4 simulations is displayed. This precise determination of low – energy neutrons is expected to play a critical role in future fission experiments, as low – energy neutrons are capable of triggering fission reactions.

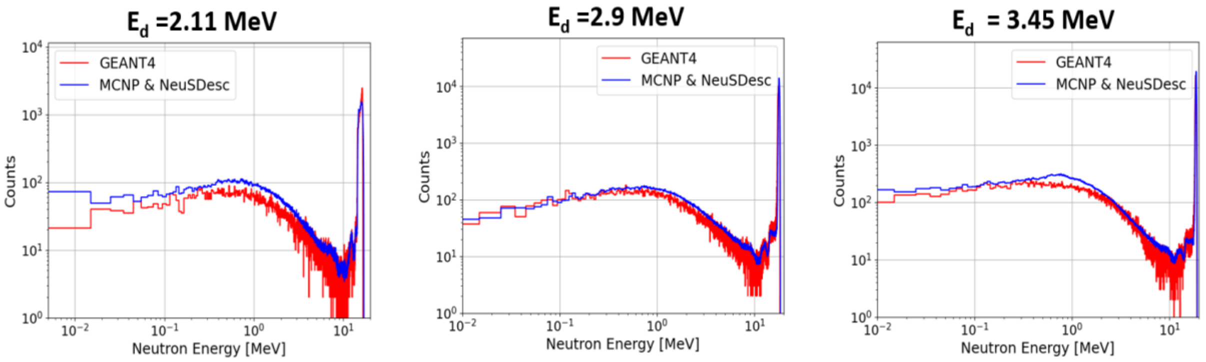

Figure 7. *Incident neutrons energy distribution in the first target of the holder. Comparison between GEANT4 and MCNP & NeuSDesc simulations.*

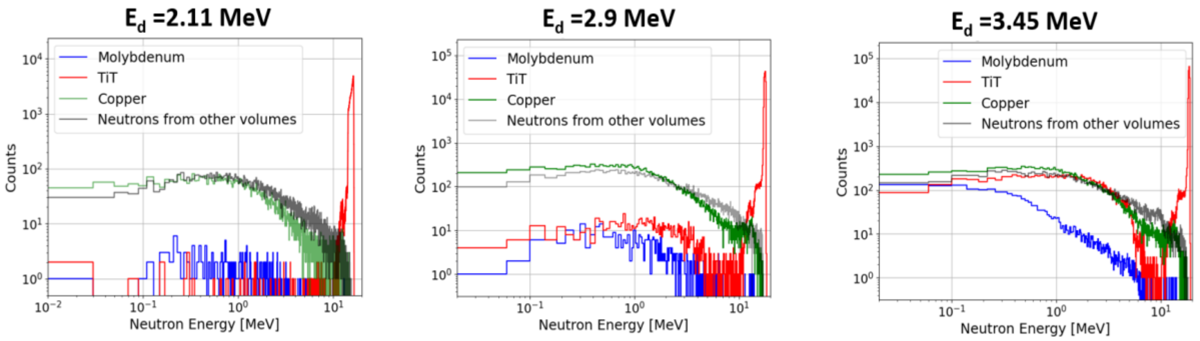

Figure 8. *Contribution of neutrons from each volume of the total geometry in GEANT4 simulations. The other volumes contributions (black color) are the parasitic neutrons from accelerator line, the collimators, the aluminum flange and the holder.*

CONCLUSIONS

From the results, it was observed that for a low-energy deuteron beam (2.11 MeV), there are significant differences between the main energy peaks produced by the GEANT4 simulation and those produced by the corresponding MCNP and NeuSDesc codes. Specifically, the main peak of MCNP has an average energy of 16.10 MeV and a maximum neutron energy of 17.06 MeV, while that of GEANT4 has an average energy of 16.36 MeV and a maximum neutron energy of 16.63 MeV. This discrepancy was attributed to the MCNP code's incapability of accounting for the energy loss of deuterons within the tritium target. To be specific, in MCNP the TiT – target is irradiated with a neutron source generated via the NeuSDesc code, so the energy loss effects (both spatial and longitudinal) of the deuterium inside the tritium target are not considered.

For the other deuteron energy levels, there was better convergence of the results concerning the events of the main neutron peak (15–20 MeV). Events beyond the main peak (parasitic neutrons) in the GEANT4 simulation were in good agreement with those of the MCNP code. This was expected as there is limited ability to observe additional parasitic neutrons due to very low cross sections in the elements of the experimental setup located in front of the flange.

Finally, it constitutes a future objective to:

a. Model the deuteron beam to be as compatible as possible with the experimental beam

b. Study possible material oxidation in the elements of the experimental setup and assess the contribution of parasitic neutrons due to (d,n) reactions with oxygen

c. Investigate reactions like $^{2}H(d,n)^{3}He$ and quantify the contribution of parasitic neutrons resulting from these reactions. Specifically, the implantation of deuterons in the flange elements is plausible, because of the repeated irradiation of the flange targets over the years

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