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Evaluation of Neutron Field Parameters at the VITA Facility using Geant4 Simulation

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Abstract—Parameters of the neutron field generated at the VITA (Vacuum Insulated Tandem Accelerator) installation are assessed using Monte Carlo simulation in the Geant4 software package. A detailed model of the target section of the installation is developed, including the output accelerator tube, frontal lithium target for neutron generation, backplate cooling system, and neutron moderator system. The simulation makes it possible to obtain the energy and spatial distributions of the neutron flux intensities in the configuration intended for irradiation of small biological objects at a proton energy of 2.05 MeV. It is shown that the obtained calculated values of the neutron flux intensities correspond to the target values, providing acceptable time intervals for irradiating biological objects. Moreover, the transverse profiles of the simulated neutron field are consistent with the experimental data and preliminary theoretical expectations. The developed model can be used for dose planning in experiments on irradiation of small biological objects *in vitro* and *in vivo* and for further optimization of the neutron beam formation system to increase a therapeutic index in neutron capture therapy.

Keywords: neutron capture therapy, accelerator neutron source, lithium target, Monte Carlo simulation, neutron field formation system

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1. INTRODUCTION

Boron neutron capture therapy (BNCT) is a promising method for treating malignant tumors. This therapy is a form of binary radiotherapy based on the high cross section of thermal neutron capture (3800 b) by nonradioactive nuclei of the boron-10 isotope [1]. The absorption of a neutron by a boron-10 nucleus leads to an instantaneous nuclear ^{10}B(n,α)^{7}Li reaction with a release of energy at 2.79 MeV. About 85% of the energy of the nuclear ^{10}B(n,α)^{7}Li reaction is released in the internal volume of one cell; therefore, with selective accumulation of boron-10 in tumor cells and subsequent neutron irradiation, it is possible to destroy tumor cells with relatively little damage to surrounding healthy tissues. The combination of high ionization density, short range, and high relative biological effectiveness (RBE) of nuclear reaction products makes it possible to effectively combat radioresistant tumors, such as glioblastoma [2–4]. The effectiveness of BNCT directly depends on the intensity of the neutron flux reaching the tumor and the neutron energy distribution.

This method of treating malignant neoplasms is being actively studied and developed at the Budker Institute of Nuclear Physics SB RAS (Novosibirsk), where the VITA accelerator neutron source was fabricated. It consists of a tandem electrostatic charged particle accelerator of original design to generate a stationary beam of protons or deuterons, a lithium target for generating neutrons in the ^{7}Li(p,n)^{7}Be reaction, and a number of systems for producing a therapeutic neutron flux with different geometric parameters and materials of neutron moderators and reflectors [5]. The installation provides an intense stationary monochromatic beam of protons or deuterons with an energy form 0.3 to 2.3 MeV and a current from 0.5 to 10 mA; it allows a high-power neutron flux (up to 2×10^{12} s^{-1}) of various energy ranges to be generated. The VITA units are already used in clinical practice at the BNCT center in Xiamen (China) and will soon be delivered to clinics in the Russian Federation and Italy [1].

The approach to determining the parameters of irradiation in BNCT, based on experimental studies, is a labor-intensive and expensive process. However, the development of modern computational methods and software has made it possible to move to *in silico* simulation of physical processes occurring during irradiation. Numerical simulation allows one to analyze the spatial and energy distribution of neutrons in the irradiated volume, to estimate radiation doses for both the tumor and healthy tissues, to study the effect of various irradiation parameters (proton energy, target thickness, irradiation geometry, etc.) on the efficacy of therapy, and to optimize irradiation parameters to achieve a maximum efficiency with minimal side effects on healthy tissues. Thus, simulation of physical processes is an indispensable method for optimizing BNCT, making it possible to predict the characteristics of irradiation, avoid unnecessary experiments, and accelerate the development of efficacious treatment methods. Today, one of the most common tools for Monte Carlo simulation of various physical processes of radiation interaction with matter is the object-oriented software environment Geant4 [6] developed at the European Center for Nuclear Research. The application areas of Geant4 include high-energy physics, space research, and medicine.

This paper presents a software model of one of the variants of the neutron field generation system for the Geant4 environment [6], the neutron field generation process is simulated, and the spatial and energy distribution of neutrons is estimated. The obtained agreement between the simulation results and experimental measurements has proven the applicability of this approach for further work on optimizing the irradiation parameters.

2. NEUTRON-GENERATING SYSTEM AND ITS COMPUTER MODEL

In accelerator sources for BNCT, lithium targets are widely used to generate neutrons, since the threshold ^{7}Li(p,n)^{7}Be reaction has a significant cross section and a relatively low energy of output neutrons, which can be effectively slowed down to thermal and epithermal energies (1 eV–10 keV), most suitable for BNCT [1, 7].

The VITA accelerator neutron source uses a stationary neutron-generating system that provides generation of a high-quality therapeutic beam [5]. The design of the neutron-generating system is shown in Fig. 1.

The neutron-generating system includes an accelerator feed pipe, a target unit, and a moderator. The 235-mm long feed pipe made of aluminum alloy AMG6 has a minimum internal diameter of 100 mm and an external diameter of 160 mm. The target unit consists of a copper disk with a diameter of 143 mm and a thickness of 8 mm, onto which a thin (60 μm) layer of lithium is deposited. On the reverse side of the copper disk, four double-ended spiral channels for water cooling are made. An aluminum element of the cooling system, which has a square shape (with a side of 175 mm) with rounded corners and holes for the supply and discharge of cooling water, fits tightly to the reverse side of the copper disk. In order to slow down the generated neutrons in the configuration for irradiating biological objects, a moderator made of organic glass with a thickness of 72 mm and a diameter of 200 mm is installed behind the target unit. In this configuration, irradiation is carried out at a proton beam energy of 2.05 MeV, current values on the order of ~1 mA, and a proton field sweep of 80 mm.

A model of the above-described neutron-generating system was created in the Geant4 environment, taking into account all the key parameters and geometric characteristics of the target unit (Fig. 2). The model includes a copper disk with spiral channels inside; it also has an aluminum element of the cooling system consisting of the AMG6 alloy, including the cooling system pipes. All cavities in the cooling system are filled with water. Some simplifications in the model affected only the accelerator feed pipe located in front of the lithium layer and the control and measuring equipment installed on it. The model accurately took into account the composition of the AMG6 alloy, which is very important, since aluminum in the AMG6 alloy is alloyed, among other things, with manganese (content up to 0.5%–0.8%), which has a high cross section for the absorption of thermal neutrons. The difference in the thermal neutron flux in the presence of manganese in the alloy and in its absence reaches tens of percent.

The processes of interaction of the proton beam with the target and the moderator were simulated using one of the standard sets of physical models in Geant4 QGSP_BIC_AllHP, which is most suitable for the purposes of this study [8]. To describe the interaction of protons with matter at low energies, which is of interest to us, QGSP_BIC_AllHP uses a set of cross sections available in the TENDL library [9]. Of greatest interest in the context of this work is the interaction of protons with ^{7}Li near the threshold. In the TENDL library, the cross section of this interaction is included using a fairly extensive set of available experimental data, while the angular distribution of the reaction products is obtained from R-matrix analysis [10]. The interaction of neutrons with matter in Geant4 is described by the JEFF-3.3 [11] and

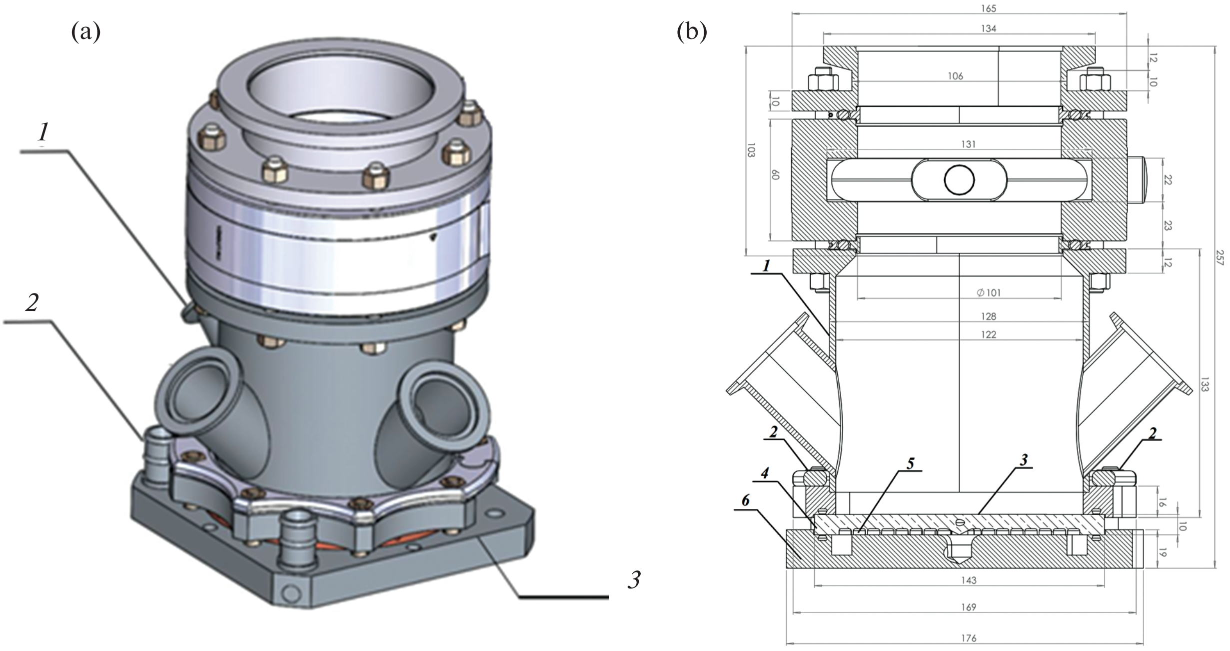

Fig. 1. (a) 3D model of the neutron-generating system of the VITA installation: (*1*) accelerator feed pipe, (*2*) cooling system nozzle, and (*3*) copper substrate (disk) with a thin lithium layer. (b) Side sectional drawing of the neutron-generating system of the VITA installation: (*1*) accelerator feed pipe, (*2*) cooling system nozzles, (*3*) thin lithium layer, (*4*) copper substrate, (*5*) spiral channels made in the copper substrate for water cooling, and (*6*) aluminum element of the cooling system.

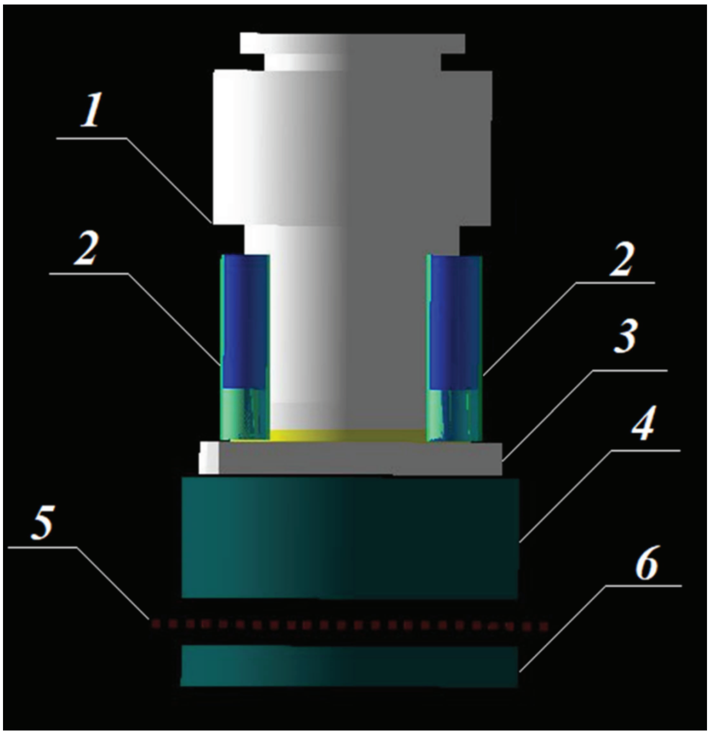

Fig. 2. Geometry of the VITA neutron-generating system model in the Geant4 environment: (*1*) accelerator feed pipe, (*2*) PVC pipes of the target unit cooling system filled with water, (*3*) target unit, (*4*) plexiglass moderator, (*5*) positions of detectors for measuring the energy release profile, and (*6*) plexiglass phantom.

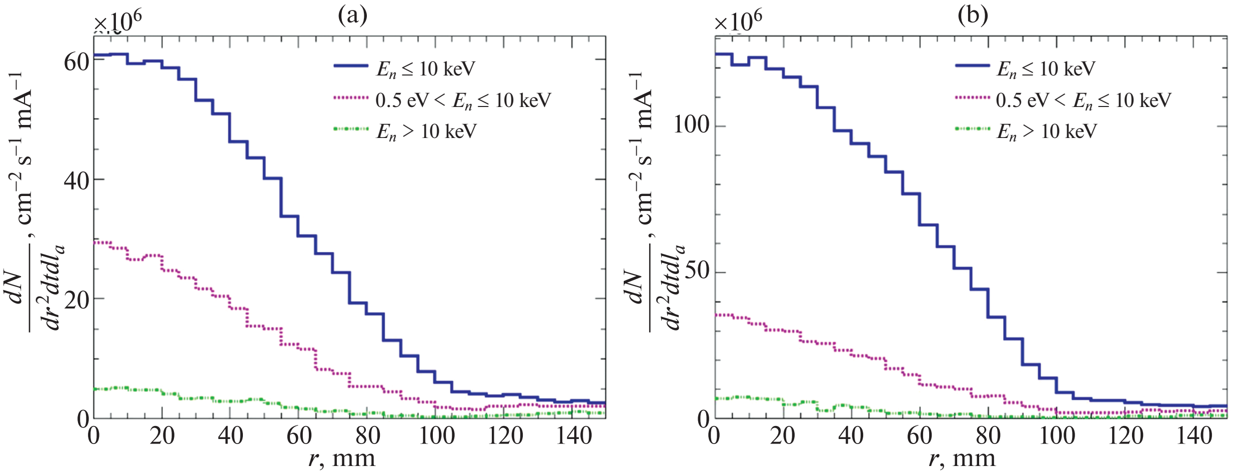

Fig. 3. Neutron flux intensity per 1 mA of proton beam current at a distance of 15 mm from the rear face of the moderator as a function of the distance to the proton beam axis for three neutron energy ranges (a) in the case when there are no objects behind the moderator and (b) in the case of placing the phantom at a distance of 25 mm from the rear face of the moderator.

ENDF/BVIII-0 (for those materials that are not contained in JEFF-3.3) libraries [12]. These libraries contain a large amount of experimental data on neutron interactions with matter.

3. RESULTS

In this paper, we simulated the formation of a neutron field at the VITA installation for irradiating small biological objects. The case of irradiating a lithium target with protons with a kinetic energy of 2.05 MeV and a scan rate of 80 mm was considered. Figure 3a shows the simulation results for a scenario where there are no objects in the path of the neutron field generated at the exit of the moderator. In the second scenario (Fig. 3b), a 200 mm diameter, 24 mm thick organic glass disk is placed at a distance of 25 mm from the rear face of the moderator, simulating a dense packing of small biological objects with a substrate for their placement in the case of BNCT, hereinafter referred to as a phantom. The resulting field is characterized by the dependence of the neutron flux intensity measured at a distance of 15 mm from the rear face of the moderator on the distance to the proton beam axis for three neutron energy ranges.

Based on the simulation results, we constructed neutron flux intensity distributions for three energy ranges (less than 0.5 eV, from 0.5 eV to 10 keV, and higher than 10 keV) in a plane located 15 mm from the rear face of the moderator as functions of the distance to the proton beam axis for the two above-described experimental geometry scenarios. In the first case, the flux intensity of thermal neutrons on the axis of the neutron-generating system reaches 0.6×10^8 cm^{-2} s^{-1} mA^{-1}; the flux intensity of epithermal neutrons, 3×10^7 cm^{-2} s^{-1} mA^{-1}; and the flux intensity of fast neutrons, 5 × 106 cm^{-2} s^{-1} mA^{-1}. These values correspond in order of magnitude to the target characteristics of the VITA installation [5], ensuring acceptable time intervals for irradiating biological objects. Namely, such values of the epithermal neutron flux intensity ensure the achievement of the required therapeutic dose for realistic irradiation times and typical therapeutic concentrations of the boron-10 isotope in the tumor. In the case of placing a disk made of organic glass, the thermal neutron flux intensity in the plane between the rear face of the moderator and the disk increases twofold. For epithermal and fast neutrons, an insignificant increase in the flux intensity is observed, up to ~20%. This phenomenon can be explained by the fact that the organic glass has elements that promote effective neutron scattering, which leads to an increase in the number of thermal and epithermal neutrons in the studied plane of space.

Then, to compare the obtained neutron flux characteristics with the experiment, we performed measurements using compact neutron counters developed at the Institute of Nuclear Physics SB RAS [13]. The sensitive element of the detector is a cylinder with a diameter of 1 mm and a length of 1 mm, made of a plastic scintillator. It is placed inside a reflective cylinder made of solid Teflon with a wall thickness of 1 mm. The scintillator is glued to the plastic optical fiber (POF) with epoxy resin, and all components are housed inside a black plastic housing. Two sensors, one with a boron-enriched scintillator and one with a boron-free scintillator, are combined into one detector head. The signal from the optical fiber is fed

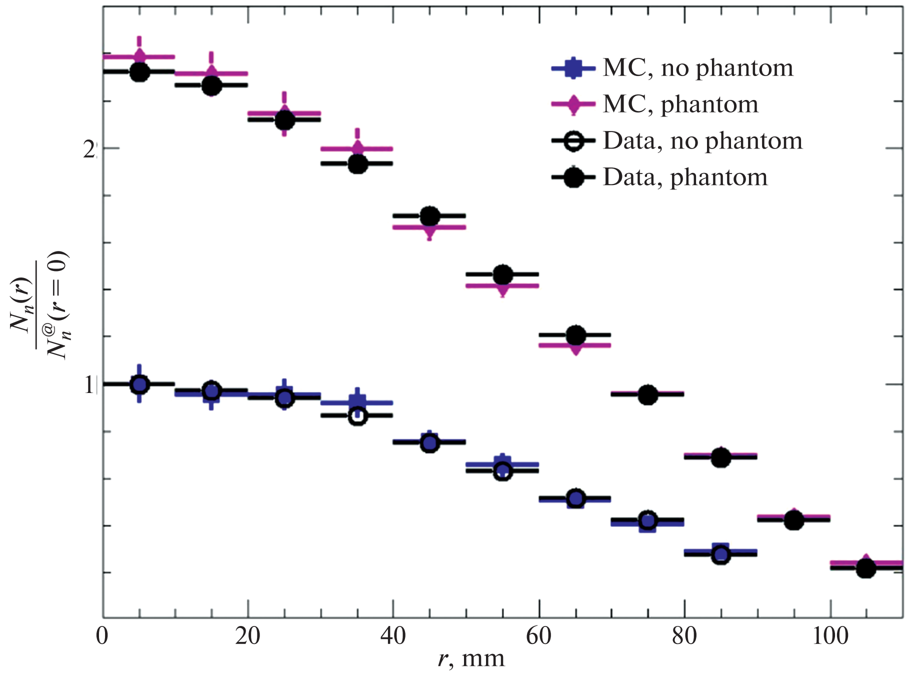

Fig. 4. Relative energy release profiles in boron-enriched scintillators measured experimentally in comparison with the results obtained by Monte Carlo methods. Normalization was performed to the measurement closest to the center of the proton beam axis in the absence of a phantom for the experimental and calculated data, respectively. The figure shows the statistical errors.

to a silicon photomultiplier with subsequent signal processing. Simultaneous use of two different recording channels—the first, sensitive to gamma radiation, and the second, sensitive to gamma radiation and neutrons—allows the contribution of the neutron component to be more accurately assessed. The detector was moved by an ER50B-2100 industrial robot (ESTUN Automation Co).

The calculated data on the radial profile of the thermal neutron flux intensity were compared with the experimental measurements obtained for the two above-described scenarios (Fig. 4). As can be seen from the plotted dependences, the simulation results are in good agreement with the experimental data. Note that in the case of the presence of a phantom, an increase in energy release in scintillation detectors reaches 2.3 times, while only a twofold increase was observed for the intensity of the thermal neutron flux. This is due to the additional softening of the neutron spectrum and increased sensitivity of the detectors in the soft region of the neutron energy spectrum.

4. CONCLUSIONS

We have shown that the obtained calculated values of the neutron flux intensities correspond to the target values, providing acceptable time intervals for irradiation of biological objects. In addition, we have found that the transverse profiles of the simulated neutron field are consistent with the experimental data. It is worth noting that the phantom placed behind the neutron field measurement plane significantly increases the intensity of the thermal neutron flux. Thus, the critical importance of the dependence of the thermal neutron flux intensity on the presence of objects in the irradiation zone has been demonstrated, which can play a key role in optimizing biological experiments. Evaluation of the effect of the material and geometry of the substrate for placing small *in vivo* objects on the dynamics and distribution of the neutron field will allow one to ensure more accurate irradiation planning and increase the efficiency of neutron use in BNCT. The developed model can be used for dose planning of biological experiments on irradiation *in vitro* and *in vivo* of small objects with a neutron flux at the VITA installation, and also can serve as a basis for further optimization of the neutron field formation system in order to improve the therapeutic index.

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CONFLICT OF INTEREST

The authors of this work declare that they have no conflicts of interest.

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