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Study of the cross section biasing technique using GEANT4 and determination of the parasitic neutrons at N.C.S.R. "Demokritos"

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Abstract   A simulation code was developed using the GEANT4 [1] toolkit in order to determine the behavior of the neutron production beams generated by proton induced reactions, while applying the cross section biasing technique [2]. As the application of the biasing technique can cause a change in the physical processes occurring during the simulation, the specific implemented technique was tested via control simulations to determine any deviations of the results from the theoretically expected ones. Different materials, geometries and biasing factors were used in order to qualify and quantify the discrepancies between the unbiased and the biased simulations. One of the main reactions used for the production of the neutron beam at the Tandem accelerator laboratory of N.C.S.R. "Demokritos" [3] is the ^{3}H(p,n)^{3}He one. In the geometry of the main tritiated target, elements such as molybdenum, copper and titanium are included. During the interaction of the proton beam with them, it is possible to produce neutrons that will "contaminate" the main neutron beam. These neutrons are called parasitic and their quantification via the proper simulated geometry and the developed code is necessary in order to avoid obtaining erroneous results in cross section measurements on the various targets under study [4].

Keywords   Cross section biasing, GEANT4, parasitic neutrons

INTRODUCTION

The neutron beams generated by proton-induced reactions are widely used in many applications. At the Tandem laboratory of N.C.S.R "Demokritos", the ^{3}H(p,n)^{3}He reaction consitutes one of the main sources of neutrons implemented in fission and neutron activation experiments. In the present work, the GEANT4 toolkit was used in order to determine the behavior of the neutron production caused by proton-induced reactions, while applying the cross section biasing technique. Different materials, geometries and biasing factors were used for the quality assessment and the quantification of the discrepancies between the unbiased and the biased cases. During the interaction of the proton beam with the materials of the main tritiated target, parasitic neutrons are produced. By constructing the proper geometry and using the developed GEANT4 code, the determination of the parasitic neutrons is achieved with optimal statistical results in short computational times, while the discrepancies between the unbiased and the biased results remain minimal.

ANALYSIS DETAILS

Biasing technique application

The biasing technique which is used for the neutron production is responsible for the biasing of the cross section of the specific reaction. The GEANT4 toolkit is using the mean free path quantity, λ, for the determination of the possibility of a reaction to take place and its value is given by the following formula:

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

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where Σ is the macroscopic cross section which is given by the microscopic cross section via the formula:

$$\Sigma(m^{-1}) = N(nuclei/m^3)\,[\sigma(m^2)]\,, \qquad (2)$$

where N is the number of the nuclei per m^3 and σ is the microscopic cross section of each proton induced reaction.

For the implementation of the biasing technique, the mean free path is multiplied by a factor (biasing factor) f_b. As a result, the probability of the proton-induced interactions increases, while the value λ decreases accordingly. This process could affect the whole procedure and cause changes in the expected physical results. Applying unconsciously the above technique could lead to the occurrence of erroneous discrepancies between the biased and the unbiased (analog) case. Schematically, the effect of the cross section change is presented in Fig. 1, using the (p,n) reaction as an example. As demonstrated in Fig.1, the application of the specific technique causes direct changes to the energy of the impinging protons due to energy loss effects. This fact, results to the change of the cross section, while the production of neutrons follows a different energy distribution in contrast to the ubiased case.
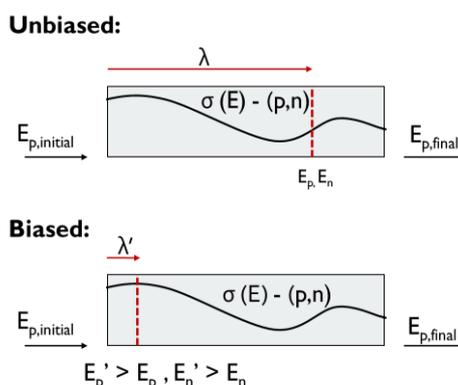

Figure 1. *Schematic representation of the cross section biasing technique behavior*

Control simulations and results

In order to choose the most suitable biasing factor which will minimize the above mentioned discrepancies, various control runs are mandatory. Different materials, geometries and biasing factor values were used for the qualification and quantification of the effective differences. It is worth mentioning that, for all the simulations, the non-elastic nuclear interactions are modeled with the G4ParticleHP package provided by GEANT4 and the data used for the (p,n) reactions correspond to the TENDL2019 [4] nuclear data library.

In Fig. 2, the setup schematic illustration of the control simulations is shown. A point source is emitting protons of 10 MeV or 6.5 MeV towards the target axis and these impinge on a thick ^{27}Al or ^{56}Fe target in each case study. A cylindrical void detector, covering almost a 2π detection angle, is placed right after the main target. The energy distribution of the neutrons passing through the detector window and the neutron production distribution as a function of target depth are recorded. For each unbiased case, the number of the primary protons is $N_p = 10^9$, while for the biased cases $N_p = 10^7$. The results of the unbiased run are used for the determination of the discrepancies caused by the application of the biasing technique.

Figure 2. *Schematic illustration of the control simulation setup*

The control runs revealed the exact behavior of the application of the specific biasing technique. In Fig. 3 and 4, the results concerning the use of ^{27}Al as main target and the proton energy $E_p = 10$ MeV are presented for the unbiased case along with the biased cases with $f_b = 150$ and $f_b = 10000$.
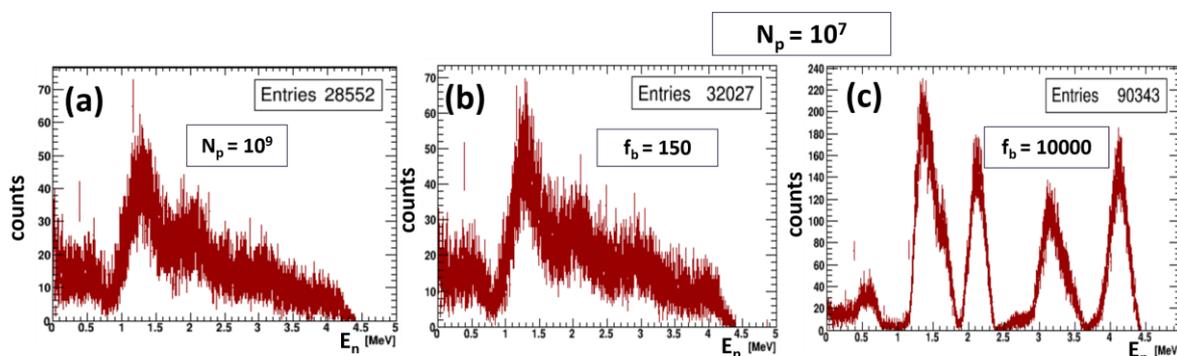

Figure 3. *Neutron spectra for (a) the unbiased case with the number of primary protons equal to $N_p = 10^9$, (b) biased case with $f_b = 150$ and $N_p = 10^7$, (c) biased case with $f_b = 10000$ and $N_p = 10^7$.*

Figure 4. *Distribution of the neutron production as a function of the depth along the target for (a) the unbiased case with the number of primary protons equal to $N_p = 10^9$, (b) biased case with $f_b = 150$ and $N_p = 10^7$, (c) biased case with $f_b = 10000$ and $N_p = 10^7$.*
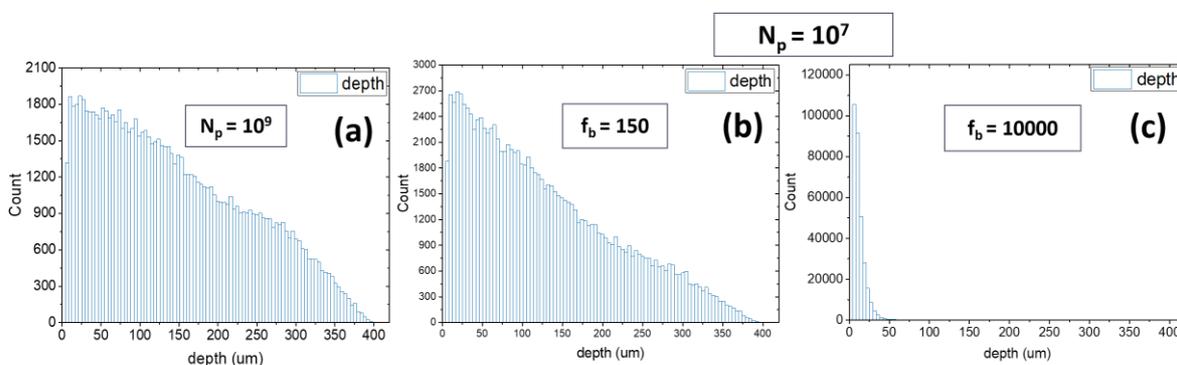
As shown above, the use of higher biasing factor values, forces the interactions to occur closer to the target surface. This fact leads to erroneous and unphysical results corresponding to the neutron energy distribution. The same behavior was observed at each case study. The effect is less intense for the low proton energy for both targets (aluminun and iron), but the discrepancies between the unbiased and the biased case are more pronounced in the case of the ^{56}Fe target. This is attributed to the differences observed between the cross-section values of the ^{27}Al(p,n) and ^{56}Fe(p,n) reactions (more specifically, the Fe cross section displays a rapidly falling behavior, in contrast to the Al one - for the same proton energy range). Furthermore, additional control simulations for the cross-check of the biased proton beam behavior were conducted, revealing no significant deviations from the analog case.

The validation of the application of the specific biasing technique, carried out by comparing the results for different materials and proton energies, lead to certain assumptions. For the choice of the most suitable biasing factor in a case study, there are three main criteria that have to be taken into consideration:

a. The total stopping power of the biased charged particles in the target
b. The energy threshold of the reaction under study
c. The cross section structure of the reaction of interest

According to the first two points, the available proton energies through the target are determined. The proton energy distribution is directly correlated to the produced neutron energies and their final distribution. High proton energy discrepancies, caused by the use of higher biasing factors, can lead to unphysical neutron energy distributions. Furthermore, with respect to the third criterion, sharp fluctuations in the cross section can also cause large deviations in the neutron distribution.

RESULTS AND DISCUSSION

In order to implement the biasing technique for the determination of the parasitic neutrons produced during the use of the ^{3}H(p,n)^{3}He reaction at N.C.S.R. "Demokritos", the appropriate geometry of the experimental setup needed to be reconstructed via the GEANT4 toolkit. The full geometry consists of the experimental beam line, the collimators and the main flange. The main flange includes the tritiated titanium foil, the molybdenum foils right before the tritiated target and the copper backing as a beam stop (Fig. 5). The parasitic neutrons are mainly produced due to the interaction of the proton beam with the materials contained in the flange and their quantitification plays a signifigant role in all the neutron-induced experiments.
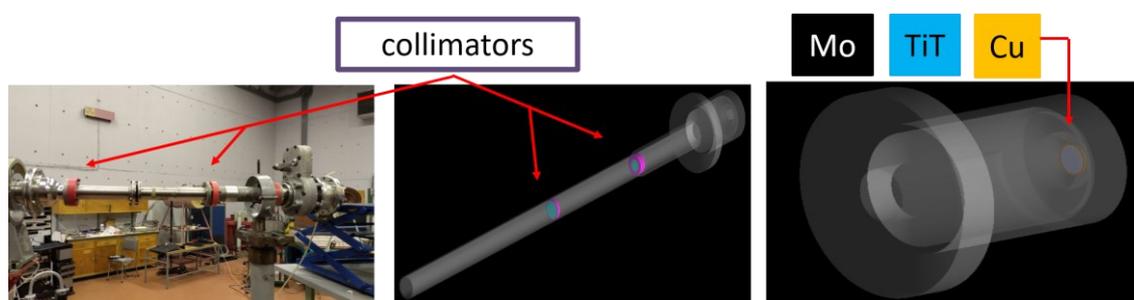

Figure 5. *The full geometry of the experimental setup. In vivo (on the left) and the simulated one (on the right). The main materials of the flange are also presented.*

The final results were extracted for 8 different proton energies chosen with respect to a previous experiment [5]. The detection of the neutrons was carried out in a void detector placed ~ 8 cm after the endpoint of the main flange. Three different runs were conducted performing the proton biasing at the three different targets (molybdenum, tritiated titanium and copper) separately. For the molybdenum and the tritiated titanium foils, the biasing factor value $f_b = 1000$ was used, while $f_b = 100$ was the most suitable value for the thick copper foil. The results corresponding to the copper foil were normalized accordindly. The number of the primary protons was $N_p = 10^9$ in all cases.

After the proper analysis, the comparison between the extracted results using the GEANT4 simulation and the combination of MCNP [6] and NeuSDesc [7] codes was conducted. The related graphs for the proton energies $E_p = 3.400, 3.849, 4.300, 4.763, 5.229, 5.550, 5.850$ and 6.500 MeV are presented in Fig. 6. Apparently, the neutrons produced due to the interaction of protons with the Mo, Cu and TiT foils are described and qualified in a quite satisfactory way. As expected, a high contribution of parasitic neutrons in the low neutron energy range is revealed for higher proton energies. For these energy values, the cross section of the (p,n) reactions on target materials exhibit significant values. A comparison between the two methods, reveals the disadvantage of the MCNP & NeuSDesk codes to reproduce the high neutron rate in the low energy range with respect to the increase of the incident proton energy values. However, for $E_p = 3.400$ MeV, the determination of low-energy neutrons seems to be less satisfactory when using the GEANT4 code, due to the limitations related to the number of primary particles used. In both methods, the scattering of the neutrons in the tritiated target is described in a quite similar way.
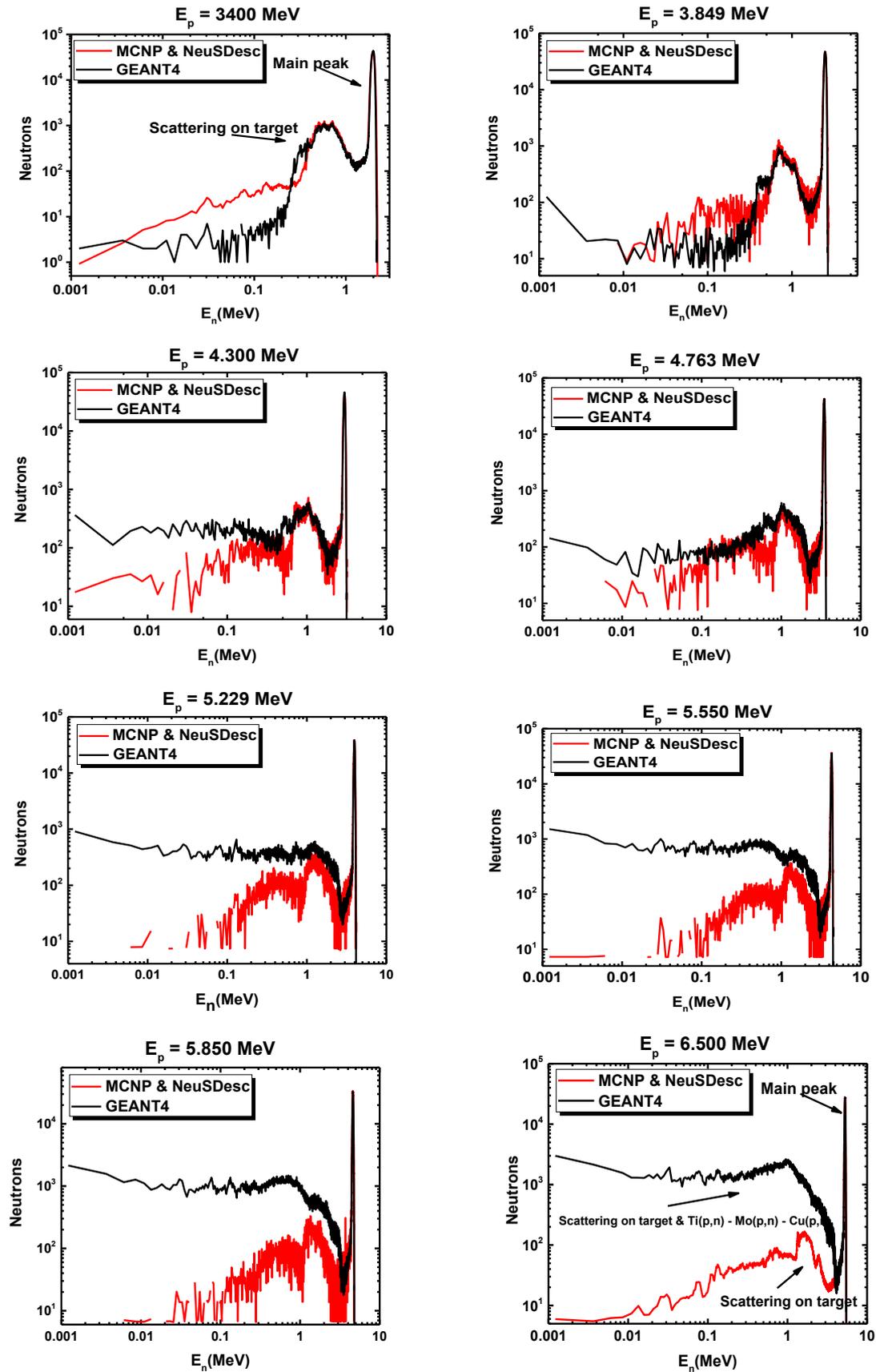
Figure 6. *Comparison on the neutron distribution produced via the GEANT4 simulation and the combination of the MCNP and NeuSDesk codes for proton energies E_p = 3.400, 3.849, 4.300, 4.763, 5.229, 5.550, 5.850 and 6.500 MeV*
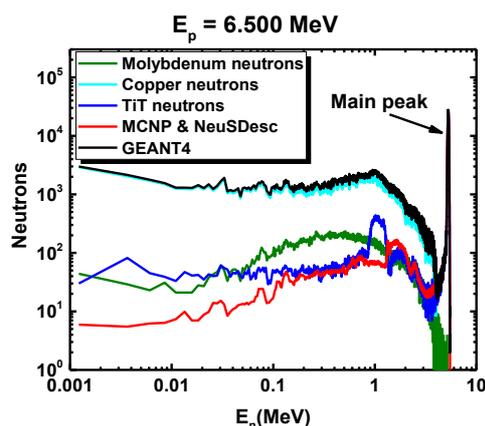
Figure 6 (continued). *At the last graph the neutrons originated from each different target foil are presented with different colors*

Finally, the last graph of Fig. 6 displays the individual contributions of the neutrons originated by the (p,n) reactions on molybdenum, tritiated titanium and copper, in the total neutron flux. This precise determination of the low energy neutrons is expected to play a critical role in future fission experiments.

CONCLUSIONS

The cross section biasing technique was applied using the GEANT4 toolkit for the determination of neutrons produced by (p,n) reactions in short computational times, while obtaining optimal statistical results. For the validation of the results, simple geometries were constructed and materials such as aluminum and iron were tested. Control runs were carried out for different proton energies and various biasing factors. The comparison of the results with the analog case revealed the complex behavior of the biasing technique and its limitations. Several assumptions for the criteria concerning the suitable value of the biasing factor in each case study had to be made. The implementation of the biasing technique in the real experimental setup, which was constructed using the GEANT4 toolkit, lead to a satisfactory description of the parasitic neutrons produced during the irradiation of the tritiated target, while the combined use of MCNP and NeuSDesk failed to reproduce the expected enhanced low-energy tail of the neutron spectra.

Further simulations, concerning a more detailed description of the experimental conditions and various experimental setups, are mandatory in order to accurate determine physical quantities concerning neutron based experiments.

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