A Monte Carlo Program for Estimating Characteristics of Neutron Calibration Fields Using a Pelletron Accelerator

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1. INTRODUCTION

Calibration fields are essential to keep measurement quality assurance of radiation measuring instruments for radiation protection purposes. The Japan Atomic Energy Research Institute (JAERI) has a calibration facility, named the Facility of Radiation Standards (FRS), and an annex is now under construction. In this annex, we have been constructing monoenergetic and spectrum-changeable neutron calibration fields using a 4MV Pelletron (Van-de-Graaff) accelerator to implement reliable neutron dosimetry. The monoenergetic field is for type-tests and the spectrum-changeable field, which can simulate the actual neutron spectrum in working places, is for realistic calibration of neutron dosimeters.

Optimization of the design of neutron target and computational estimation of neutron fluence and energy distribution in the calibration field are necessary for providing a high-quality calibration field. For example, in general, neutron emission rate increases with increasing target thickness but energy resolution decreases. It also needs to reduce scattered neutrons from such as structural and cooling materials of the target. Such design and calculation require a computer program to calculate the transport of both charged particles and neutrons produced by nuclear reaction. Although many transport calculation programs exist independently for charged particles and for neutrons, there is no appropriate program for the design of accelerator-produced neutron field since nuclear reaction is not included in the programs for charged particles. Therefore, we have developed a program that simulates the transport of charged particles and the neutron production in a target, as well as the transport of neutrons. This paper describes an overview of the developed Monte Carlo program and discusses the applicability of the program to calculation of the characteristics of neutron calibration fields.

2. PROGRAM DESCRIPTION

2.1 Outline

We have developed a Monte Carlo computer program, MCNP-ANT (MCNP™ for Accelerator Neutron Target) as an expanded version of MCNP (version 4B), a three-dimensional continuous energy Monte Carlo transport program for neutron, photon and electron(1). A newly developed Monte Carlo subprogram was integrated into MCNP-4B as a source-subroutine for calculating the transport of charged particles and the neutron production. It allows executing a series of the transport calculations of both charged particles and neutrons with a single program. Figure 1 shows an outline of the calculation flow of the program.

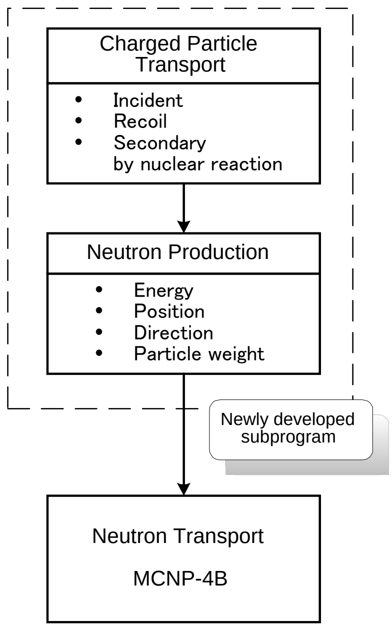

Fig.1 Outline of calculation flow of MCNP-ANT program.

2.2 Charged particle transport and neutron production

The developed Monte Carlo subprogram in MCNP-ANT deals with protons and deuterons up to an energy of 4MeV as incident charged particles. Users can specify the shape and energy distribution of incident beam as an ellipsoid and Gaussian, respectively. The methods of simulating slowing down and scattering of charged particles are based on TRIM(SRIM) (2,3), which is one of the most widely used programs for transport calculation of ions in matter. The data of stopping power coefficients are taken from those in SRIM-98. The subprogram traces the histories of not only the incident and recoil particles from the interaction but also secondary particles resulting from neutron production reactions that could generate neutrons by subsequent nuclear reactions.

Neutrons are generated by nuclear reactions of charged particles with target nuclei. The reactions of $^{2}H(d,n)^{3}He$, $^{3}H(d,n)^{4}He$, $^{3}H(p,n)^{3}He$, $^{7}Li(p,n)^{7}Be$ and $^{7}Li(p,n)^{7}Be^{*}$ are available in the subprogram. The differential cross-sections of the reactions and neutron energies as functions of incident particle energies are taken from the data of Liskien and Paulsen (4,5). The direction of a produced neutron is determined so that it is consistent with the angle-differential cross-section at the energy of charged particle. The neutron energy is calculated using the kinematics of the reaction.

In the subprogram, every incident particle produces a neutron with the particle weight corresponding to the cumulative probability of the neutron production along with the history. The position, energy and direction of a generated neutron are calculated and stored in each step in a history, and one of the data is sampled finally. This procedure makes the calculation of neutron production efficient.

The subprogram treats the same three-dimensional geometry and material configuration as MCNP, and thus the input of geometries and material specifications is common to both the subprogram and the main part of MCNP.

2.3 Neutron transport

The transport of produced neutrons is calculated with MCNP-4B. There is no modification in the program files of MCNP. Therefore, users can use all of the features and techniques, such as nuclear data, tallies, output and variance reduction, in the same manner as MCNP, except for the original source cards.

3. CALCULATION

To demonstrate the applicability and reliability of MCNP-ANT, a number of representative calculations have been performed. We selected some cases that calculated results were able to be compared with measurements. Baba *et al*. have reported the monoenergetic neutron calibration fields using $^{2}H(d,n)^{3}He$, $^{3}H(d,n)^{4}He$, $^{3}H(p,n)^{3}He$, $^{7}Li(p,n)^{7}Be$ and $^{45}Sc(p,n)^{45}Ti$ reactions at 4.5MV Dynamitron accelerator facility (6). These data are suitable for the comparison since information on the neutron targets is almost sufficient for calculation and the neutron fluence and spectra were measured precisely, although the data of incident particle energy are not shown in detail. In the comparison, the results are presented for $^{3}H(d,n)^{4}He$ (E_n=15MeV) and $^{7}Li(p,n)^{7}Be$ (E_n=250 and 550keV) sources, hereinafter expressed as d-T and p-Li sources, respectively.

In calculation of the d-T source, deuterons of 0.5MeV were incident on the tritium-loaded titanium (Ti-T) target. This incident energy is equal to the energy per deuteron of molecular beam (D_3^+) of 1.5MeV, which has been actually used in the experiment. The target had a thickness of 2.5mg·cm^{-2} and the Ti/T ratio was assumed to be the maximum value of 1/1.5 because of lack of the data. The Ti-T target was surrounded with a Cu cylinder having a thickness of 0.5mm. For the p-Li source, protons of 2.03 and 2.29MeV bombarded a LiF target with a thickness of 0.2mg·cm^{-2}. These incident energies were determined from the reaction data of Liskien and Paulsen, mentioned above. A Pt disk of 0.3mm in thickness was placed as a backing.

In all cases an ion beam with a radius of 10nm was normally incident on the targets since TRIM can treat only a pencil beam. Neutron spectrum and fluence at a distance of 10cm from the target were scored with a spherical track-length estimator, *i.e.* “cell tally” in the term of MCNP, with a radius of 0.5cm.

4. RESULTS AND COMPRISONS

Figures 2 and 3 show the depth distributions of 0.5MeV deuterons in the Ti-T target and of 2.03MeV protons in the LiF+Pt target, respectively, together with the results calculated with TRIM. The shapes of the depth distributions with both programs are in good agreement with each other. The peaks of the MCNP-ANT results slightly shift to shallower side compared with those of TRIM. This is because MCNP-ANT treats the upper energy in energy struggling more rigorously than TRIM.

Figure 4 illustrates the distribution of the positions where d-T neutrons were produced in the Ti-T target. It was found that the positions of neutron production spread out in lateral direction as increasing the depth of penetration.

Table 1 shows the calculated neutron fluence at 10cm from the d-T and p-Li sources in comparison with the typical values listed in the reference (6). The calculated values agree with the measured results within ±50% even though the calculations employed quite a simple geometrical model of the target structure. Figures 5 and 6 illustrate the calculated neutron spectra at 10cm from the target for d-T (E_d=0.5MeV) and p-Li (E_p=2.29MeV) reactions, respectively. The measured spectra by the time-of-flight (TOF) technique are included in the figures for comparison. The peak and shape of the spectra are rather different in both cases. For the d-T source, the peak energy of MCNP-ANT result is just 15MeV while the measured one is about 16MeV. This is probably caused by the difference in the incident energy used in the calculation and that in the measurement. It should be studied whether the molecular beam (D_3^+), which was actually used, is different in behavior in the target from D^+ beam. For the p-Li reactions, the peak energy of the measured spectrum is also slightly higher than 0.55MeV. The neutron energy produced by the p-Li reaction is quite sensitive to incident proton energy. Therefore, further comparison requires the detailed information about the incident proton energy in the measurements. The peak widths in the calculations are narrower than those in the TOF measurements. This is because, as pointed out by Baba *et al.*, the time resolution of the TOF measurements affects the measured spectra. The widths of energy spread calculated with MCNP-ANT were approximately agreed with the tabulated values of the reference, as shown in Table 1. It is found in Fig.5 that low energy contaminant neutrons via parasitic reactions, such as D(d,n), C(d,n) and O(d,n) reactions, are not shown in the calculated spectrum. The present version of MCNP-ANT does not treat such reactions due to lack of the cross-section data. But the program has been upgrading so that such contaminant neutrons can be calculated successfully.

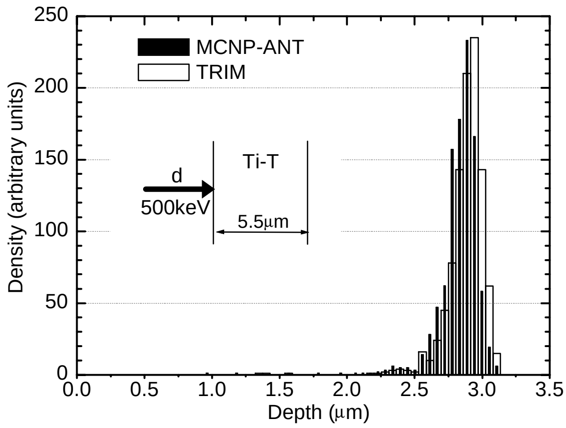

Fig.2 Comparison of depth distribution of 0.5MeV deuterons in Ti-T target between MCNP-ANT and TRIM.

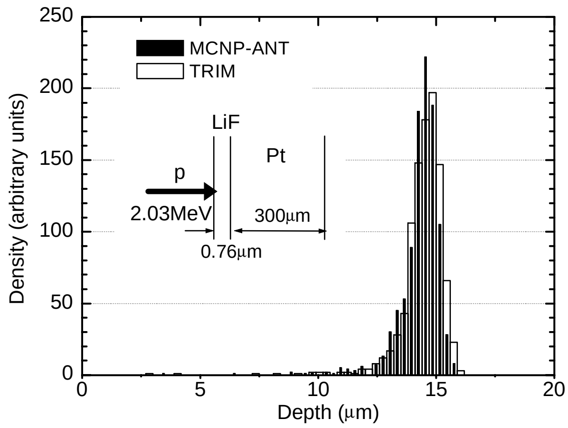

Fig.3 Comparison of depth distribution of 2.03MeV protons in LiF+Pt target between MCNP-ANT and TRIM.

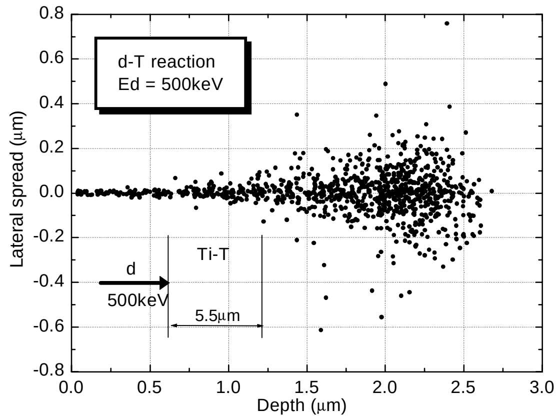

Fig.4 Distribution of the position where d-T neutrons were produced in Ti-T target, calculated with MCNP-ANT. (Incident beam size: 20nmϕ)

Table 1 Comparison of energy spread and neutron fluence for monoenergetic neutron sources between calculated with MCNP-ANT and measured by Baba *et al.*

Source reaction	Target/ Backing	Neutron energy	Energy spread		Neutron fluence at 10cm ($cm^{-2}\cdot\mu C^{-1}$)	
			MCNP-ANT	Baba *et al.*	MCNP-ANT	Baba *et al.*
$^3H(d, n)^4He$	Ti-T / Cu	15 MeV	400 keV	~500 keV	1.4×10^5	8.0×10^4
$^7Li(p, n)^7Be$	LiF / Pt	550 keV	55 keV	~50 keV	2.5×10^4	3.2×10^4
$^7Li(p, n)^7Be$	LiF / Pt	250 keV	60 keV	~50 keV	6.5×10^3	1.0×10^4

5. SUMMARY

A Monte Carlo program, MCNP-ANT, has been developed to simulate the transport of charged particles and the neutron production in an accelerator neutron target, in addition to the transport of neutrons. In the program, the newly developed Monte Carlo subprogram was integrated into MCNP-4B to calculate the transport of charged particles and the neutron production. The results of the calculations for typical monoenergetic neutron calibration fields indicate generally good agreement with the experimental ones. It is necessary to improve the program so that contaminant neutrons can be treated, which stem from such reactions that the incoming charged particles with matter other than the intended target isotope. The program will promote the construction of high-quality neutron calibration fields using an accelerator.

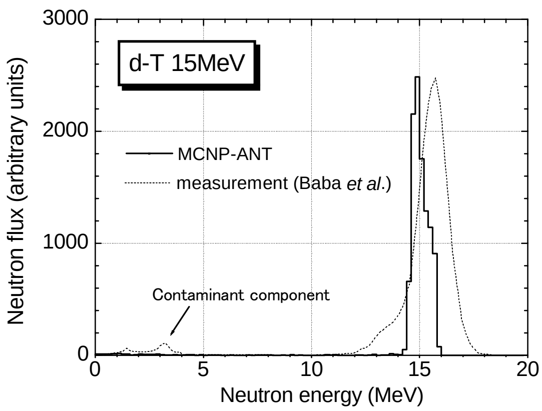

Fig.5 Comparison of neutron spectra of d-T source between calculated with MCNP-ANT and measured by TOF technique (6).

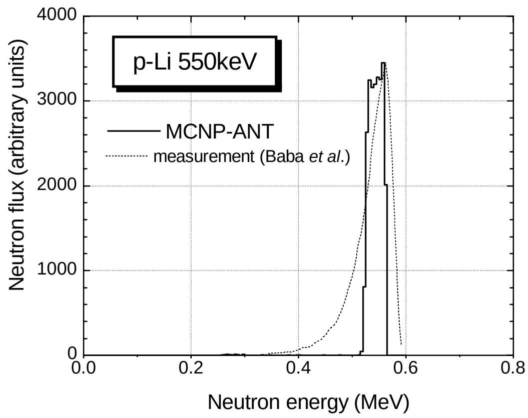

Fig.6 Comparison of neutron spectra of p-Li source between calculated with MCNP-ANT and measured by TOF technique (6).

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