Development and verification of a Monte Carlo dose calculation program "MagicDose" for boron neutron capture therapy

Authors: Aikou Sun, Zhenping Chen, Tao Yu, Zhenping Chen

Date: 2026-03-24T22:44:33+00:00

Abstract

Dose calculation is the foundation of boron neutron capture therapy (BNCT). MagicDose, a dose calculation program for the BNCT treatment planning system, is developed based on the Monte Carlo method. First, the voxel phantom of the modified Snyder head with 16 and 8 mm is constructed, and the results from MagicDose and MCNP are presented as two-dimensional coordinate points (Xn , Yn), comparing their relationship relative to the y=x linear function, while analyzing their respective calculation time. A modified Snyder head phantom with a tumor at three different spatial resolutions of 16, 8, and 1 mm was constructed, and the depth-dose-rate curves and spatial distribution maps are analyzed. Finally, the patients' head CT data were used for the application. The results indicate that the calculations from MagicDose and MCNP exhibit high consistency anddemonstrate that MagicDose offers superior computational efficiency compared to MCNP, with improvements of approximately 31.24% and 28.65% at spatial resolutions of 16 and 8 mm, respectively. As the spatial resolution increased, the variability in the dose rate results decreased. The voxel size and number of threads are both inversely proportional to the calculation time. For the CT model, a voxel phantom with a spatial resolution of 1mm$\times 1mm \times$1 mm is successfully constructed. The calculation results showed that the boron dose rate contribution significantly exceeds that of the other dose components, with the spatial distribution of the total relative biological effect dose rate clearly delineating the boundaries between the high- and low-dose-rate regions. The above results verify the correctness of MagicDose, which also provides a reference for optimizing the design ofvoxel phantoms for clinical treatment.

Full Text

Preamble

Development and verification of a Monte Carlo dose calculation program "MagicDose" for boron neutron capture therapy Ai-Kou Sun, Zhen-Ping Chen, 1, 2, 3, Ke-Kun Gao, Lin Zhu, Cheng-Wei Liu, Zhi-Qiang Chao Yang, Tong Liu, Song Wang, Zi-Zhu Zhang, Yi-Zheng Chong, and Tao Yu 1, 2, 1 School of Nuclear Science and Technology, University of South China, Hengyang, Hunan 421001, China Key Lab of Advanced Nuclear Energy Design and Safety, Ministry of Education, Hengyang, Hunan 421000, China State Key Laboratory of Radiation Medicine and Protection, Soochow University, Suzhou, Jiangsu 215123, China Graduate School of Biomedical Engineering, Tohoku University, Sendai, Japan Beijing Nuclear Industry Hospital, Beijing 102413, China China National Nuclear Corporation Overseas Ltd, Beijing 100044, China Dose calculation is the foundation of boron neutron capture therapy (BNCT). MagicDose, a dose calculation program for the BNCT treatment planning system, is developed based on the Monte Carlo method. First, the voxel phantom of the modified Snyder head with 16 and 8 mm is constructed, and the results from MagicDose and MCNP are presented as two-dimensional coordinate points ( ), comparing their relationship relative to the linear function, while analyzing their respective calculation time. A modified Snyder head phantom with a tumor at three different spatial resolutions of 16, 8, and 1 mm was constructed, and the depth-dose-rate curves and spatial distribution maps are analyzed. Finally, the patients' head CT data were used for the ap- plication. The results indicate that the calculations from MagicDose and MCNP exhibit high consistency and demonstrate that MagicDose offers superior computational efficiency compared to MCNP, with improvements of approximately 31.24% and 28.65% at spatial resolutions of 16 and 8 mm, respectively. As the spatial resolu- tion increased, the variability in the dose rate results decreased. The voxel size and number of threads are both inversely proportional to the calculation time. For the CT model, a voxel phantom with a spatial resolution of 1 1 mm is successfully constructed. The calculation results showed that the boron dose rate contri- bution significantly exceeds that of the other dose components, with the spatial distribution of the total relative biological effect dose rate clearly delineating the boundaries between the high- and low-dose-rate regions. The above results verify the correctness of MagicDose, which also provides a reference for optimizing the design of voxel phantoms for clinical treatment.

Keywords

Boron neutron capture therapy (BNCT), Monte Carlo, Dose calculation, MCNP, Voxel phantom, Spatial resolution

INTRODUCTION

Cancer is a leading cause of death worldwide. According to cancer statistics from the National Cancer Center (NCC) of China, 4.82 million new cancer patients and 2.57 million deaths are expected in China in 2022 [1]. Cancer is a major problem affecting national health. Currently, cancer treat- ment modalities include surgery, chemotherapy, and radiation therapy.

Almost 50% to 70% of cancer patients in China receive radiation therapy during treatment, which has been playing an increasingly important role in cancer treatment.

Among these, boron neutron capture therapy (BNCT), a state- of-the-art tumor radiotherapy technology based on neutron radiotherapy, has been developed in various countries world- wide. The main principle is to inject boron-containing drugs

This work was supported by the National Natural Science Foundation of China (Nos. 12475174 and U2267207), the YueLuShan Center In- dustrial Innovation (No. 2024YCII0108), the Project of State Key Laboratory of Radiation Medicine and Protection, Soochow University (No. GZK12023031), the Science and Technology Innovation Project of Hengyang (No. 202250045336) and the Graduate Research Innovation Project of Hunan Province (No. QL20230228).

(boronophenylalanine, BPA, and sodium boronophenylala- nine, BSH) with tumor specificity into the patient’ s body. Af- ter a period of metabolism of the boron drug in the patient’ s body, the drug is enriched in the tumor area, and then the tumor is irradiated with a neutron beam generated by the neu- tron source. Owing to the very large thermal neutron absorp- tion cross-section of B, a large amount of B undergoes the Li reaction, which releases two high Linear Energy Transfer (LET) particles, Li. Through these two parti- cles, energy is deposited in the range of approximately 12-13 m, causing irreparable damage to cellular DNA in the area of the deposited energy and ultimately killing tumor cells [The BNCT reaction formula and a basic schematic are shown in Fig.

BNCT treatment is based on the calculation and analysis of the distribution of irradiation doses in the patient’ s body, which is used to determine the optimal treatment plan for the duration and angle of orientation of neutron beam exposure, while observing the dose limitations that jeopardize normal tissues and organs. The tissue dose in BNCT comprises the following four parts [(1) Boron dose. It is produced by the Li reaction, and because the absorption cross-section of boron for thermal neutrons is very large (3840 b), the reaction releases much energy; thus, the boron dose contributes significantly to the total dose and is the main component [

Li reaction formula; schematic. (2) Thermal neutron doses. Thermal neutrons react with N atom in the human body to generate recoil nuclei and protons, and this dose is generated by the deposition of energy in the cells of the human body. (3) Epithermal and fast neutron doses.

Dose result- ing from energy deposited by epithermal and fast neutrons 0.5 eV) through elastic scattering with various nuclides.

Over 90% of this dose arises from the elastic scattering contri- bution of neutrons with H, whereas the remaining portion is contributed by scattering from nuclides such as C and (4) Photon dose. There are three main production pathways: rays produced by the accompanying incident neutron beam, rays produced by the boron neutron capture reaction, rays produced by the thermal neutron capture reaction with H atoms in the human body.

The calculations of these four dose components are compli- cated, and no empirical formula for accurate dose calculations has been reported to date. At this stage, Monte Carlo (MC) simulations are mainly used in the BNCT Treatment Plan- ning System (TPS) to calculate the radiation dose distribution of patients [ ]. Moreover, the TPS of BNCT is significantly different from the photon or electron TPS of conventional ra- diotherapy. In conventional radiotherapy, only a single dose from a primary photon or electron must be calculated, and a simple numerical-model-based approach is applied to ac- celerate the calculation. For the calculation of the dose of BNCT, many factors are involved, such as the neutron source, boron content, distribution of the neutron energy in tissues, and the total dose composed of different doses with differ- ent biological effects, which makes its TPS more compli- cated than traditional methods and requires greater accuracy and technical support to ensure the effectiveness and safety of the treatment. Currently, the international TPS technol- ogy for BNCT is maturing, and a variety of BNCT treatment software programs have been developed, including NCTPlan and SERA in the United States [ ], BDTPS in Italy [JCDS-FX, TsukubaPlan, and NeuCure in Japan [ ], and NeuMANTA, THORPlan, and MCDB in China [ ]. The characteristics of each BNCT treatment planning system are presented in TABLE The TPS of BNCT consists of three parts: pre-processing, post-processing, and dose calculation (Fig.), in which pre- processing is used to read and display the CT/MRI medical image data (including the body geometry and material) and cooperates with the neutron irradiation conditions to generate the input file required for dose calculation, which will pro- cess the output of the dose calculation and display the results in graphs, which is convenient for users to analyze the results of the calculation. The dose calculation is the core part of the whole TPS, and the MC method is usually used to simulate the dose of particles produced by neutron beams. As shown in TABLE , MCNP has been widely used as a TPS dose calcu- lation program for BNCT because it supports neutron-photon multiparticle simulation, is relatively easy to use, provides flexible source definitions, has a large number of users, and has been fully validated by experiments. However, the MCNP program system is enormous, and its application is limited not only to the field of nuclear medicine but also to the fields of nuclear energy, nuclear engineering, nuclear technology, and other related theoretical calculations. MCNP, as commercial software, is subject to strict licensing restrictions, especially in certain countries (e.g., China) or specific application ar- eas, while Fortran programming has weak support for object- oriented programming, which is not as comprehensive and flexible as C++ and is not conducive to the subsequent de- velopment of specific areas of need. Therefore, a program specifically for dosimetry computation in BNCT is required, which should be characterized by a small program size, a high degree of autonomy, and friendly extensibility.

In this study, MagicDose, a dose calculation program for BNCT treatment planning, is developed using MC particle transport and C++. Compared to MCNP, it features com- pact size, specialization, and autonomy, with modular design enabling independent development and maintenance of func- tional modules. It provides functions like fine-voxelization phantom construction, a human tissue composition library, a Kinetic Energy Released in Matter (Kerma) factor library, and spatial plane rotation for BNCT dose calculation. It supports server parallel computing and results visualization for effi- cient analysis. To validate MagicDose, this paper: (1) Pre- pared voxel phantom of modified Snyder head with 16 and 8 mm resolution as benchmark, verifying that neutron and pho- ton dose rates calculated by MagicDose and MCNP are con- sistent, with MagicDose showing better computational effi- ciency; (2) Using material-located method with central point algorithm, constructed voxel phantom of modified Snyder head with tumor at 16, 8, and 1 mm resolutions to analyze the influence of model voxel sizes through depth-dose-rate curves and spatial distribution maps. The parallel computational ef- ficiency was analyzed across different spatial resolutions and thread numbers; (3) Applied MagicDose to a clinical BNCT case using a patient’ s CT head model.

Country/Institution Geometry Dose program Cross section NCTPlan USA/Harvard-MIT voxel MCNP4B/5 continuous energy USA/INEEL-MSU univel seraMultigroup multigroup BDTPS Italy/University of Pisa/JRC voxel continuous energy JCDS-FX Japan/JAEA voxel/multi-voxel MCNP5 continuous energy TsukubaPlan Japan/Tsukuba University voxel PHITS continuous energy NeuCure Japan/Sumitomo Heavy Industry voxel PHITS continuous energy NeuMANTA China/Neuboron voxel COMPASS continuous energy THORPlan China/Tsing Hua University voxel MCNP4C continuous energy China/IAPCM,Beijing voxel MCNP4C continuous energy “univel,” an abbreviation for uniform volume element, is a geometric modeling approach in BNCT. Unlike the voxel model, it represents a single pixel within a medical imaging sequence and does not require the use of mixed-material filling.

MATERIAL AND METHOD MagicDose program development & framework Dose calculation is the core part of the whole BNCT treat- ment planning system, which is based on the MC particle transport method. MagicDose, a dose calculation program dedicated to the BNCT treatment planning system, is devel- oped in C++, which is convenient for future development and maintenance of the BNCT treatment planning system. The MagicDose program consists of seven functional modules, including the Geometry module, Source module, Database module, Particle Transport module, Tally module, Output module, and Auxiliary module. Figure illustrates the Mag- icDose development framework. (1) Geometry module:

In the BNCT treatment planning system, the 3D voxel phantom is the most commonly used ge- ometric modeling technique and is usually constructed based on image information from computed tomography (CT) or magnetic resonance imaging (MRI). According to statis- tics, when MC particle transport simulations are performed, approximately 30–80% of the computational time is spent on geometry processing; therefore, the MagicDose program combines the characteristics of CT/MRI image information and the advantages of the lattice structure geometry process- ing method, which has a better average efficiency compared to the constructive solid geometry (CSG) method.

First, based on the CSG method, each tissue is defined as a cu- bic universe according to the surface equation; then, multi- ple universes are arrayed and discharged to form a repetitive lattice structure, which is then combined with the database module to fill in the nuclide composition and ratio of the corresponding tissue region to construct a complex dose calcula- tion model. Figure shows a lattice mapping of the geometric model [(2) Source module:

It is important to determine the source of BNCT irradiation in TPS because it involves a 5- dimensional ( ) probability distribution that ac- curately describes the spatial, energy, and angular character- istics of the neutron beam. The MagicDose program supports a variety of commonly used source terms, including the point source of monodirectional angular distribution, point source of isotropic angular distribution, spatial source of isotropic angular distribution, and spatial plane source with translation

and rotation. It is capable of simulating neutrons, photons, and neutron-photon coupled transport and supports a variety of probability distributions (discrete, continuous, histogram, and mixed distribution) for the corresponding source param- eters, thus providing an effective tool for simulating complex source beams for BNCT [Figure (a) shows the schematic of an in-hospital neutron irradiator type I reactor (IHNI-I), which is the first proto- type in the world that meets the requirements of the IAEA- specialized neutron source device BNCT [The site se- lection is located approximately 2 kilometers from the Bei- jing Nuclear Industry Hospital rather than being directly in- stalled within the hospital premises. This decision stems from the consideration of various uncertainties, such as the distri- bution and control of radiation dose levels, with the aim of accumulating experience and establishing a technical foun- dation for the future construction and application of BNCT neutron sources [ ]. The IHNI-I has a “tank-pool” structure with a rated power of 30 kW and two beam holes for thermal and epithermal neutrons. To avoid the significant computational time required to track particles from the reactor core for simulating the dose distribution in the human body, Mag- icDose establishes equivalent surface sources at the exits of the two beam flow orifices of IHNI-I to facilitate rapid dose calculations. The equivalent surface source, denoted as , is a function of the spatial position, energy, and direc- tion, where represents the radial distance (cm), denotes the energy (MeV), and is the cosine of the scattering an- gle (ranging from -1 to 1). Given that the collimator aper- ture diameter of IHNI-I is 12 cm, to more accurately capture the particle information emitted from the beam ports in con- structing the equivalent surface source, this study divides the radial direction into three intervals: 0 10, and 15, as shown in Fig. (b) [ ]. The energy spec- tra shown in Fig. (c) originate from an equivalent surface source at the thermal neutron beam port of IHNI-I, whereas the energy spectrum in Fig. (d) originates from the equiv- alent surface source at the epithermal neutron beam port of IHNI-I [(3) Database module:

In the particle transport calculation, the microscopic cross-section and angular distribution data of nuclear reactions induced by particles of various energy

Lattice in input card; Model. segments and nuclides are involved. Because a low-energy neutron contributes significantly to the dose of BNCT, when the neutron energy is reduced to a few eV, the thermal mo- tion of the scattering target nucleus has a strong effect on the collision, which affects the energy of the emitted neutron and the exit angle, eventually leading to errors in the results.

MCNP provides an S( ) thermal scattering model for this case, which directly calls the S( ) thermal scattering model data from the corresponding nuclides [ ]. The MagicDose program also saved the same S( ) thermal scattering data for the thermal neutron scattering of H in the voxel phantom material. The MagicDose program stores the physically rel- evant data of each reaction cross section in particle transport based on the ENDF/B-VIII.0 evaluation database using the HDF5 data format, which has the advantages of a hierarchi- cal structure and can handle large datasets [ ]. The actual tissue components must be simulated in the calculation of the BNCT dose, according to the ICRU46 and ICRU63 re- ports [ ], a material library including 106 human tissue components (TABLE), and the corresponding Kerma factor library (Fig.) with functions that support the addition, mod- ification, and editing of the related data. In the Kerma factor library, the neutron energy range spans from 0.0253 eV to 29 MeV, divided into 117 energy groups, while the photon en- ergy range extends from 0.01 MeV to 100 MeV, divided into 33 energy groups.

In the boron dose calculation of Magic- Dose, a Kerma factor of 1 ppm is adopted. The Kerma factor library is constructed according to Eq. ( ) and Eq. (

$K\ g =$

where is the average Kerma factor of the neutron or photon in group g with the unit of Gy is the width of the energy group region of group g; is the neutron or -photon energy spectrum with the unit of n/cm is the Kerma factor at energy point with the unit of Gy Data from the ICRU46 report can be used directly for neu- trons in different tissues of the human body. However, photons must be derived by conversion from Eq. (

$K\ \gamma\ (\ E\ ) = E\ \cdot \mu\ en\ (\ E\ )\ \rho$ (2)

where is the mass-energy absorption coefficient -photons in the ICRU46 report in units of cm is the -photon energy in units of J. The Kerma factor database of multigroup neutron and -photon is obtained by combining Eq. ( ) and Eq. ( ) with the energy spectra of the ICRU46 report. (4) Particle transport module:

BNCT dose calculation is the neutron-photon coupled transport process, and this module deals mainly with the MagicDose program to sim- ulate the particle production-to-disappearance process. Neu- tron–matter interactions mainly involve elastic scattering, in- elastic scattering, and absorption, in which absorption con- tains the dose-dependent reactions of interest to BNCT (n, (n,p), and (n,). During this process, the photons generated by a neutron are stored in the particle bank for subsequent photon transport. With respect to the photon-matter inter- actions, the photoelectric effect, electron pair effect, coher- ent scattering, and Compton scattering are primarily consid- ered [ ]. Figure shows a particle transport flow diagram. (5) Tally module:

After particle transport is completed, users can set different statistical parameters to invoke the tally module according to their own needs, among which the pa- rameters include selection of the region of interest. The pro- gram supports two ways of statistics—cell statistic and virtual superposition mesh statistic—and supports setting of energy region and particle type, etc. The corresponding quantity of is obtained in various statistical ways, and the data for

Schematic of in-hospital neutron irradiator type I reactor (IHNI-I); Schematic of the IHNI-I equivalent surface source; Energy spectrum of the equivalent surface source at the thermal neutron beam port of IHNI-I; Energy spectrum of the equivalent surface source at the epithermal neutron beam port of IHNI-I.

Tissue Density (g/cm Elemental composition (mass percentage %) Brain (whole) Heart

each dose component can be obtained by combining Eq. (3) and the Kerma factor library in the database module.

Dose (j) = ϕ (j, E) V (j) · Kerma (j, E) dE (3)

where is the normalized flux value in n cm/s for the voxel mesh with energy is the volume of the voxel mesh, and Kerma is the neutron/photon flux dose conversion factor for the voxel mesh with energy . In this paper, the Kerma factor for the adult brain rela- Fetus (14weeks) Newborn Infant (18months) Adult Fetus (17-40 weeks) Adult (healthy) 0.26 (Inflated) Adult (congested) Fetus (17-40 weeks) Child (2 years) Child (4-18 years) Adult (healthy) Adult (fatty)

tive to ICRU46 given by ICRU63 in the MagicDose program database is used, but the lowest energy corresponding to the Kerma factor given in the report is 0.0253 eV, and for the dose of the BNCT, the neutron contribution to the thermal neu- tron dose for energy lower than 0.0253 eV is very important.

Therefore, double logarithmic interpolation is adopted to ex- trapolate the Kerma value corresponding to less than 0.0253 eV to the data corresponding to 0.0001 eV. The Kerma factor of the photon in this study is obtained based on the mass- energy absorption coefficients calculated by Seltzer [(6) Output module:

The data counted by the tally mod- ule are transferred to the output module, through which the data of boron dose, thermal neutron dose, epithermal and fast neutron dose, and photon dose of interest in BNCT treatment are exported. As different types of ionizing radiation cause different biological effects in living organisms, and BNCT involves mixed-field irradiation of several different radiation dose components, for BNCT treatment, it is necessary to mea- sure the relative biological effectiveness (RBE) of each dose component and assess its killing effect on normal tissues and tumors. The RBE experimentally measured is used to char- acterize the high or low biological effect dose of the thermal neutron dose, epithermal and fast neutron dose, and photon dose. To convert the local high LET radiation dose produced Li into an equivalent dose, the use of a com- pound biological effect (CBE) factor is required to more accu- rately assess its actual biological effects on biological tissues, especially tumors and normal tissues [ ]. Multiplying each of the above four dose components by their correspond- ing weighting factors yielded the total relative biological ef- fect dose (Eq. (

$$H = W B D B + W \gamma D \gamma + W n D n + W p D p \quad (4)$$

where is the CBE factor for the boron dose; are the RBE factors for the photon, epithermal and fast neutron, and thermal neutron dose, respectively; and , and are the boron dose, the photon dose, the ep- ithermal and fast neutron dose, and the thermal neutron dose from nitrogen capture, respectively. (7) Auxiliary module:

The auxiliary module is used to enhance the main functions and improve program maintain- ability and user-friendliness, including the provision of re- lated function libraries, such as mathematical libraries related to each mathematical probability sampling in source sam- pling (Math) and file manipulation functions, to improve code reusability. Simultaneously, the program stability is enhanced by the exception-catching mechanism (fatal error, warning), which detects and handles abnormalities during operation to prevent the whole program from crashing. The visualization tool in the auxiliary module shows the results of the output module, which presents the results of each BNCT dose field in 2D/3D form. The interface information outputs provide key information to the user, including run status, progress re- ports, run date, and number of threads, to facilitate user inter- action with the program.

The MagicDose program adopts the particle transport mod- ule as the core, interconnects with the upstream geometry, source, and database modules, and simultaneously supports the downstream tally and output modules. Each module is in- dependent of the others, and module functions are realized by messages passing through the interface, which is conducive to the maintenance and expansion of the program.

Calculation conditions and models To verify the accuracy and efficiency of MagicDose, three models are selected for testing. First, because the MCNP program can be used as a standard for all types of MC cal- culations and is often used to calibrate the correctness tests of other MC programs, the results of MagicDose calculations are compared with MCNP. The two programs select the voxel phantom of a modified Snyder head with 16 and 8 mm res- olution, which is commonly used internationally. Under the same irradiation conditions, we compare the calculated spa- tial neutron and photon dose rates to see if they are consistent and count the computational efficiency of both. Subsequently, to explore the influence of voxel phantom on the calculation results under different spatial resolutions, the MCNP compu- tational analytical model is used as the reference result. The voxel phantom of the modified Snyder head with a tumor hav- ing three different spatial resolutions of 16, 8, and 1 mm was constructed using MagicDose combined with the material- located method using the central point algorithm. The depth- dose-rate curves and spatial value distribution plots are used to analyze the effect of model voxel size on the results and to statistically calculate the computational efficiency of Mag- icDose with different resolutions and the number of threads.

Finally, based on the CT head model of a patient given by DICOM data, we initially verify whether MagicDose can be applied to the clinical case of BNCT.

All the calculations in this study are performed on an In- tel (R) Core(TM) i7-10700 K CPU @ 3.8 GHz with 32 GB RAM and 16 threads. To minimize the impact of the results from the deep penetration of the MC program, the number of

particles is set to 1 for both MagicDose and MCNP to ensure that the number of samples is adequate [ ]. In the actual BNCT treatment, some photons are produced by the accompanying neutron source, which cannot be avoided.

We assume the absence of accompanying photon contamina- tion from the neutron source and only discuss the induced photons produced by the reaction of neutrons with nuclides in the voxel. (1) Voxel phantom of the modified Snyder head with 16 and 8 mm Currently, the benchmark problem commonly adopted in- ternationally for BNCT dose calculation is the modified Sny- der head phantom, which consists of three ellipsoidal surfaces to define the boundaries of different tissues, dividing the head

from inside to outside into three parts: brain tissue, skull, and scalp tissue. The whole head is surrounded by air, which is usually called the analytical model (Fig.). The densities of air, scalp, skull, and brain tissue are 0.001293, 1.09, 1.61, and 1.04 g/cm , respectively, and the corresponding elements of the human tissue are obtained from the MagicDose database module with the specific parameters listed in TABLE The surface analytical equations for the modified Snyder head phantom with tumor at each interface are expressed as follows:

Boundary surfaces of the scalp and air x, y, z) = (Boundary surfaces of the skull and scalp x, y, z) = (Boundary surface between brain and skull x, y, z) = (

In clinical treatment, owing to the different shapes, loca- tions, and sizes of patients' tumors, it is not possible to use analytical equations to describe the phantom; therefore, it is common to use a continuous and uniform cubic mesh to approximate the phantom structure in international clinics, which are generally called voxel phantoms. Goorley et al. [3] constructed 16 and 8 mm voxel phantoms as an international benchmark problem based on the modified Snyder' s analyt- ical model, which is mixed with four basic materials (brain, skull, scalp, and air); the volume share of each basic material

(Color online) Elemental composition and density of tissues.

Elemental composition Tissue (mass percentage %) Scalp Skull Brain in the mix is a multiple of 10% to produce the mixed mate- rials and corresponding mixing densities, and a total of 286 hybrid materials are derived. Therefore, to verify the accu- racy of MagicDose, identical 16 and 8 mm voxel phantoms are constructed based on MagicDose and MCNP respectively (Fig. 16 [Figure 16: see original paper] mm, 8 mm.

For the irradiation condition, in this paper, the international wide-spectrum epithermal mixed neutron beam proposed for the modified Snyder head phantom is adopted, in which the thermal neutron with energy less than 0.5 eV accounts for 10%, the epithermal neutron with energy between 0.5 eV and 10 keV accounts for 89%, and the fast neutron with energy between 10 keV and 2 MeV accounts for 1%. The overall neutron source spectra obeyed the distribution according to the energy-dependent probability function 1/E, uniformly dis- tributed on a disk surface with a radius of 5 cm and a source strength of 10]. Figure presents the energy spectrum of the neutron source. (2) Voxel phantom of the modified Snyder head with tu- mor based on the material-location method with a central point algorithm To study the influence of the voxel phantom on the calcula- tion results under different spatial resolutions and to simulate the situation of glial tumors in the brain in the clinic. Based

(Color online) Energy spectra of the wide-spectrum ep- ithermal mixed neutron beam. on the model illustrated in Fig. , a sphere with a radius of 1.5 cm is added to the brain tissue as the tumor boundary, and the coordinate origin is at the center of the entire analyti- cal model. Fig. shows the modified Snyder head phantom with tumor [ ], in which the equation for the boundary surface of the tumor and brain is given by Eq. (x, y, z) = ((Color online) Schematic transverse of modified Snyder head with tumor.

For the analytical model, the materials can be accurately described, but the voxel phantom will be difficult to deal with because the voxel mesh may be at the interface of the two substances. The traditional way to deal with this is to fill by obtaining the exact volume ratio of different materials inside each cubic mesh (Fig.), which is extremely time consum- ing and results in bias when the number of voxel meshes is large. As described above, the model material was derived 286 from 4 materials as the hybrid materials. In this study, to reduce the complexity of the simulation problem, the ma- terial of the center point of the mesh is used in the phantom construction of MagicDose, and the material density of the whole mesh is determined according to the location of the center point of each mesh, which is reduced from the original 286 kinds of material to four types of materials [ ], Fig. shows the material-location method with a central point al- gorithm. In Fig. denotes the center point position of each voxel mesh, and denote the boundary equations Eq. ( ) as follows: When the position of the center point is substituted in the boundary equations with a value less than 1, it is "True" , the mesh material is the tis- sue component inside the boundary equation, otherwise it is "False" , the mesh material is the tissue component outside the boundary equation.

Based on the material-located method with the central point algorithm, MagicDose constructed three voxel phan- toms of the modified Snyder head with tumor of different spatial resolutions (16, 8, and 1 mm), and the corresponding voxel mesh numbers of are 2744, 21952, and 11239424, respectively [ ]. As shown in Fig. show trans- verse views of different voxel phantoms. 16 mm, 8 mm, spatial resolution.

In this study, MCNP is used to construct a modified Snyder head analytical model with a tumor. The results of the MCNP computation are used as the reference result, which is com- pared and verified with the results of MagicDose under differ- ent resolutions, and are used to explore the influence of voxel phantom on the computational results under different spatial resolutions. The tissue compositions of the voxel phantom of the modified Snyder head with tumor and the modified Sny- der head analytical model with tumor are shown in TABLE The tissue compositions of the tumor are consistent with that of normal brain tissues, except for the different boron con- tents, according to the relevant literature [ ]. According to the current clinical trials requirements, the B content (T) of the tumor must be higher than the B content (N) of the normal tissue by a factor of 2.5 or more (T/N 2.5), and the calculations in this paper set the boron concentration of scalp tissue and normal tissue in the brain at 10 ppm and the boron concentration within the tumor tissue at 30 ppm, with no boron in the skull [ ]. MagicDose and MCNP both utilize the wide-spectrum epithermal mixed neutron beam spectrum shown in Fig. for the simulated dose calculations. To make the calculated results comparable to international BNCT dose results, according to Eq. ( ). The RBE and CBE factors are

selected with reference to the values obtained from the MIT and BNL in BNCT clinical trials [40 , 41], as shown in TA- BLE 4 .

(Color online) RBE and CBE factors for tumor and healthy tissues at different dose compositions in voxel phantom of modified Snyder head with tumor.

BNCT dose components Healthy tissue (brain, skull, scalp) Tumor 10 B(n, -CBE) N(n, p) -RBE) Epithermal and fast neutron -RBE) (3) CT head model of a patient based on DICOM data In a preliminary application, MagicDose was used to con- struct a voxel phantom based on DICOM data from a patient' s head (Fig. shows coronal, transverse, and sagittal CT im- ages [ ]. The dimensions of the phantom in the X-, Y-, and Z-directions are 18, 18 and 16.5 cm, respectively, and the size of the constructed voxel is 1 mm 1 mm. An equivalent source of the epithermal neutron beam plane of the IHNI- I reactor with the MagicDose source module is used for the irradiation conditions (Fig. (d)), and the irradiation direction was vertical to the back of the head (Fig. (g)).

RESULT AND DISCUSSION Correctness testing of MagicDose Coronal, Transverse, and Sagittal of CT images; Coronal, Transverse, and Sagittal of MagicDose constructed model; Schematic of irradiation direction. of the modified Snyder head at spatial resolutions of 16 and 8 mm for MagicDose and MCNP. Using MCNP as a refer- ence result [ ], the slope ratio method is used in this study to distinguish how close the dose rate results calculated by MagicDose are to the MCNP results. For any voxel in the model, the dose rate result of MCNP is taken as the horizontal coordinate value , and the dose rate result of MagicDose is the vertical coordinate value , and the points ( ) are labeled sequentially on the coordinate system, and it is ob- served that all the images formed by scattering the points are scattered near the straight line equation of . As illustrated

in Fig. , the number of model voxels with a spatial resolu- tion of 16 mm is fewer than that of the 8 mm model voxels.

Consequently, the number of coordinate points in the 16 mm model are lower than that in the 8 mm model. However, the points ( ) generated by MagicDose and MCNP are pre- dominantly concentrated near the line . Furthermore, the locally magnified graphs of the respective dose rates reveal that the deviation of the dose rate results from is mini- mal. This observation indicates that the results computed by MagicDose and MCNP are in strong agreement, thereby val- idating the accuracy of MagicDose.

In the model calculations, both MagicDose and MCNP are performed under the same conditions, as listed in TABLE At a spatial resolution of 16 mm, the calculation times for MCNP and MagicDose are 1373 and 944 s, respectively, with MagicDose achieving an efficiency improvement of approx- imately 31.24% compared to MCNP. At a spatial resolution of 8 mm, the calculation times for MCNP and MagicDose are 2042 and 1457 s, respectively, with MagicDose demon- strating an efficiency improvement of approximately 28.65% over MCNP. The numerical results demonstrate that Mag- icDose outperforms MCNP in terms of computational effi- ciency, while ensuring the accuracy of the BNCT calcula- tions. (Color online) Time comparison of different computa- tional programs based on 16 and 8 mm voxel phantoms.

Exploration of MagicDose at different spatial resolutions The result of each dose rate of the modified Snyder head analytical model with tumor simulated by MCNP calculation is used as the reference in this section. In the comparative validation calculations, using the parameter setup described above (including material and source terms, etc.) as well as the nuclear cross-section database, MagicDose is used to con- struct voxel phantoms with three different spatial resolutions of voxel sizes of 16, 8, and 1 mm, and to compare the vari- ability in the results of the phantom-depth correlation dose- rate curves along the Z-axis computed by the two MC particle transport programs. Simultaneously, the relevant spatial dose rates of the head phantom at different voxel resolutions are statistically calculated to explore the effect of the voxel size of the voxel phantom on the results and to provide reference opinions for the optimization of the voxel phantom design for clinical treatment.

Figure - Fig. show the boron dose rate, thermal neu- tron dose rate, epithermal and fast neutron dose rates, induced photon dose rate, total relative biological effect dose rate, rel- ative deviation with depth, and spatial dose rate distributions at different voxel resolutions. The relative deviation is the percentage of deviation obtained by comparing the Magic- Dose voxel phantom results with the MCNP analytical model results as the reference result, and the ICRU24 report sug- gests that the relative deviation between the actual treatment and the planned dose of BNCT should not exceed 5%; oth- erwise, the risk of tumor recurrence persists, and radiological complications increase in normal tissues [As shown in Fig. (a), the boron dose rate calculated by MagicDose at different resolutions of the voxel is compared with the reference result, which is consistent with the results at 1 mm. However, the variability of the results is more obvi- ous with an increase in the resolution of the voxel. Fig. shows that the relative deviations of 1 mm are within 5% of the clinical allowable for BNCT, whereas 8 and 16 mm have greater relative deviations between depths of 0.5–1.5 cm, 5.4–8.2 cm, and 14.2–18.2 cm. By integrating the phantoms de- picted in Fig. with the spatial dose-rate distribution derived from Fig. (c)–Fig. (e), it becomes evident that significant relative deviations can be ascribed to the depth ranges of 0.5–1.5 cm, 14.2–18.2 cm, which corresponds to the skull, and 5.4–8.2 cm, which pertains to the tumor. The phantoms with dimensions of 8 mm and 16 mm lack high-resolution repre- sentation of tissues in these specific regions, ultimately result- ing in inaccuracies in the dose rate calculations. Figure (e) demonstrate that the results derived from the voxel phantom at high resolution exhibit greater accuracy. Analysis of the spatial dose rate values clearly indicates that the skull does not contribute to the boron dose rate, as it lacks boron content. Conversely, in the tumor region, the elevated boron content leads to a substantial increase in the boron dose rate, thereby facilitating more precise tumor localization in clinical settings.

From Fig. (f)–Fig. (j) and Fig. (f)–Fig. (j), we ob- serve that the thermal dose and induced photon dose rates for 1 and 8 mm are consistent with the reference result, and the relative deviations are limited to 5%. However, the calcu- lated results are biased owing to the large resolution of the 16 mm voxel. The distribution curves of the thermal dose rate and induced photon dose rate exhibit the same trend, because the induced photon comes from the neutron capture reaction and the -ray is generated by the capture reaction between thermal neutrons and H-atoms in the body; the photon is gen- erated in place of the higher neutron dose, and the greatest damage is produced in the superficial tissues of the head.

This is shown in Fig. (a), (c), (d), and (e), because 89% of the neutron source radiation is epithermal neutrons, neu- trons slowing down to thermal neutrons occur initially and the dose rate gradually decreases as the depth increases. From (b), it is understood that when the depth is less than 12 cm, the relative deviations of both 1 mm and 8 mm are basi- cally kept within 5%; when the depth is greater than 12 cm, it will cause the problem of deep penetration, at which time the MC program calculates the number of particles arriving at the depth to be less, resulting in the statistical results of the relative deviation to be larger.

The dose rates are shown in Fig. to Fig. are com- bined according to the corresponding factors of CBE or RBE to obtain the total dose rate of the relative biological effect,

(Color online) (a)(b) Thermal neutron dose rate based on voxel phantom of modified Snyder head; (c)(d) Epithermal and fast neutron dose rate based on voxel phantom of modified Snyder head; (e)(f) Induced photon dose rate based on voxel phantom of modified Snyder head. as shown in Fig. . As shown in Fig. (a)(b), the total dose rate at 1 mm is consistent with the reference result, and the

relative deviations are kept within 5%; the discrepancy of the results at 8 mm and 16 mm is due to the boron dose as the main dose component, and the effect of the resolution of the voxel phantom on the boron dose, which ultimately leads to the deviation of the total dose rate. Overall, Fig. to Fig. show that the dose rates and relative deviations of the high- resolution voxel phantoms calculated from MagicDose are consistent with the reference result and remain within indicating that as the size of the constructed voxel mesh gets smaller, the better it converges to the analytical model, the better the computed results match, highlighting the effect of the voxel size of the voxel phantoms on the results Because the boron concentration of BNCT changes rapidly with the body' s metabolism after boron injection, BNCT is highly demanded owing to its speed of dose calculation, which ensures that the dose calculation can be completed in a very short period of time (3600 s). The number of vox- els also affects the efficiency of the calculation. Therefore, to verify the computational efficiency of MgaicDose, simula- tions are performed using 1, 4, 8, and 16 threads for the voxel phantom of the modified Snyder head with tumor at 16, 8, and 1 mm, respectively, to test the computational efficiency of the program at different spatial resolutions and with differ- ent numbers of threads. Figure compares the computation time (s) for different mesh scales and different numbers of thread 3D histograms. Evidently, under the same computa- tional conditions, the smaller the voxel size, the longer the simulation computation time. However, with an increase in the number of parallel threads, the time used for the simulation becomes increasingly shorter, with increasingly obvious acceleration effects.

C. Initial application of MagicDose based on DICOM data

MagicDose constructes a voxel phantom of the head us- ing DICOM data, and

Fig. shows that the schematics of MagicDose in the coronal, transverse, and sagittal planes are consistent with the CT images of the corresponding locations.

Based on the irradiation from an equivalent surface source at the epithermal neutron beam port of IHNI-I, as shown in (d), Fig. (a), (b), (c), and (d) show the boron dose rate, thermal neutron dose rate, epithermal and fast neutron dose rates, and induced photon dose rate, respectively. The total relative biological effects of the dose rate (Fig. (d)) is de- rived by integrating TABLE with the aforementioned dose- rate values. The spatial distributions of the boron and thermal neutron dose rates are similar to those shown in Fig. and Fig. (b) because both doses are related to thermal neu- trons, and the boron dose rate is significantly higher than the contribution of the epithermal neutron dose rates presented in Fig. (c) is mainly located in the shallow region of the posterior cerebral epidermis. Fig. (d) shows that the in- duced photon dose rate is distributed throughout the space and presents the complete human head profile; combining the CBE and RBE factors, the total relative bioeffect dose rate shown in Fig. (e) is obtained, and the highest dose region appears in the irradiated region of the back of the head.

CONCLUSION

To further develop the TPS-dedicated dose calculation pro- gram for BNCT, this study presents the BNCT MC dose cal- culation program MagicDose, which was developed using the MC particle transport method. Compared to MCNP, Magic- Dose features a small program size due to its exclusive fo- cus on BNCT, in contrast to MCNP' s extensive applications across nuclear medicine, reactor design, and detection, which result in a larger codebase; it exhibits enhanced specialization through a modular design tailored to BNCT needs, such as a source module preconfigured with the IHNI-I reactor' s equiv- alent surface beam sources and a database module optimized with Kerma values for 106 human tissue materials; Magic- Dose exhibits greater autonomy.

Unlike MCNP, which is subject to stringent licensing restrictions—including an em- bargo on China—and is developed in Fortran, limiting its ca- pabilities in object-oriented programming and hindering ex- tensions for BNCT' s future needs, such as GPU-based MC particle transport, MagicDose is independently developed in C++. This license-free approach, coupled with a modular, reusable, and easily maintainable design, significantly en- hances developmental flexibility and enables independent op- erations without relying on external tools. MagicDose in- volves seven functional modules: geometry, source, database, particle transport, tallies, output, and auxiliary. With particle transport as the core, connected upward with the geometry, source, and database modules and supported downward by the tally and output modules, the program adopts a modular design so that each functional module can be developed and maintained independently, facilitating the secondary develop- ment of the BNCT' s subsequent needs. To test the correct- ness of MagicDose, two international benchmark voxel phan- toms, i.e., the voxel phantom of modified Snyder head with 16 and 8 mm, are first selected in this paper, and the neutron and photon dose rates computed by MagicDose and MCNP are compared with each other, which are used to validate the correctness of the program; Subsequently, based on the material-located method with central point algorithm, three different spatial resolutions (16, 8 and 1mm) of voxel phan- tom of modified Snyder head with tumor are constructed us- ing MagicDose, and the depth-dose rate curve results and spa- tial value distribution plots are used to explore the influence of the voxel phantoms on the calculation results under differ- ent spatial resolutions; Finally, based on the CT head model of a patient given by DICOM data, MagicDose is used to con- struct a voxel phantom with a voxel size of 1 mm mm, and the corresponding dose rate values are calculated and obtained, demonstrating the application of the program in clinical cases of BNCT. Based on these three models, the following conclusions were drawn: (1) For the modified Snyder head voxel phantom with spa- tial resolutions of 16 mm and 8 mm, taking the dose rate val- ues calculated by MCNP as the reference, denoted as , and those computed by MagicDose as , a comparison of their relationship relative to the linear function reveals that the two-dimensional coordinate points ( ) are consistently distributed near the line. Thus, the results of Magic-

(a)(b) Boron dose rate and relative deviation vs. depth; (c)(d)(e) Boron dose rate at 16, 8, and 1 mm; (f)(g) Thermal neutron dose rate and relative deviation vs. depth; (h)(i)(j) Thermal neutron dose rate at 16, 8, and 1 mm.

Dose are well-consistent with those of MCNP calculations, validating MagicDose.

According to TABLE , at spatial resolutions of 16 and 8 mm, MagicDose reduced the com- putation time by 31.24% and 28.65%, respectively, compared with MCNP, demonstrating its overall superior computational efficiency over MCNP.

(Color online) (a)(b) Epithermal and fast neutron dose rate and relative deviation vs. depth; (c)(d)(e) Epithermal and fast neutron dose rate at 16 mm, 8 mm and 1 mm; (f)(g) Induced photon dose rate and relative deviation vs. depth; (h)(i)(j) Induced photon dose rate at 16 mm, 8 mm and 1 mm. (2) For the voxel phantom at high spatial resolution, the boron dose rate, thermal neutron dose rate, epithermal and fast neutron dose rates, induced photon dose rate, and total relative biological effect dose rate calculated by MagicDose

(Color online) (a)(b) Total relative biological effect dose rate and relative deviation vs. depth; (c)(d)(e) Total relative biological effect dose rate at 16 mm, 8 mm and 1 mm. (Color online) Comparison of computation time (s) for different mesh scales and different number of threads 3D histograms.

align closely with MCNP reference results, with a relative de- viation of less than 5%. This consistency confirms the com- putational reliability of MagicDose, although its applicability to clinical treatment requires further validation using experi-

mental data. The results show that the variability of the results decreases with increasing spatial resolution, which provides reference opinions for optimizing the design of voxel phan- toms for clinical treatment. In tests at different spatial reso- lutions and with different numbers of threads, it is concluded that the smaller the size of the voxel constructed by Magic- Dose, the longer the simulation computation time. However, with an increasing number of parallel threads, the time used for the simulation becomes increasingly shorter, and the ac- celeration effect becomes increasingly obvious.

(3) MagicDose can be used to construct an appropriate voxel phantom based on DICOM data, and the results of the calculations provide a preliminary validation of the use of the program in clinical cases, particularly its ability to develop high-resolution CT-based phantom dosimetry calculations.

Given the potential for further optimization of the Magic- Dose program, future efforts will focus on developing a set of four-dimensional dynamic MC programs specifically for BNCT pharmacokinetics. This development will be under- taken alongside the investigation of time-dependent MC par- ticle transport methods to enhance the efficiency and accuracy of dose calculations.

Boron dose rate distribution based on head CT; Thermal neutron dose rate distribution based on head CT; Epithermal and fast neutron dose rate distribution based on head CT; Induced photon dose rate distribution based on head CT; Total relative biological effect dose rate based on head CT.

U2267207), YueLuShan Center Industrial Innovation (No. 2024YCII0108), Project of State Key Laboratory of Radi- ation Medicine and Protection, Soochow University (No.

ACKNOWLEDGMENT

This work was supported by the National Natural Science Foundation of China (Nos. 12475174 and

GZK12023031), Science and Technology Innovation Project of Hengyang (No. 202250045336), and Graduate Research Innovation Project of Hunan Province (No. QL20230228).

CREDIT AUTHORSHIP CONTRIBUTION STATEMENT

Aikou Sun : Methodology, Software, Validation, Inves- tigation, Visualization, Formal analysis, Writing -original draft, Writing -review & editing.

Zhenping Chen : Con- ceptualization, Methodology, Validation, Supervision, Fund- ing acquisition, Writing -review & editing.

Kekun Gao :

B.F. Han, R.S. Zheng, H.M. Zeng et al., Cancer incidence and mortality in China. J. Natl. Cancer Cent. , 47–53 (2024).

International Atomic Energy Agency, Advances in boron neu- tron capture therapy. (Non-serial Publications, IAEA, Vienna, 2023). boron-neutron-capture-therapy J.T. Goorley, W.S. Kiger III, R.G. Zamenhof, Reference dosimetry calculations for neutron capture therapy with com- parison of analytical and voxel models. Med. Phys. , 145-156 (2002).

F. Tian, C.R. Geng, X.B. Tang et al., Analysis of influencing factors on the method for determining boron concentration and dose through dual prompt gamma detection. Nucl. Sci. Tech. , 35 (2021).

X. Guan, I.M.T. Wang, Monte Carlo optimization of an epither- mal neutron flux monitor for BNCT. J. Nucl. Sci. Technol. 1118-1122 (2017).

S.J. Gonz´alez, NCTPlan, the new PC version of Mac- NCTPlan: improvements and verification of a BNCT treat- ment planning system. (10th International Congress on Neu- tron Capture Therapy for Cancer, Essen, Germany, 2002).

T. Seppaelae, L. Kankaanranta, H. Joensuu et al., BNCT Rtpe and sera dose planning programs: phantom and patient studies.

Proc. Ninth Int. Symp. Neutron Capture Ther. Cancer. 175-176 (2000).

N. Cerullo, G.G. Daquino, L. Muzi, An overview on the de- velopments and improvements of a treatment planning sys- tem for BNCT. IEEE Trans. Nucl. Sci. , 1333-1338 (2006).

H. Kumada, K. Yamamoto, A. Matsumura et al., Verifica- tion of the computational dosimetry system in JAERI (JCDS) for boron neutron capture therapy. Phys. Med. Biol. , 3353 (2004).

H. Kumada, K. Takada, T. Aihara et al., Verification for dose estimation performance of a Monte-Carlo based treatment planning system in University of Tsukuba. Appl. Radiat. Isot. , 109222 (2020).

N. Hu, H. Tanaka, K. Ryo et al., Evaluation of a treat- ment planning system developed for clinical boron neutron capture therapy and validation against an independent Monte Carlo dose calculation system. Radiat. Oncol. , 243 (2021).

Methodology, Investigation, Visualization, Writing –review & editing.

Lin Zhu : Methodology, Investigation, Visualiza- tion, Writing –review & editing.

Chengwei Liu : Method- ology, Investigation, Visualization, Writing –review & edit- Zhiqiang Wu : Methodology, Investigation, Visualiza- tion, Writing –review & editing.

Chao Yang : Methodol- ogy, Investigation, Visualization, Writing –review & editing.

Tong Liu : Methodology, Investigation, Writing –review & editing.

Song Wang : Methodology, Investigation, Writing –review & editing.

Zizhu Zhang : Methodology, Investigation, Writing -review & editing.

Yizheng Chong : Methodology, Investigation, Writing -review & editing.

Tao Yu : Supervi- sion, Writing -review & editing, Funding acquisition.

W.B. Zhong, J. Chen, Y.C. Teng et al., Introduction to the Monte Carlo dose engine COMPASS for BNCT. Sci. Rep. 11965 (2023).

Development verification THORplan—A treatment planning system THOR.

Appl. Radiat. Isot. (2011). L. Deng, G. Li, T. Ye et al., MCDB Monte Carlo code with fast track technique and mesh tally matrix for BNCT. J. Nucl. Sci. Technol. , 1518–1525 (2007).

Z.T. Wang, Q. Zheng, B. Wang et al., Recent research progress of BNCT treatment planning system. Nucl. Eng. Technol. 103264 (2025).

R.Y. Wu, C.R. Geng, F. Tian et al., GPU-accelerated three- dimensional reconstruction method of the Compton camera and its application in radionuclide imaging. Nucl. Sci. Tech. , 52 (2023).

W. Jiang, P. Cao, Y.M. Wu et al., FPGA-based position re- construction method for neutron beam flux spatial distribu- tion measurement in BNCT. Nucl. Sci. Tech. , 56 (2024).

J.Y. Chen, J.F. Tong, Z.L. Hu et al., Evaluation of neutron beam characteristics for D-BNCT01 facility. Nucl. Sci. Tech. (2022).

Y.N. Zhu, Z.K. Lin, L.Y. Lu et al., Design of beam shaping assembly for boron neutron capture therapy based on D-T neutron source. Nucl. Tech. , 010202 (2022). (in Chinese) Y.N. Zhu, X.B. Jiang, L.X. Chen et al., Study on quality pa- rameters of neutron beams in IHNI-I reactor ducts. Prog. Rep.

Nucl. Sci. Technol. China (Vol. 4). Proc. Acad. Annu. Meet.

China Nucl. Soc. 2015, No. 7-Nucl. Phys. sub-volume. (2016).

Chinese) Y.M. Zhou, Neutron capture therapy (NCT) & in-hospital neu- tron irradiator (IHNI)—–a new technology on binary tar- geting radiation therapy of cancer. Eng. Sci. , 2–21 (2009).

Y.N. Zhu, X.B. Jiang, Z.M. Zhao et al., Numerical cal- culation for the equivalent surface source of the ther- mal neutron duct of in-hospital neutron irradiator mark 1 reactor. Strateg. Study CAE. 56–59+68 (2012).

Chinese)

Y.N. Zhu, Z.K. Lin, H.Y. Yu et al., Study on the optimal incident proton energy of Li(p, n) Be neutron source for boron neutron capture therapy. Nucl. Sci. Tech. , 60 (2024).

C.J. Werner, J.S. Bull, C. Solomon, MCNP users manual - Code version 6.2. Los Alamos National Laboratory, Report LA-UR-17-29981 (2017).

P.K. Romano, N.E. Horelik, B.R. Herman et al., OpenMC: state-of-the-art Monte Carlo research development.

Nucl. Energy. (2015). ICRU, Photon, electron, proton and neutron interaction data for body tissues. ICRU Report 46, International Commis- sion on Radiation Units and Measurements, Bethesda (1992).

ICRU, Nuclear data for neutron and proton radiotherapy and for radiation protection. ICRU Report 63, International Commission on Radiation Units and Measurements, Bethesda (2000). and-proton-radiotherapy-and-for-radiation-protection-report- X.Y. Luo, R. Qiu, Z. Wu et al., THUDosePD: a three-dimensional Monte Carlo platform for phantom dose assess- ment. Nucl. Sci. Tech. , 164 (2023). 023-01315-y S.M. Seltzer, Calculation of photon mass energy-transfer and mass energy-absorption coefficients. Radiat. Res. , 147–170 (1993).

S. Ishiyama, Deterministic parsing model of the compound bi- ological effectiveness (CBE) factor for intracellular 10B dis- tribution in boron neutron capture therapy. J. Cancer Ther. 1388 (2014).

Zhang, Chong, review planned, ongoing clinical studies and recent development of BNCT in mainland of China. Cancers , 4060 (2022).

Q.Q. Pan, L.J. Wang, Y. Cai et al., Density-extrapolation global variance reduction (DeGVR) method for large-scale radiation field calculation. Comput. Math. Appl. , 10–22 (2023).

Q.Q. Pan, H.W. Lv, S.Q. Tang et al., Pointing probabil- ity driven semi-analytic Monte Carlo method (PDMC) - Part I: Global variance reduction for large-scale radiation trans- port analysis. Comput. Phys. Commun. , 108850 (2023).

Albritton, Computational aspects treatment planning neutron capture therapy.

Ph.D. disser- tation, Massachusetts Institute Technology (2009).

Y.N. Zhu, Z.K. Lin, H.Y. Yu et al., Conceptional design of an adjustable moderator for BNCT based on a neutron source of 2.8 ´aMeV proton bombarding with Li target. Nucl. Eng. Tech- , 1813–1821 (2024).

Research Monte Carlo simulation

method

software development BNCT. Master’ s thesis, China Academy Engineering Physics (2005).

Chinese M. Golshanian, A.A. Rajabi, Y. Kasesaz, Evaluation of the medical staff effective dose during boron neutron cap- ture therapy using two high resolution voxel-based whole body phantoms. Nucl. Eng. Technol. , 1505–1512 (2017).

H. Yu, C. Zheng, L. Sun, Boron neutron capture therapy dose calculation for tumor modified Snyder head phantom us- ing MCNP. Atom. Energy Sci. Technol.

, 89-94 (2010). in Chinese M. Marashi, Analysis of absorbed dose distribution in head phantom in boron neutron capture therapy. Nucl. In- strum. Meth. A , 446-452 (2000). 9002(99)00827-X C.L. Lee, L. Zhou, R.J. Kudchadker et al., A Monte Carlo dosimetry-based evaluation of the Be reaction near threshold for accelerator boron neutron capture therapy. Med.

Phys. , 192-202 (2000). R. Zamenhof, E. Redmond II, G. Solares et al., Monte Carlo- based treatment planning for boron neutron capture therapy using custom designed models automatically generated from CT data. Int. J. Radiat. Oncol. Biol. Phys. , 383-397 (1996).

Y. Liu, T. Meng, H. Zhang et al., Development and verifica- tion of a novel system for computed tomography scanner model construction in Monte Carlo simulations. Nucl. Eng. Technol. , 4244-4252 (2022).

G. Leunens, J. Verstraete, A. Dutreix et al., Assessment of dose inhomogeneity at target level by in vivo dosimetry: can the recommended 5% accuracy in the dose delivered to the target volume be fulfilled in daily practice? Radiother. Oncol. 242-250 (1992).

Note: Figure translations are in progress. See original paper for figures.