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Assessment of the power deposition on the MEGAPIE spallation target using the GEANT4 toolkit

Abdesslam Lamrabet[1,2] · **Abdelmajid Maghnouj**[1] · **Jaouad Tajmouati**[1] · **Mohamed Bencheikh**[1]

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Abstract This work aims at evaluating the reliability of the GEANT4 (GEometry ANd Tracking 4) Monte Carlo (MC) toolkit in calculating the power deposition on the Megawatt Pilot Experiment (MEGAPIE), the first liquid–metal spallation target worldwide. A new choice of codes to study and optimize this target is provided. The evaluation of the GEANT4 toolkit is carried out in comparison with the MCNPX and FLUKA MC codes. The MEGAPIE is an international project led by the Paul Scherrer Institute in Switzerland. It aims to demonstrate the safe operation of an intense neutron source to power the next generation of nuclear reactors, accelerator-driven systems (ADSs). In this study, we used the GEANT4 MC toolkit to calculate the power deposited by fast protons on the MEGAPIE target. The calculation focuses on several structures and regions. The predictions of our calculations were compared and discussed with that of the MCNPX and FLUKA codes, adopted by the MEGAPIE project. The comparison shows that there is a very good agreement between our results and those of the reference codes.

Keywords GEANT4 · Simulation · MEGAPIE target · Spallation · Power deposition

1 Introduction

The Megawatt Pilot Experiment (MEGAPIE) is an international project led by the Paul Scherrer Institute (PSI) in Switzerland and supported by many international research institutions, such as the Commissariat à l'énergie atomique in France (CEA), Forschungszentrum Karlsruhe in Germany (FZK), Centre national de la recherche scientifique in France (CNRS), Agenzia Nazionale per le Nuove tecnologie in Italy (ENEA), StudieCentrum voor Kernenergie in Belgium (SCK-CEN), Department of Energy in the USA (DOE), Japan Atomic Energy Research Institute (JAERI), and Korea Atomic Energy Research Institute (KAERI), and the European commission [1]. The MEGAPIE initiative was launched in 1999 to design, build, and operate a high-power 1-MW liquid lead–bismuth (PbBi) spallation target [2]. This target is powered by a high-energy proton beam (575 MeV) emitted by an accelerator that consists of three units: the preaccelerator (Cockroft–Walton; 860 keV), cyclotron injector (272 MeV), and main ring cyclotron [3]. The power deposited by protons on the target is one of the crucial parameters for the design of this target. In fact, this parameter affects the choice of materials, dimensions, and heat removal. Moreover, the production of neutrons in the target is also related to the rate of power deposition, particularly in the spallation region. This work explores the power deposition in various areas and structures of the MEGAPIE target (Fig. 1) using the GEANT4 [4–6] MC code. The calculation focuses on structures such as the liquid PbBi metal, main flow guide tube, lower target container, two walls of the lower target enclosure, helium gas of the insulation gap, safety hull D_2O, and moderator D_2O. In addition to these structures, two very critical zones

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✉ Abdesslam Lamrabet
abdesslam.lamrabet@usmba.ac.ma

[1] Faculty of Sciences Dhar El Mahraz, Laboratory of Integration of Systems and Advanced Technologies, University Sidi Mohamed Ben Abdellah, 30000 Fes, Morocco

[2] El Hajeb, Morocco

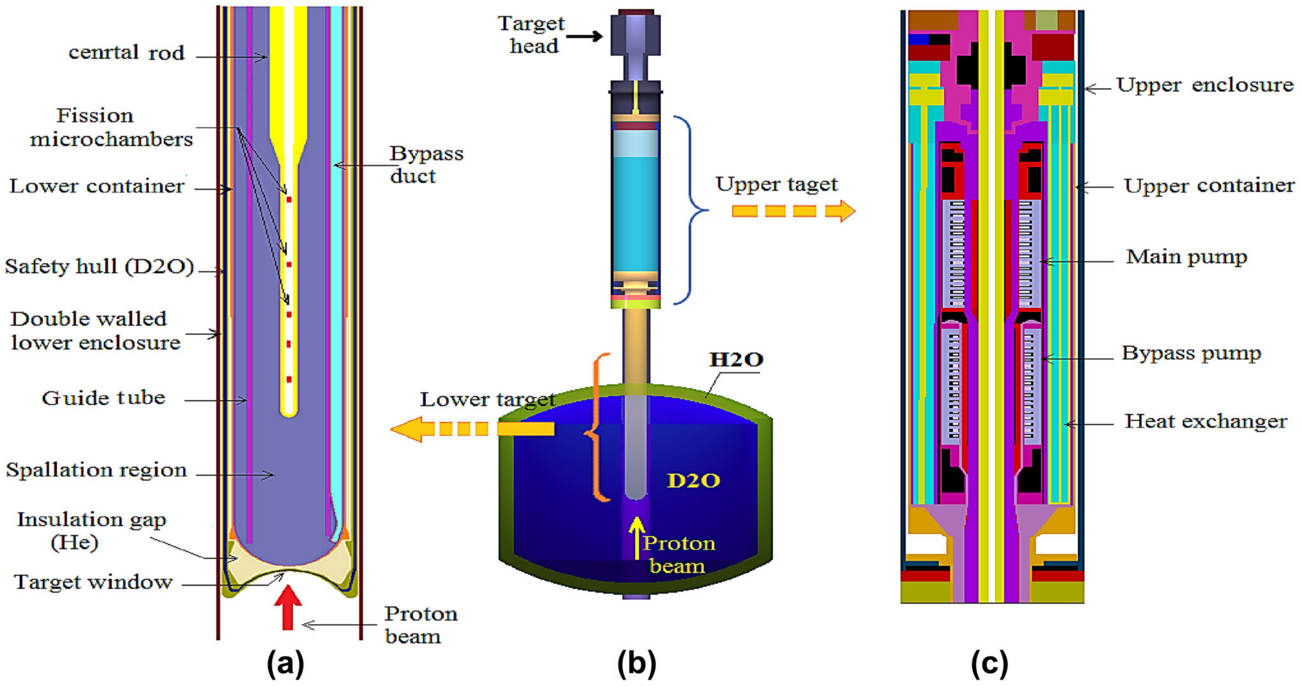

Fig. 1 (Color online) Geometry of the MEGAPIE target implemented by GEANT4. **a** Vertical cut of the lower part of the target. **b** Overview of the geometry of the target. **c** Vertical cut of the upper part of the target

are analyzed, that is the target window and axial area of the spallation zone.

Although GEANT4 has many advantages, it is very difficult to handle. Advanced knowledge of C++ language is necessary for optimal utilization of GEANT4. In addition to the complexity of the code, the geometry and distribution of the primary particles are also complex. In fact, the primary particles constitute a proton beam, which has a nonregular, two-dimensional distribution. In general, the simulation of the MEGAPIE target by the GEANT4 code itself represents a challenge.

We used the two MC codes such as MCNPX [7] and FLUKA [8, 9] as references to evaluate the predictions of our calculations. This choice is based on the conclusions of a benchmark exercise led by the X9 research group of the MEGAPIE project [10]. Based on these conclusions, MCNPX and FLUKA were adopted as reference codes for the project. In addition, most neutronic studies regarding the MEGAPIE target have been carried out with these two codes.

2 Materials and methods

2.1 GEANT4 toolkit

The GEANT4 toolkit is a C++ library designed to simulate the passage of particles using the MC method. It is a universal code that is widely used worldwide. It covers several physical areas: nuclear physics, particle physics, astrophysics, and medical physics. The GEANT4 is not a simple code, where the user only manipulates predefined components, but a very flexible toolkit full of features. It provides the users the possibility to fully customize their application. It is always allowed to modify available implementations and/or add others according to the problem and equipment needs. On the other hand, the GEANT4 toolkit is used as a basis for several specific codes such as the Gate code [11, 12] and MCADS model [13–16]. The Gate code is specifically used for medical applications, whereas the MCADS model, which was developed by the Frankfurt Institute for Advanced Studies in Germany (FIAS), is intended to simulate the spallation targets.

In the present simulation, we used GEANT4 version 10.2 [17]. Several improvements were made in this version, in particular, with respect to the compatibility with parallel calculations. The GEANT4 code considers two types of parallelism: clustering [18] and multithreading [19]. Clustering refers to the parallelism with separate memory that requires multiprocessor equipment, while multithreading represents parallelism with shared memory, which requires multicore processors. In this work, we adopted the multithreading technique, which is based on the optimization approach of memory management. Based on this technique, it was possible to reduce the computation time by a factor that is almost equal to the number of cores. Our simulation was performed using an application with many input files. The physics, geometry, materials, source (proton beam), and methods of results extraction in these files are all described using C++ language or command lines. These elements are mentioned in our previous work [20] and explained in more detail in the following sections.

To ensure the optimal functioning of the GEANT4 toolkit in this simulation, we built GEANT4 version 10.2 in an environment consisting of the scientific Linux version 7.4 [21], a Class Library for High Energy Physics (CLHEP) version 2.3.1.1 [22], data analysis framework ROOT version 6.12 [23], and Qt development frameworks version 5.6.2 [24].

2.2 Modeling physics

As a toolkit, GEANT4 does not provide physics models to use by default but provides a wide variety of several models. It is up to the user to choose which model is appropriate for the problem. The choice is made according to the energy field and type of the particle followed. The energy field of the MEGAPIE target is lower than 1 GeV. Therefore, we chose the predefined physics list FTFP_INCLXX_HP to treat the physics processes that may be produced in the MEGAPIE target, which is one of the reference physics lists provided by GEANT4. It was already validated as the most appropriate physics list for this type of problem [25]. This list includes the following models: FRITIOF model (FTF) [26, 27] coupled with the precompound one, Liège Intranuclear Cascade Model, C++ version (INCL++ or INCLXX) version 5.2.9.5 [28, 29], and high-precision model (HP). The FTF is used in GEANT4 to simulate the interactions between hadrons, nucleus, antibaryons, and antinucleus–nucleus. It is suitable for energies higher than 3 GeV. The precompound model is intended to manage the preequilibrium emission of protons, neutrons, and light ions [30]. The INCLXX model is used the most for spallation reactions. Its original version, INCL [31] was written in Fortran 77 and translated to C++ such that it can be implemented in GEANT4. The translation was started by Kaitaniemi et al. [32] and finalized by Mancusi et al. [29]. The Liège Intranuclear Cascade Model is designed to govern medium-energy reactions such as spallation reactions. It is permanently maintained and extended to cover more energies. The INCL++ version 5.2.9.5 implemented in GEANT4 10.2.03 has 20 GeV as an upper limit. As an intranuclear cascade model, INCL needs to be coupled with a de-excitation model to describe the two stages of the spallation reactions. Such reactions are assumed to start and finish with an avalanche of independent binary collisions and de-excitation phase, respectively. The nucleus remaining at the end of the first stage relaxes by emitting low-energy particles or by fissioning [33]. To control the processes corresponding to this stage, we coupled INCL++ with the ABLA version 3 statistical de-excitation model [34–36]. This model is one of the best de-excitation models based on the International Atomic Energy Agency (IAEA) benchmark of spallation models [37, 38]. As mentioned above, the FTFP_INCLXX_HP physics list also includes the high-precision model HP, which is appropriate for neutron tracking below 20 MeV. Finally, note that it is necessary to add the thermal neutron scattering model [39, 40] to the previously mentioned models if one is interested in thermal neutrons.

The threshold energy of secondary production (or Cut) is one of the most important physics parameters. It has a great impact on the calculation of the power deposition, especially for narrow volumes. The smaller this energy is, the more accurate the power deposition is. However, this precision comes at a cost. The calculation time increases. Therefore, a judicious choice of this parameter is essential for an optimal calculation within a reasonable time.

2.3 Geometry and materials

The MEGAPIE target is a complex device with respect to the geometry and materials. It consists of two parts that include many components (Fig. 1). The lower part in which the spallation reaction occurs is constituted by a guide tube for the proton beam ($AlMg_3$), double-walled enclosure ($AlMg_3$), safety hull (D_2O) between the two walls, lower liquid–metal container (martensitic steel T91), guide tube for the main flow of the liquid metal, central rod with microdetectors, bypass duct, and filling and draining tubes. The last five elements are all made of austenitic stainless steel SS316L. The upper part of the target that is dedicated to heat removal mainly consists of two electromagnetic pumps (copper and ferromagnetic), upper enclosure, upper liquid–metal container, heat exchanger, two Diphyl-THT (DTHT) oil boxes, heavy water box, and expansion tank. All these parts are made of stainless steel SS316L. In addition to all the previously mentioned elements, there are shielding blocks (tungsten) and the target head with its equipment. Figures of the geometry obtained with GEANT4 were published in the previous work [19]. The dimensions of the above-mentioned elements and other details can be found elsewhere [41, 42].

2.4 Proton beam

In the MEGAPIE target, a monoenergetic proton beam with an energy of 575 MeV and intensity of 1.74 mA induces the spallation reaction. As already mentioned, the target is supplied with this beam by an accelerator with three units. Each unit raises the energy of the protons to a given value until it reaches 575 MeV. The spatial distribution of the proton beam (Fig. 2) is a parameter that strongly impacts the functioning of the target. It affects the production of neutrons, power deposition, and life of the materials (mechanical stress). Consequently, the safety of the device is affected by this parameter. On the other hand, the results of the calculations are very sensitive to any change in the distribution of the proton beam. Therefore, a precise description of the proton beam profile is essential to obtain correct results. The definition of the source (proton beam) in the present simulation was a difficult task. The difficulty is due to the complexity of the beam distribution and the lack of a function describing it correctly. To overcome this difficulty, we proceeded with a superposition of many sources, each with its own distribution and probability/intensity. The description was made in a macrofile, and the implementation was accomplished using a dedicated class, that is, G4GeneralParticleSource. Note that previous trials were made to determine a function that can describe the proton beam profile. Equation (1) [10] represents one of the functions adopted by the scientific community in charge of the MEGAPIE project. However, based on γ mapping and the results obtained from the MCNPX simulation, Eq. (1) does not accurately describe the proton beam profile [43].

$$I_{x,y}\left[\frac{\mu\mathrm{A}}{\mathrm{cm}^2}\right] = \frac{I_0}{2\pi\sigma_x\sigma_y\left(1-\mathrm{e}^{\frac{-c^2}{2}}\right)}\mathrm{e}^{\frac{-1}{2}\left[\left(\frac{x}{\sigma_x}\right)^2+\left(\frac{y}{\sigma_y}\right)^2\right]^2} \qquad (1)$$

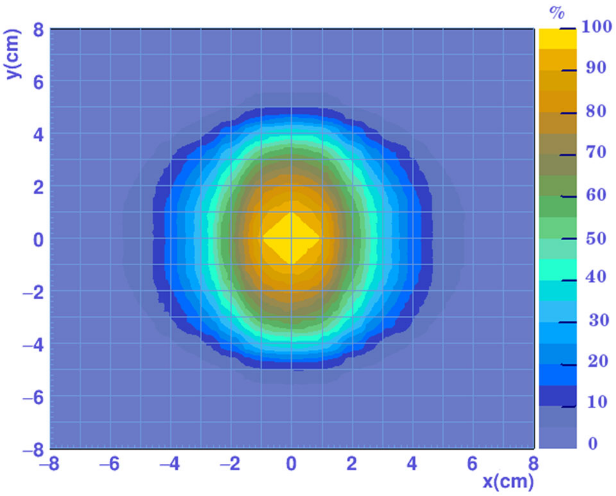

Fig. 2 (Color online) Two-dimensional distribution of the proton beam implemented by GEANT4

3 Results and discussion

3.1 Power deposited on the target

The MEGAPIE target is designed in a way that the maximum power of protons (1 MW) can be dissipated in its lower part, particularly in the spallation region (Fig. 1). The simulation shows that approximately 85.1% of this power is dissipated in this part of the target. Approximately 71% of the power is deposited in the liquid PbBi metal (actual target), whereas 14% of the power is divided between the confining structures (SS316L, T91, and $AlMg_3$), coolant (D_2O), and moderator (D_2O).

The power deposited in each component depends on the position, dimensions, and constituent material. Table 1 shows the power dissipated in the various elements of the MEGAPIE target. The power values were previously calculated with the FLUKA and MCNPX codes [44]; the GEANT4 toolkit was used in this work. Table 1 indicates that the GEANT4 results are all framed by those of MCNPX and FLUKA, except for the power deposited on the insulation gap "gas_Gap." This difference is quite normal because it is due to the type of gas used in this area of the target. The MCNPX and FLUKA calculations were based on argon (Ar). Conversely, helium (He) was used as a gas for the GEANT4 calculation [40]. The fact that all our results are in good agreement with that of the references indicates that the GEANT4 code provides accurate results. This conclusion can mainly be justified by the fact that the version of GEANT4 used is very recent compared with those of FLUKA and MCNPX. Therefore, the GEANT4 code has the potential to provide good results. However, the results need to be compared with experimental data to support this conclusion.

3.2 Power deposited in the target window

The window represents the most critical zone of the MEGAPIE target. It constitutes the interface between the proton beam and target. Thus, it is the most irradiated part of the target. Consequently, the window is the part that is most vulnerable to temperature increase and structural stress. Moreover, it is subjected to mechanical constraints due to the weight of the liquid PbBi metal and the difference in the pressure between the PbBi and helium gas sides. Therefore, the life of the target and its operation safety are directly related to the quantity of the power deposited in its window. Figure 3 shows the distribution of the power deposited in this part calculated by GEANT4 and FLUKA as a function of x at $y = 0$. Gaussian curves were obtained, with a maximum at the center ($x = 0$, $y = 0$). The agreement between the results of GEANT4 and

Table 1 Power deposition on structure materials calculated by GEANT4, FLUKA, and MCNPX

Material	Power deposition (kW)			Relative difference (%)		
	GEANT4	FLUKA	MCNPX	GEANT4/FLUKA	GEANT4/MCNPX	MCNPX/FLUKA
PbBi	709.7	710.8	708.2	0.15	0.21	0.37
T91	8.72	8.60	8.94	1.40	2.46	3.95
$AlMg_3$_in	4.56	4.48	4.60	1.79	0.87	2.68
$AlMg_3$_ext	4.19	4.15	4.21	0.96	0.48	1.45
Gas_Gap	0.00076	0.012	0.016	–	–	33.33
D_2O	3.92	3.83	3.96	2.35	1.01	3.39
Moderator	114.9	114.4	115.4	0.44	0.43	0.87
Guid_Tub	5.33	5.55	5.23	3.96	1.91	5.77
Total	851.4	851.8	850.6	0.05	0.09	0.14

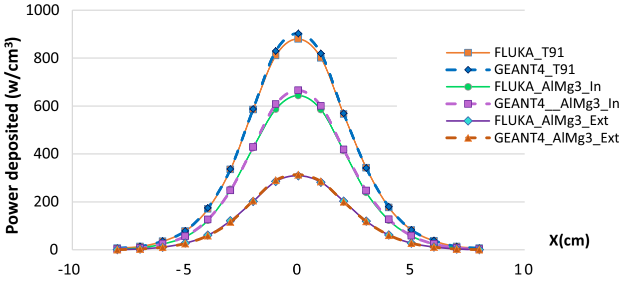

Fig. 3 (Color online) Power deposited in structures of the window of the MEGAPIE target calculated by FLUKA and GEANT4

that of the reference code FLUKA [44] is very clear based on these curves. Note that the difference does not exceed 4% (maximum) and on average is 0.3% (Fig. 4). Table 2 shows a comparison between the maximal power values deposited in the structures of the target window. These data were calculated with GEANT4, FLUKA, and MCNPX. Once again, the values computed by GEANT4 are framed by the reference values. This confirms the ability of GEANT4 to provide results with satisfactory precision.

Table 2 Maximal power deposited in the window structures

Material	Maximal deposited power (w/cm^3)		
	GEANT4	FLUKA	MCNPX
T91	902.7	879.5	924.8
$AlMg_3$_in	332.6	321.9	330.4
$AlMg_3$_ext	313.6	309.4	321.1

3.3 Power deposited along the *z*-axis of the target

The assessment of the power along the *z*-axis of the target is both of neutronic and thermohydraulic interest. It allows the location of the Bragg peak and therefore the identification of the spallation region, which will be useful for the dimensioning of any reactor powered by a similar target. The determination of the power deposited in the axial zone of the target also allows to consider which heat removal system should be used. Figure 5 represents the map of the volume density of the power deposited in the

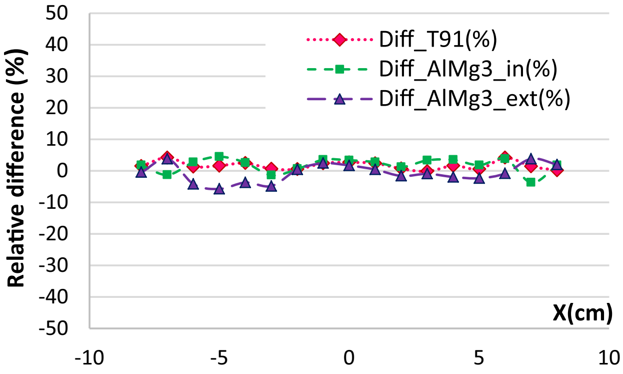

Fig. 4 (Color online) Local relative difference between the results of GEANT4 and FLUKA

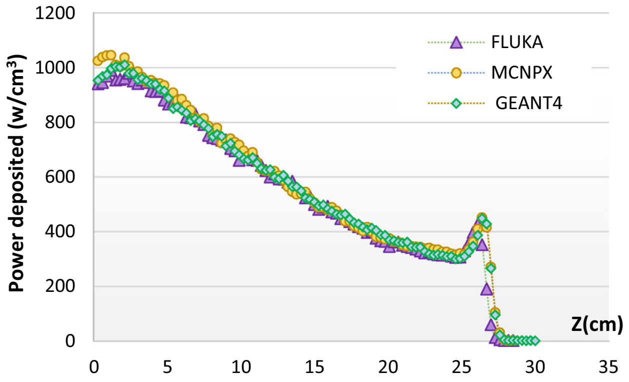

Fig. 5 (Color online) Power deposition map along the z-axis of the target, calculated with GEANT4, FLUKA, and MCNPX

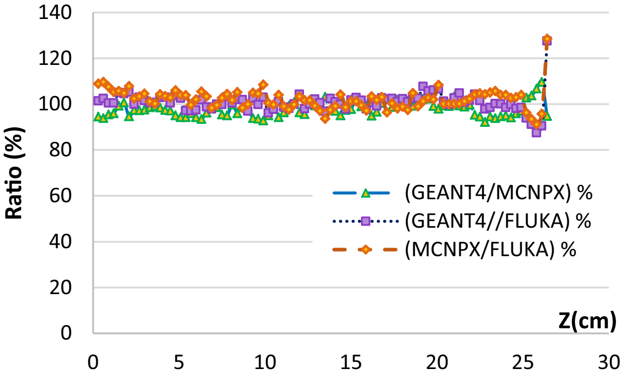

Fig. 6 (Color online) Local ratio between the power values calculated with GEANT4, FLUKA, and MCNPX

central region of the target. The radius of this region is $r < 0.3$ cm; the calculations were made using GEANT4, FLUKA [44], and MCNPX [44]. The power deposition reaches its maximum of ~ 1 kW/cm^3, approximately 2 cm from the window. It then decreases with the altitude z up to 26 cm, where a peak can be observed, that is the Bragg peak. Above 26 cm, the deposited power significantly decreases until it is practically null at approximately 27.5 cm. The curves show that the results are in very good agreement. The curves in Fig. 6 representing the local ratios between GEANT4/FLUKA, GEANT4/MCNPX, and MCNPX/FLUKA confirm this agreement. The only observed disparity is related to the position of the Bragg peak. A lag of $\sim$ 0.3 cm was observed between the FLUKA and GEANT4 and MCNPX results. This difference is mainly due to the physical choices adopted by each code.

4 Conclusion

In this paper, we evaluated the power deposition on the MEGAPIE spallation target using a MC method based on the GEANT4 toolkit. We faced many challenges during the accomplishment of this work: (1) the definition of a very complicated geometry; (2) the definition of a two-dimensional and nonregular proton beam; (3) the choice of the suitable physics for the problem; and (4) the development of a program providing correct results. The implemented geometry and proton beam are very similar to that of the references, as indicated in Figs. 1 and 2. The physics are governed by the combination of physics models used in this work: FTFP_INCLXX_HP coupled with the ABLA model. The results are in very good agreement with those of the reference codes FLUKA and MCNPX. Furthermore, the difference between our results and that of FLUKA and MCNPX is smaller than that between the FLUKA and MCNPX data. It is remarkable that the GEANT4 predictions are closer to that of the MCNPX code than to that of FLUKA. In general, the differences are mostly due to geometry and proton beam approximations, especially due to physics models and methods of sampling adopted by each code. However, our results are framed by the results of the references, which indicate that the GEANT4 simulation might be optimal. Finally, the GEANT4 toolkit reproduced the geometry and power deposition of MEGAPIE experiment well. Therefore, GEANT4 can be considered to be one of the most reliable and competitive codes for the simulation of great physics experiments.

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