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Original Article

GEANT4 characterization of the neutronic behavior of the active zone of the MEGAPIE spallation target

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ABSTRACT

The increasing interest that GEANT4 is gaining nowadays, because of its special capabilities, prompted us to address its reliability in neutronic calculation for the realistic and complex spallation target MEGAPIE of the Paul Scherrer Institute of Switzerland. In this paper we have specifically addressed the neutronic characterization of the active zone of this target. Three physical quantities are evaluated: neutron flux spectra and total neutron fluxes on target's z-axis, and the neutron yield as a function of the target's altitude and radius. Comparison of the obtained results with those of the MCNPX reference code and some experimental measurements have confirmed the impact of the geometrical and proton beam models on the neutron fluxes. It has also allowed to reveal the intrinsic influence of the code type. The resulting differences reach a factor of ~2 for the beam model and 4–18% for the other parameters cumulated. The analysis of the neutron yield has led us to conclude that: 1) Increasing the productivity of the MEGAPIE target cannot be achieved simply by increasing the thickness of the target, if the irradiation parameters are not modified. 2) The size of the spallation area needs to be redefined more precisely.

1. Introduction

The MEGAPIE spallation target [1,2] is a neutron source specially designed to demonstrate the feasibility of external neutron supply for accelerator-driven systems (ADS). The neutron performance of such a device has always been the main issue in its development. The neutronic characterization of the MEGAPIE target (Fig. 1 a) has already been carried out with Monte Carlo calculations in the R&D phase, and with experimental measurements in the irradiation phase (2006) [3,4]. The transport codes used in this characterization include the MCNPX code [5,6] and a little less the FLUKA code [7,8]. In this paper, we propose to address this topic using the GEANT4 toolkit [9–11]. The relevance of the use of the GEANT4 code is justified by the fact that this code is one of the most powerful modern codes, based on the new programming technology (C++/OO) and having several advantages. As toolkit, GEANT4 benefits from a wide variety of models and implementing modes of physics, geometry, and primary particles. As an example, GEANT4 includes, among numerous physics models, "INCLXX-ABLA" (§ 2.4) which are the most suitable models for spallation reaction. In addition, GEANT4 can simulate problems in almost all energy ranges using together the detailed and condensed methods; it is a class II code [12 and refs.]. Another raison to use GEANT4 is to give a new numerical tool to study the MEGAPIE spallation target that can't be completely characterized only by experiment. Several constraints prevent this characterization as: 1) The available area for neutron detectors is very narrow (Ø1.3 cm) and inaccessible during the irradiation period. 2) Strong and frequent temperature gradients (500 K–690 K) caused by repetitive extinctions of the proton beam. 3) Intense irradiation: 10^{13}-10^{14} n/cm^2/s and the same level of γ radiations. 4) Strong electromagnetic perturbations caused by electromagnetic pumps ensuring the liquid metal circulation. Finally, this work also aims to demonstrate the reliability of GEANT4 to accurately model a realistic and complex neutron source such as the MEGAPIE spallation target. It is worth noting here that GEANT4 is constantly being updated and improved through international collaboration [13].

In this paper, we have evaluated three physical quantities, namely: the neutron flux spectrum at the first two stages of the neutron micro-detectors embedded in the target (Fig. 1 b & c), the

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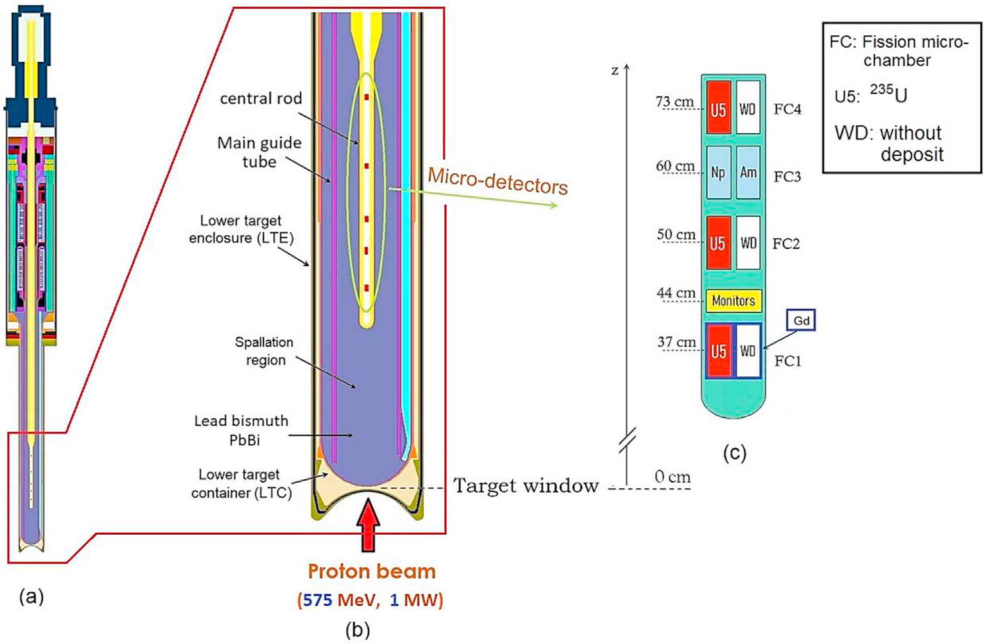

Fig. 1. (a) vertical cut of the MEGAPIE target geometry modeled with GEANT4. (b) Active zone of the target including the micro-detectors. (c) Illustration of micro-detectors and their positioning.

total neutron flux at the five stages of these micro-detectors and the neutron production rate per incident proton, as a function of the altitude z and radius r. These quantities are chosen to provide an overall characterization of the neutronic behavior of the most active region in the MEGAPIE target. They provide relevant information on the neutron generation capabilities of such a target. We talk about the neutron flux intensity, its energy distribution, and the neutron yield: "number of generated neutrons/incoming proton". Obviously, the neutron production efficiency is one of the main objectives of the MEGAPIE target, and this efficiency is directly affected by the neutronic behavior of the spallation region.

It should be noted that in this simulation, we have used the same geometrical model and proton beam profile as in our publications [12,14]. The main modifications that have been made to the present simulation are the addition of the physical model managing thermal neutron scattering (§ 2.4) and the use of parallel geometry (§ 2.2).

To evaluate the obtained results and thus the reliability of GEANT4 to reproduce correct results for the realistic spallation target "MEGAPIE", we have compared the results of our simulation with those obtained either with the MCNPX reference code, or by some experimental measurements. The comparison revealed a satisfactory agreement between our results and those of reference, and consequently demonstrated the validity of our GEANT4 modeling of a complex system like the MEGAPIE target.

2. Materials and methods

2.1. GEANT4 toolkit

GEANT4 (GEometry ANd Tracking 4) is a complete environment for simulating the passage of particles through matter. Taking advantage of the experience gained in its precursor "GEANT3**"** and based on the new C++/OO programming technology, the GEANT4 tool was initiated in 1994 as part of the RD44 project [15]. This initiative was undertaken by the European Organization for Nuclear Research (CERN) and the Japanese Research Organization for High Energy Accelerators (KEK). The first version GEANT4.1.0 was released in December 1998.

GEANT4 is not just a simple code, but a whole simulation environment that allows users to build their own application without being limited to pre-defined components. Thanks to the object-oriented (OO) technology, it is all time possible, in a GEANT4 application, to modify available implementations and/or add others without affecting the basic architecture of the code. GEANT4's capabilities have made this toolkit a platform for building other more specific codes including codes dedicated to medical applications such as GATE [16,17] and GAMOS [18,19], and the MCADS model [20–23] for modelling spallation targets.

In this work we have used the GEANT4.10.2.p03 version [24] built on a scientific Linux v7.4 system [25] together with many other components to insure a better performance. The required components are: The class library for high-energy physics CLHEP v2.3.1.1 [26], the data analysis framework ROOT v6.12 [27] and the development framework Qt v5.6.2 [28].

2.2. Parallel geometry in GEANT4 [29]

In order to overcome the difficulties related to the complexity of the detectors and to give more flexibility to the applications, GEANT4 proposes two concepts of geometry: mass geometry and parallel geometry. Mass geometry is the actual geometry with real materials of the simulated detector. For instance, the mass geometry in this simulation is the actual geometry of the MEGAPIE target (Fig. 1 a). Parallel geometry is a fictitious geometry to which no material is attributed. This geometry is defined in the same way as the mass geometry, but without restrictions related to volume limits. Overlapping and sharing of surfaces are not forbidden. The only restriction is that the parallel geometry must not extend beyond the world volume.

Parallel geometry is an important feature added to GEANT4 code to enhance its toolkit aspect. Thanks to its free nature of restrictions, it allows to carry out, so easily, many tasks such as: data extraction and variance reduction implementation, etc. A volume in parallel geometry is just like any other volume in mass geometry, it can serve as: 1) Sensitive volume, for scoring purposes. 2) Region, to define user limits such as: maximum step, range cuts [12], minimum energy for particle tracking … 3) Region to define biasing, e.g., assign an artificial weight. in the present modeling, we have used parallel geometry for two main purposes: Implementation of the geometric importance-based variance reduction technique (§ 2.3), and definition of sensitive volumes that cover multiple mass geometry volumes. It should be noted here that in the MEGAPIE target, data extraction task becomes so delicate if parallel geometry is not used. Indeed, the extraction of a given physical quantity requires to associate to each concerned volume a separate sensitive detector. However, with parallel geometry, only one volume containing previous volumes can be used to achieve the task.

2.3. *Variance reduction by geometric importance: “splitting/killing”*

Rare events simulation is always very slow to converge. To overcome this problem, variance reduction techniques [30,31] are often used. They allow to accelerate the calculation convergence without affecting the results quality. In general, variance reduction is about favoring events that can generate more results.

Most simulations that require the use of variance reduction techniques are simulations that are interested in counts in volumes that are either small, far from the source, or separated from the source by a highly stopper screen. In our case, the fission micro-chambers (Fig. 1 c), in which we want to determine the neutron flux, are small volumes and considerably far from the entrance of the proton beam (Fig. 1 b). In this situation, the convergence of neutron spectra calculations is indeed very slow. That is why we have proceeded with a variance reduction in order to accelerate calculations convergence. The chosen technique is based on geometric importance [32]. It is a splitting/killing or splitting/(Russian roulette) technique. Splitting consists of clone particles that move towards the counting volume. Each time a particle accesses a geometrical cell i, it undergoes cloning by a coefficient n_i. The n_i coefficients are chosen by the user. The particles resulting from cloning each bear a weight of (W/n_i). Where W is the weight of the mother particle. Killing or Russian roulette consists in killing with a probability of $(1/n_i)$ any particle leaving cell i moving away from the count volume. However, if the particle is survival, its weight is multiplied by the n_i coefficient. To implement this technique, we have subdivided the area below the fission micro-chambers into several cylindrical cells of 1 cm thickness. To each cell we have assigned a number n_i designating its geometric importance. The importance of a cell increases as it approaches the relevant fission micro-chamber. This technique made it possible to significantly accelerate the convergence of calculations while preserving the quality of the results.

2.4. *Modeling physics*

To govern the physics of the problem, we have used the “FTFP_INCLXX_HP” physics list. This is a predefined list of physics, provided by GEANT4. It is already validated as the most appropriate physics list for spallation problems [33]. The FTFP_INCLXX_HP list includes the following physical models: the Fritiof model (FTF) [34,35], the Pre-compound model (P) [36], the Liège Intranuclear Cascade model, C++ version (INCLXX) and the Hight Precision model (HP). The FTF model is used in GEANT4 to simulate interactions between hadrons, nuclei, anti-baryons and anti-nucleus−nucleus. It is suitable for energies above 5 GeV. The Pre-compound model manages the pre-equilibrium emission of protons, neutrons, and light ions [36]. INCLXX is the C++ version of the INCL model [37,38] which is designed to govern the medium energy reactions of such as spallation reactions. Several improvements in terms of energy and type of particles have been made to this model. Currently, it can manage reactions induced by light ions and nuclei up to carbon. Further, INCL4.6 version and higher can also describe the emission of light clusters up to alpha particles or even heavier particles [39−41]. In order to be integrated into GEANT4, the INCL model is translated into C++ (INCLXX) by Kaitaniemi et al. [42] and Mancusi et al. [40]. In this simulation, we have used the INCLXX 5.2.9.5. version. It covers an energy range up to 20 GeV as upper limit. In fact, the INCL model can well describe only the intranuclear cascade stage, and to be able to describe the two stages of the spallation reaction, it should be coupled with one or more de-excitation models. For this purpose, we have coupled it with the statistical model ABLA v3 [43−45]. According to the spallation benchmarks of the International Atomic Energy Agency (IAEA) [46,47], the ABLA model is currently considered one of the best de-excitation physics models. We recall that the physics list used in this work also includes the HP physics model for low energy neutrons ($<$ 20 MeV).

In fact, the set of physics models mentioned above is sufficient to calculate certain physical quantities concerning the MEGAPIE target, as shown in the publications [12,14]. However, this is not sufficient to evaluate other quantities such as neutron distributions: fluxes, spectra, etc. To calculate such quantities, it is necessary to add a physics model able to handle the thermal neutrons scattering processes. The GEANT4 toolkit includes a special thermal neutron scattering model *“G4NeutronHPThermalScattering”* ($<$ 4 eV). This model is recently added to the GEANT4 code with corresponding data library *“G4NeutronHPThermalScatteringData”*. many validation and improvement studies of this model have been conducted in recent years, such as [48−51].

In the thermal energy range, the De Broglie neutron wavelength is comparable to the interatomic distance of materials. Therefore, the thermal neutron interactions with mater is affected by the chemical structure of materials. In such a situation, atoms cannot be treated as free, but rather as linked. Thus, neutron scattering on the same atom vary according to the type of the material. For this reason, defining an element for scattering, in a GEANT4 simulation, needs to specify the material type. For instance, to process neutron scattering in water, hydrogen must be defined as follow: “TS_H_of_Water”. Currently, the data library *“G4NeutronHPThermalScatteringData”* integrated into GEANT4 provided data for 20 different materials.

3. Results and discussion

To overcome the experimental constraints mentioned in the introduction, the “Commissariat à l'Énergie Atomique” (CEA) of France has designed and developed innovative detectors [52] capable of taking, with accuracy better than 5%, online neutron flux measurements in the MEGAPIE target. These detectors are micro-metric fission chambers (FC) designed specifically to withstand the harsh operating conditions of the MEGAPIE target. They are 8 pairs, arranged side by side in four stages along the target's axis (Fig. 1 c). Each pair is made of two micro fission chambers: one with fissile deposit and another without deposit (WD). The empty chamber is used for background compensation. The closest pair (FC1) to the spallation region is shielded with a thin layer (200 μm) of natural Gadolinium (Gd) to eliminate the thermal component of neutron spectrum. The pair of the FC2 contains ^{241}Am deposit in a chamber and ^{237}Np in the other chamber. This is intended to estimate the incineration rate of these minor actinides. To provide reference measure, a ninth detector is used as a monitor. It is placed in a Titanium (Ti) box between the first and second FCs pair. More details about these micro-detectors: dimensioning, material composition and other characteristics, are given in references [3,52,53].

Before discussing the results of this simulation, we would like to point out that the neutron fluxes presented below (§ 3.1. and § 3.2.) do not result from an actual simulation of the micro-detectors, but are fluxes calculated at their positions, as part of an overall modelling of the MEGAPIE target. Nevertheless, the overall structures of these micro-detectors are taken into account in the modelling.

3.1. Estimating of neutron flux spectra along the target's axis

For reasons related to computing equipment, we have been limited to the calculation of the neutron flux spectra at the first two stages of the micro-detectors. In fact, the small size of these micrometric detectors makes it very unlikely that neutrons can pass through, which makes the calculation of the neutron spectrum an extremely time-consuming process. The computing time becomes even longer when the micro-detector is further away from the neutron production area. The use of variance reduction techniques is not always the magic solution to make short a successful calculation. Indeed, if the number of events that generate results is very small, the excessive amplification of some events can cause convergence concern. In such a situation, a large number of simulated events and sophisticated computing equipment becomes the unique solution to achieve good results.

Fig. 2 jointly illustrates the neutron flux spectra obtained with GEANT4 and MCNPX. The results of MCNPX are already experimentally validated and published in Refs. [3,54]. Analysis of Fig. 2 shows that in the FC1 stage, the thermal component of the spectrum is fully absorbed due to the existence of the Gadolinium (Gd) layer. Instead, in the monitor stage where there is no Gd layer, this component (up to 1 eV) represents ~ 39% of the total flux. The rest of the flux is divided into epithermal (1–10 keV) and fast (10 keV ˂) components with ~22% and ~39% respectively. For MCNPX, these rates are of the order of 42% for the thermal component, 20% for the epithermal component and 38% for the fast component. The maximum difference between the proportions obtained with the two codes is about 5 percentages for the FC1 pair, and about 4 percentages for the monitor. In general, it is remarkable that the spectra obtained with GEANT4 tend more towards epithermal range compared to those obtained with MCNPX.

Fundamental factors that can naturally cause the remarked differences between the two results are in particular: 1) The specific characteristics of each code such as the particle tracking way and the limits associated with this tracking-up: minimum energy, maximum step, etc. 2) The tolerated approximations in each simulation, especially in geometry, materials and proton beam profile definition. 3) The used physical models. Indeed, The MCNPX code uses by default the coupling “BERTINI [55] - DRESNER [56]” to manage the spallation reaction, while we have used in this simulation the coupling “INCLXX-ABLA”. It is important to be noted here that not using the thermal neutron scattering model (§ 2.4) in GEANT4 simulation leads to flux spectra without thermal and part of the epithermal component.

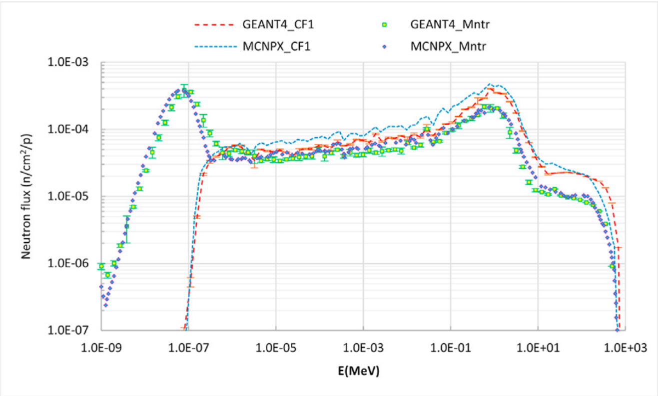

Fig. 2. Neutron flux spectra on the FC1 and monitor stages, calculated with GEANT4 and MCNPX.

As mentioned above, we have not processed in this work in actual simulation of the micro-detectors. This has motivated the testing of the effect of the geometry and the material composition of the micro-detectors. In fact, we have made many arbitrary changes to reveal whether these parameters affect or not the neutron flux spectra. This operation has shown that the geometry and material composition of the micro fission chambers are also factors that influence the neutron flux distribution.

In conclusion, although the number of factors influencing the determination of flux spectra is important, the obtained results present a remarkable agreement that can be considered satisfactory.

3.2. Estimation of total neutron fluxes along the target's axis

In addition to previous spectra, we have also evaluated total neutron fluxes in the micro-detectors placed on the target's axis (Fig. 1 b). But this time, the calculations have covered all the five stages of these detectors. The convergence time issue encountered when calculating the flux spectra is not strongly raised here because neutrons are not divided into many energy groups. The GEANT4 results are shown together with the experimental results and those of the MCNPX reference code in Fig. 3. The experimental and MCNPX data are extracted from the reference [57]. The first observation that can be made from this figure is that the simulations, whether with GEANT4 or with MCNPX, overestimates neutron fluxes compared to experimental measurements. This issue has in fact already been raised in the validation studies of the MCNPX results [57]. In this later reference, the authors have noticed that the results of the MCNPX simulation are sharply higher than the experimental measurements. To reveal the source of this large difference, several factors were examined. Thus, the study revealed that the angular dispersion of the proton beam is the main cause of this flagrant disagreement between the simulation and the experiment. [3,57]. Indeed, when irradiating the target and taking measurements, the proton beam has been focused below the

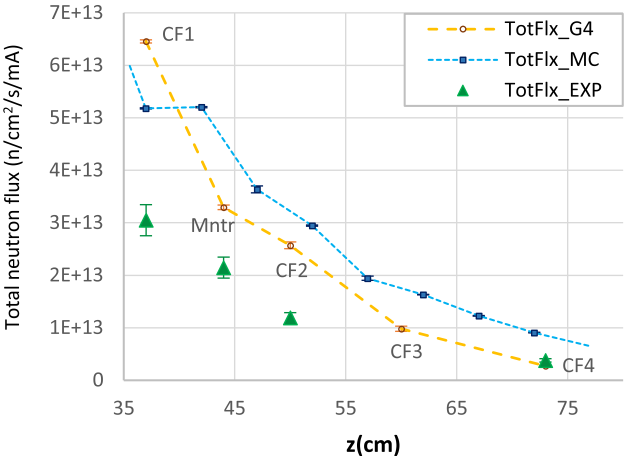

Fig. 3. Total neutron fluxes at different positions along de target's axis, calculated with GEANT4 and MCNPX, and measured.

window to prevent excessive damage to it. In contrast, in the simulations, the proton beam is considered as one-dimensional and parallel to the target's axis as it has actually been designed for this target. We note that the MEGAPIE target is designed to be powered by a mono-energetic proton beam (575 MeV and 1.74 mA) having a planar spatial distribution with a quasi-double Gaussian profile, and travelling parallel to the target's axis [3]. To ensure that there is a real impact on the neutron flux due to the angular distribution of the proton beam, we have performed several flux calculations using proton beams with different angular distributions. The results are shown in Fig. 4. This figure shows that this parameter had a real impact on the calculated fluxes.

Fig. 3 also shows that there is a remarkable difference between the fluxes calculated with GEANT4 and those calculated with MCNPX. Obviously, this difference is not due to angular distribution of the proton beam because both simulations (GEANT4 and MCNPX) use a parallel beam. However, the study published in the paper [4] have showed that this kind of difference is mainly due to the shielding geometry of the target. The shielding structures are part of the SINQ facility where the MEGAPIE target is placed. This interpretation seems very appropriate with our model, which accurately describes only the geometry of the target. The external structures constituting the SINQ facility are roughly defined due to a lack of data of the SINQ's geometry.

The fact that the geometrical model plays an important role in the calculation of neutron fluxes does not mean that it is the only factor of influence. On the contrary, many other factors as mentioned above can actually influence the calculated fluxes. But the impact of these factors might not necessarily be in favor of the MCNPX code. It is very likely to be in favor of GEANT4 for novelty reasons: While the results of GEANT4 are very recent, those of MCNPX are dated more than 15 years before. Indeed, the GEANT4 release used here benefits from all the recent improvements, both in the code itself, in the physical models and nuclear data. In general, the two results of GEANT4 and MCNPX remain comparable despite the important differences between the two simulations as especially in physical models, geometry, etc.

3.3. Neutron yield evaluation in the spallation zone

The spallation area is the most active area in the MEGAPIE target. The proton beam dissipates the largest part of its energy (~71%) in this area. Thus, rare are the incident protons that can escape from this zone. i.e., most of the interactions induced by primary protons, whether electromagnetic or hadronic, occur in the spallation zone. Electromagnetic interactions are particularly relevant in the assessment of the power deposition, while hadronic ones determine the neutronic performance of the target. The reactions that contribute the most to neutron production in the MEGAPIE target are, first, the spallation reaction that occurs mainly in the liquid metal lead bismuth (PbBi), and second, the multiplication reactions (n, xn) that is the main production source in the target structures.

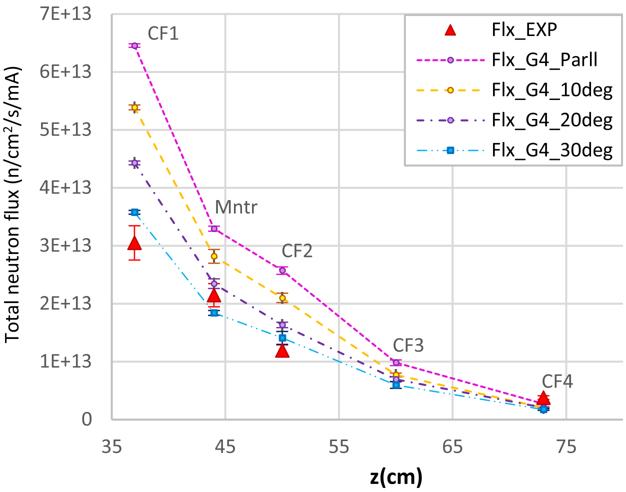

Fig. 4. Influence of the angular aperture of the proton beam on the calculated fluxes with respect to the measured ones.

Fig. 5 illustrates the neutron production of the target, as function of the z-altitude at various radius and Table 1 summaries principal values of this production in (n/p). These results show that the number of neutrons produced by an incident proton does not exceed 14 n/p as an average limit. It is reached at about $z = 48$ cm and $r = 15$ cm. The containment structures of the liquid metal, especially the lower target container (LTC) and the lower target enclosure (LTE) (Fig. 1), are therefore included. The production of neutrons in the area covered by the liquid metal ($r = 8.8$ cm) reaches its limit value 13.5 n/p at the altitude $z = 40$ cm. The remaining 0.5 n/p from the total number 14 n/p is therefore produced in containment structures, mainly (LTC) and the lower target enclosure (LTE), via mainly (n, xn) reactions. It is also remarkable that from $z = 30$ cm, the liquid metal produces almost no neutrons, as shown by the curve corresponding to $r = 6$ cm. As a result, we can estimate the total number of neutrons produced by all the liquid metal ($r = 8.8$ cm) at around ~ 13 n/p. Thus, the remaining 0.5 n/p is mainly due to reactions (n, nx) occurred in structures inside the liquid metal. Another finding is that more than 89% of the liquid metal's neutronic productivity (~11.6 n/p) comes from its part inside the guide tube ($r = 6$ cm), and less than 11% comes from the remaining part (~3 cm). A more subtle analysis of the obtained results (Fig. 5 and Table 1) show that the evolution of neutron production is significant only within the interval $0 \le z \le 25$ cm. This alludes to the fact that the spallation zone is actually shorter than what is commonly considered (30 cm). It should be noted here that the same conclusion is obtained differently in our study concerning the impact of the production threshold of secondaries on the power deposition in the MGAPIE target [12]. All results presented in this section have been obtained with a statistical error of less than 1%.

Finally, this analysis has allowed us to conclude that: 1) With the same irradiation conditions as these described when designing the target, the neutronic productivity cannot be improved by a simple increase in the thickness of the target. Nevertheless, this can be achieved by in spatial and/or energetic changing in the proton beam, or by changing in material composition of the target [58]. 2) More information is needed to accurately delimit the spallation region.

4. Conclusion

In this work we have overcome the complexity of the GEANT4 Monte Carlo toolkit and dealt, for the first time, the neutronic characterization of the MEGAPIE target with this code. The validate results are reproduced and the impact of several parameters on the neutron fluxes near the spallation zone is confirmed. The resulting curves have generally a clear trend towards the reference curves despite the remarkable differences between GEANT4 and MCNPX simulations. These differences are, in particular, due to the type of codes, and to the physical and geometrical models. The impact of the geometrical model is actually quite clear from Figs. 2 and 3. However, the impact of physical models requires even more results to be properly evaluated. We have also shown the important influence of the angular distribution of the proton beam on neutron

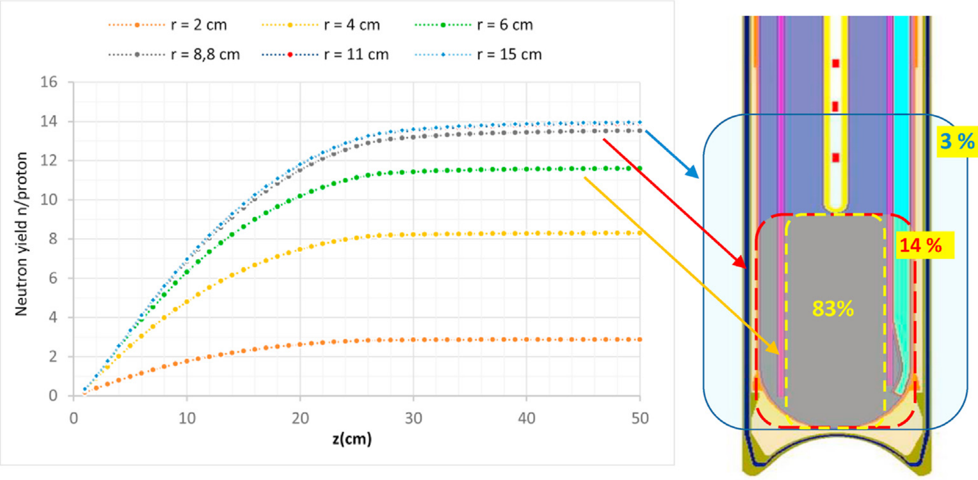

Fig. 5. Neutron yield per incident proton as a function of altitude z for different radial distance.

Table 1
Mean neutronic productivity according to the altitude (z) and radius (r) of the target.

r(cm) *z(cm)*	2	4	6	8.8[a]	11	15
5	1.0	2.5	3.2	3.3	3.3	3.3
10	1.8	4.8	6.3	6.9	7.0	7.0
15	2.3	6.4	8.6	9.6	9.8	9.8
20	2.6	7.5	10.2	11.5	11.8	11.8
25	2.8	8.1	11.1	12.8	13.0	13.1
30	2.9	8.3	11.5	13.3	13.7	13.8
40	2.9	8.3	11.6	13.5	13.8	13.9
50	2.9	8.3	11.6	13.5	13.9	14.0

[a] Actual radius of the liquid metal PbBi.

fluxes, as shown in Fig. 4. In general, the larger the dispersion angle, the smaller the neutron flux.

In addition to neutron fluxes, we assessed the evolution of the neutron yield in the spallation zone as a function of altitude and radius. The results of this part have shown that 94% of (neutrons/primary proton) are particularly generated in the liquid metal PbBi, and more than 87% of this rate is produced in the region bounded by the main guide tube. The interpretation of all the results allowed us to conclude that, first, the neutron productivity of the MEGAPIE target cannot be improved by just increasing the target radius, and second, the spallation region seems to be smaller than currently considered. A more rigorous redefinition of this region is therefore required.

Finally, a more detailed characterization of the MEGAPIE target in terms of neutron productivity is still necessary in order to envisage a real optimization for this target.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.net.2021.05.002.

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