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Evaluation of $D(d,n)^3He$ reaction neutron source models for BNCT irradiation system design

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Abstract A mathematical method was developed to calculate the yield, energy spectrum and angular distribution of neutrons from $D(d,n)^3He$ (D-D) reaction in a thick deuterium-titanium target for incident deuterons in energies lower than 1.0MeV. The data of energy spectrum and angular distribution were applied to set up the neutron source model for the beam-shaping-assembly (BSA) design of Boron-Neutron-Capture-Therapy (BNCT) using MCNP-4C code. Three cases of D-D neutron source corresponding to incident deuteron energy of 1000, 400 and 150 keV were investigated. The neutron beam characteristics were compared with the model of a 2.45 MeV mono-energetic and isotropic neutron source using an example BSA designed for BNCT irradiation. The results show significant differences in the neutron beam characteristics, particularly the fast neutron component and fast neutron dose in air, between the non-isotropic neutron source model and the 2.5 MeV mono-energetic and isotropic neutron source model.

Key words $D(d,n)^3He$ reaction neutron source, Neutron energy spectrum, Neutron angular distribution, Neutron beam characteristics in air, BNCT

CLC numbers O571.52, O571.53

1 Introduction

An accelerator neutron source based on $^3H(d,n)^4He$ (D-T) or $^2H(d,n)^3He$ (D-D) fusion reactions is advantageous in its relative higher neutron yield achieved with a lower energy and higher current deuteron beam, which can be produced with a small accelerator. In recent years, compact neutron generators based on the D-T and (D-D) fusion reactions have been widely investigated for boron-neutron-capture therapy (BNCT).[1,2] The application of D-T neutron generators, however is hindered because of the cost and safety concerns regarding tritium, though the D-T reaction yields much more neutrons (approximately two orders of magnitude) than the D-D reaction. Therefore, for developing a BNCT facility of longer target lifetime and better manageability, this feasibility study uses accelerator neutron source based on D-D reaction and focuses on a compact neutron generator and beam-shaping-assembly (BSA) design.

In previous investigations concerning the BSA design for BNCT, D-D neutron source was generally assumed to generate mono-energetic 2.45 MeV neutrons emitted isotropically[3,4]. A D-D neutron source, however, has a distinct angular distribution and intrinsic energy distribution. In order to perform more accurate estimations in relation to the BSA design and dose simulation for BNCT based on a D-D accelerator neutron source, a better modeling of D-D neutron source based on the neutron energy spectrum and the angular distribution should be required. In this paper, a calculation method and a computer program were developed for computing the yield, energy spectrum and angular distribution of neutrons generated by the D-D reaction for thick TiD*x* target. The neutron source data proposed in this study were applied to design the BSA for BNCT using MCNP-4C code[5]. An example BSA was presented. In-air neutron beam parameters at the

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exit window of this example BSA were calculated for three D-D neutron source cases corresponding to incident deuteron beams of 1000, 400 and 150 keV, and a 2.45 MeV mono-energetic and isotropic neutron source. The results were compared to evaluate the previous model of 2.45 MeV mono-energetic and isotropic neutron source.

2 Methods

2.1 Methods for calculating neutron energy spectrum and angular distribution

For a D-D neutron source using a thick target, the differential neutron yield is derived from

$$\frac{\mathrm{d}Y}{\mathrm{d}\Omega}(\theta,E_\mathrm{d}') = \int_{E_{\mathrm{d}0}}^{0} I_0 N_\mathrm{d}\sigma(\theta,E_\mathrm{d})\frac{1}{S(E_\mathrm{d})}\mathrm{d}E_\mathrm{d} \tag{1}$$

where θ is the neutron emission angle, E_d' the incident deuteron energy, I_0 the intensity of incident deuteron ion beam, N_d the atomic density of deuterium in the target, $\sigma(\theta,E_\mathrm{d})$ the differential cross section of D(d,n)^{3}He reaction, E_d the deuteron energy in the target, and $S(E_\mathrm{d})$ the stopping power of deuteron in the target. The neutron energy of the D(d,n)^{3}He reaction is determined by the Q-value equation

$$E_\mathrm{n}(\theta,E_\mathrm{d}) = \left\{\frac{\sqrt{2E_\mathrm{d}}}{4}\cos\theta + \left[\left(\frac{1}{4}+\frac{1}{8}\cos^2\theta\right)E_\mathrm{d} + \frac{3}{4}Q\right]^{\frac{1}{2}}\right\}^2 \tag{2}$$

where E_n and Q are the neutron energy and the Q-value of D(d,n)^{3}He reaction, respectively.

In order to calculate the differential neutron yield, the thick target is divided into very thin layers with the differential neutron yield in each thin layer given by

$$\frac{\mathrm{d}Y_j}{\mathrm{d}\Omega}(\theta,E_{\mathrm{d},j}) = I_0 N_\mathrm{d}\sigma(\theta,E_{\mathrm{d},j})\frac{1}{S(E_{\mathrm{d},j})}\Delta E_{\mathrm{d},j} \tag{3}$$

where j is the index corresponding to each thin layer, $E_{\mathrm{d},j}$ is the deuteron energy impinging the j-th layer, $\triangle E_{\mathrm{d},j}$ is the energy loss of the deuteron in the j-th layer, and the other variables are defined the same as those in Eqs.(1) and (2). For a very thin target layer, $E_{\mathrm{d},j}$ can be regarded as the deuteron energy at the front interface of the j-th layer. If $E_{\mathrm{d},0} = E_\mathrm{d}'$ and $\triangle E_{\mathrm{d},0} = 0$, $E_{\mathrm{d},j}$ and $\triangle E_{\mathrm{d},j}$ can be computed with the following recursion formulas

$$E_{\mathrm{d},j} = E_{\mathrm{d},j-1} - \Delta E_{\mathrm{d},j-1} \tag{4}$$

$$\Delta E_{\mathrm{d},j-1} = S(E_{\mathrm{d},j-1})\cdot\Delta x_{j-1} \tag{5}$$

where $\triangle x_{j-1}$ is the thickness of the (j-1)-th layer. $E_{\mathrm{n},j}$ of the neutron produced in the j-th layer is related to the deuteron energy $E_{\mathrm{d},j}$ and the neutron emission angle θ by Eq.(2).

The differential yields and energies of neutrons produced in each thin layer are computed using Eqs.(2), (3), (4) and (5), and the calculation terminates when $E_{\mathrm{d},j} \leq 0$. The distribution data of $\mathrm{d}Y_j/\mathrm{d}\Omega$ as a function of $E_{\mathrm{n},j}$ and θ are then obtained. The total differential neutron yield in each θ emission direction, that is, the neutron angular distribution data for the thick target, is computed by

$$\frac{\mathrm{d}Y}{\mathrm{d}\Omega}(\theta) = \sum_j \frac{\mathrm{d}Y_j}{\mathrm{d}\Omega}(\theta,E_{\mathrm{d},j}) \tag{6}$$

and the corresponding neutron angular yield is obtained from

$$\frac{\mathrm{d}Y}{\mathrm{d}\theta}(\theta) = 2\pi\sin\theta\frac{\mathrm{d}Y}{\mathrm{d}\Omega}(\theta) \tag{7}$$

If $E_{\mathrm{n},j}(\theta)$ and $E_{\mathrm{n},j+1}(\theta)$, emitted both in the θ direction, is the energy of neutron produced in the j-th and in the (j+1)-th layer respectively, the energy difference of these neutrons is

$$\Delta E_{\mathrm{n},j}(\theta) = |E_{\mathrm{n},j}(\theta) - E_{\mathrm{n},j+1}(\theta)| \tag{8}$$

and the energy spectrum in the $\triangle E_{\mathrm{n},j}(\theta)$ energy interval is given by

$$\frac{\mathrm{d}Y_j}{\mathrm{d}\Omega\mathrm{d}E_\mathrm{n}}(\theta,E_{\mathrm{n},j}) = \frac{\frac{\mathrm{d}Y_j}{\mathrm{d}\Omega}(\theta,E_{\mathrm{d},j})}{\Delta E_{\mathrm{n},j}} \tag{9}$$

where $\mathrm{d}Y_{\mathrm{n},j}/\mathrm{d}\Omega$ is the total differential neutron yield in the $\triangle E_{\mathrm{n},j}(\theta)$ energy interval.

This study focused only on neutron production in a thick TiDx target. It was assumed that the atomic ratio of deuterium to titanium in the TiDx target was 1.5 and homogenous throughout the target. The number of incident deuterons in the target was considered constant within the deuteron mean path length, and only the incident deuterons in energies of 1000 keV and lower were investigated. The differential cross section data of the D(d,n)^{3}He reaction recommended by Liskien et al.[6] and the stopping power obtained from SRIM-2003 code[7] were used.

For this calculation method, sufficiently accurate results can be obtained as long as the layers are thin enough. A computer simulation program based on the above calculation model was developed. The program can estimate the yields, energy spectrum and angular distribution of the neutrons generated by the $D(d,n)^3He$ reaction in a thick TiD*x* target.

2.2 The example BSA for BNCT

In order to evaluate the differences between the new D-D neutron source data proposed in this study and the previous model of 2.45 MeV mono-energetic/ isotropic neutron source in the BSA design for BNCT, an example BSA for BNCT is employed. Configuration of the example BSA is shown in Fig.1. The BSA is a cylindrical assembly consisting of a moderator, a reflector and a delimiter. The moderator is composed of a 10 cm layer of tungsten alloy (75%W/25%Fe) and a 40 cm layer of 40%Al/69% AlF_3. Maximum diameter of the moderator is 60 cm. The moderator is surrounded by a 20 cm lead layer as side-reflector and a 35 cm lead back-reflector. A 9 cm-thick lithiated polyethylene and a 1cm-thick lead are used as delimiters. The neutron beam channel is a cone with *Φ*20 cm entrance and *Φ*12 cm exit. A 1 cm bismuth layer is placed at the exit of neutron beam channel to decrease the photon dose.

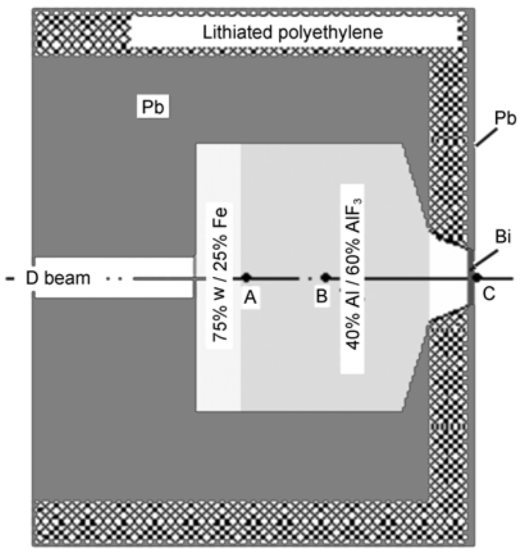

Fig.1 The configuration of the BSA.

3 Results and discussion

Three examples on the neutron energy spectrum from the D-D neutron source corresponding to 1000, 400 and 150 keV deuterons incident are shown in Fig.2, which indicates that the neutron energy spectrum from a D-D neutron source with a thick TiD_x target is closely dependent on the incident deuteron energy, and the neutron energy spectra in different directions differ from each other. The maximum and minimum energy neutrons are emitted in 0° and 180° directions, respectively, with their magnitudes being dependent on the incident deuteron energy. The maximum neutron energy is about 4.14, 3.37 and 2.96 MeV, and the minimum neutron energy is about 1.76, 1.93 and 2.09 MeV, for the D-D neutron sources corresponding to 1000, 400 and 150 keV incident deuteron energies, respectively. Fig.3 shows the neutron angular distributions of D-D neutron source with different incident deuteron energies.

The neutron energy spectrum and the neutron angular distribution are the relative distribution of differential neutron yields. The uncertainty in the differential neutron yield is mainly derived from the stopping power data of deuteron in the TiD*x* target. Averagely, the SRIM-2003 data of stopping power is about 18.8 keV/μm larger than the experimental data presented by Malbrough *et al* [8]. It is roughly estimated that the neutron yields computed using SRIM-2003 stopping power data are averagely 15% lower than those using the stopping power data in Ref.[8]. If Malbrough's stopping power data are regarded as the benchmark data, the relative error of the neutron energy spectrum and angular distribution will be less than 15% because they are only the relative distribution of the differential neutron yields.

The neutron transport simulation in the example BSA shown in Fig.1 was carried out using MCNP-4C with D-D neutrons of 1000, 400 and 150 keV and with a 2.45 MeV mono-energetic and isotropic neutron source (named as Case 1, 2, 3 and 4, respectively). The four neutron sources were modeled as a circular surface source with a 5 cm diameter in MCNP simulation. A cylindrical cell tally in *Φ*12 cm×0.5cm and a circular surface tally of *Φ*12 cm were respectively positioned at 0.5 cm from the exit window to record the average neutron flux, the average photon flux and the average neutron current of the neutron beam.

The simulation results on the neutron flux as a function of the neutron energy at the exit window of the BSA for the four neutron sources are shown in Fig.4. It indicates that the neutrons from the four sources can be moderated as the desired neutron beam for BNCT. In order to find detailed difference of the neutron beams at exit window of the example BSA for the four source cases, we calculated the thermal neutron flux Φ_{th} ($E_n \leq 1.0\times10^{-6}$ MeV), epithermal neutron flux Φ_{epi} (1×10^{-6}MeV$<E_n\leq2.0\times10^{-2}$ MeV), fast neutron flux Φ_{fast} ($E_n>2.0\times10^{-2}$ MeV), the ratio of the fast neutron physical dose in air to the epithermal neutron flux D_{fast}/Φ_{epi}, the ratio of the gamma physical dose in air to the epithermal neutron flux D_γ/Φ_{epi}, and the ratio of the neutron current to the neutron flux J/Φ. The neutron kerma factors and photon mass energy absorption coefficients of air from ICRU-44[9] were used in calculating the neutron and photon doses. The neutron beam parameters of the four sources are presented in Table 1.

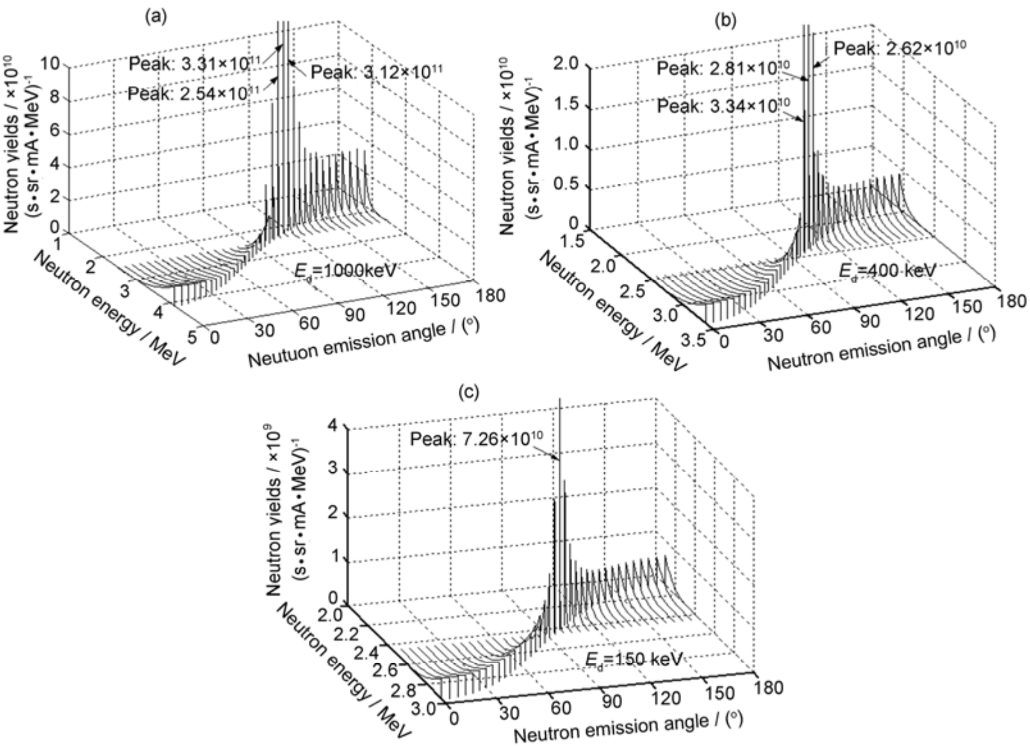

Fig.2 The neutron energy spectra of the D-D neutron source with various incident deuteron energies and the $TiD_{1.5}$ thick target. (a) 1000 keV incident deuteron energy; (b) 400 keV incident deuteron energy; (c) 150 keV incident deuteron energy.

Table 1 Neutron beam parameters at the exit window of the BSA for different source cases

Neutron sources	Φ_{th}	Φ_{epi}	Φ_{fast}	D_{fast}/Φ_{epi}	D_γ/Φ_{epi}	J/Φ
	/10^{-6} cm^{-2} per source neutron			/10^{-13} Gy•cm^2 per source neutron		
Case 1 (1000keV incident deuteron)	0.344 (1.08)#	18.3 (1.08)	1.71 (1.32)	1.47 (1.60)	1.69 (1.09)	0.721
Case 2 (400keV incident deuteron)	0.341 (1.07)	17.8 (1.05)	1.51 (1.16)	1.20 (1.30)	1.64 (1.06)	0.722
Case 3 (150 keV incident deuteron)	0.330 (1.03)	17.6 (1.04)	1.44 (1.11)	1.06 (1.15)	1.61 (1.04)	0.721
Case 4 (2.45MeV mono-energetic/ isotopic source model)	0.320 (1.00)	16.9 (1.00)	1.30 (1.00)	0.92 (1.00)	1.55 (1.00)	0.723

Values in parenthesis indicate the values relative to Case 4

Large differences in Φ_{fast} and D_{fast}/Φ_{epi} were found among the four cases. Respectively, the fast neutron flux of Cases 1, 2 and 3 were 1.32, 1.16 and 1.11 times larger than that of Case 4, while the D_{fast}/Φ_{epi} of Cases 1, 2 and 3 were 1.60, 1.30 and 1.15 times larger than that of Case 4. These suggest that the use of 2.45 MeV mono-energetic and isotropic source mode in the design of the BSA for BNCT might lead to choosing inadequate thick moderator, which will result in high fast neutron component in the neutron beam.

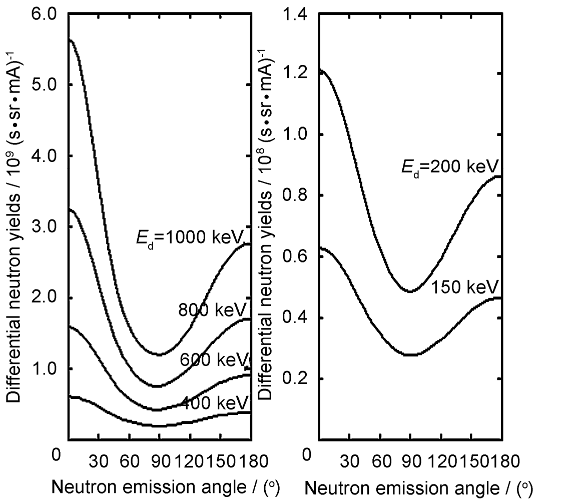

Fig.3 Neutron angular distributions of D-D neutron source for $TiD_{1.5}$ thick target.

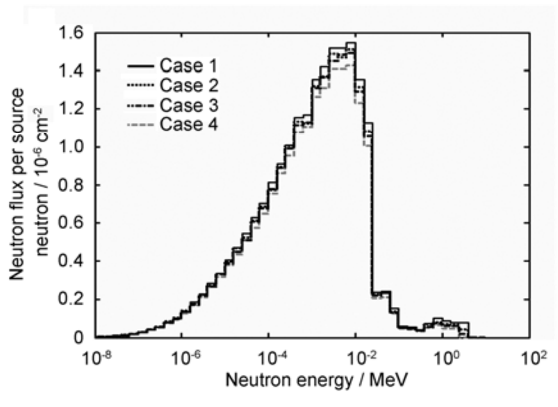

Fig.4 Neutron flux as a function of the neutron energy at the exit window of BSA.

The neutron beam parameters listed in Table 1 also show that respective Φ_{th}, Φ_{epi} and D_r/Φ_{epi} of the four neutron sources have relatively similar values. For example, Φ_{th}, Φ_{epi} and D_γ/Φ_{epi} of Case 1 are only 1.08, 1.08 and 1.09 times larger than that of Case 4, while Φ_{th}, Φ_{epi} and D_γ/Φ_{epi} of Case 3 is only 1.03, 1.04 and 1.04 times larger than that of Case 4. These results imply that 2.45 MeV mono-energetic and isotropic source model can generate similar neutron beam parameters except the fast neutron flux and the fast neutron dose.

4 Conclusion

A mathematical model for computing the yield, energy spectra and angular distribution of neutrons generated by D(d,n)^{3}He reaction in a thick deuterium-titanium target were developed for incident deuterons in energies of lower than 1.0 MeV. Available deuteron cross-section data and stopping power data derived from the SRIM-2003 code were combined to model the neutron production in an accelerator-based D(d,n)^{3}He neutron source.

In air neutron beam parameters at the exit window of an example BSA for BNCT were calculated for three cases of D-D neutron source and a 2.45 MeV mono-energetic and isotropic neutron source. The results indicate that significant calculation deviation on the fast neutron flux and fast neutron dose may be caused if the approximate model with 2.45 MeV mono- energetic and isotropic neutron emission is only applied to design the BSA based on D-D neutron source for BNCT irradiation. The neutron source model based on the neutron energy spectrum and angular distribution data should be applied to replace the previous model of the 2.45 MeV mono-energetic and isotropic neutron source to perform more accurately the BSA design and dose calculation for BNCT.

In this study, we only use the neutron beam parameters at exit window of the BSA to evaluate the D-D neutron source models. Although it is a convenient way, the neutron beam parameters do not directly provide any information on the dose profile in tissue. Further investigations on dose calculation in tissue should be performed to obtain more accurate evaluation result.

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