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Technical Note

A model of the 14 MeV neutrons source term, for numerical solution of the transport equation to be used in BNCT simulation

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ABSTRACT

The use of neutron generators has been growing with the development of Neutron Capture Therapies (NCTs), mainly in Boron Neutron Capture Therapy (BNCT). In the absence of nuclear reactors in Brazil the neutron generators plays an important role for medical application. So the neutron transport calculation and neutron generators experiment analysis is very important to implement BNCT in Brazil. The aim of this work was to develop a method of calculating the 14 MeV neutron angular and energetic distribution for the *D–T* reaction in realistic conditions to compare with experimental data produced in our Neutron Generator Laboratory. The angular and energetic spectrum is obtained in a format as input for the discrete ordinates method used to solve the neutron transport equations, ANISN, DORT and TORT are the codes that will be used for this purpose.

1. Introduction

The neutron spectrum and angular distribution are basic quantities to understand the transport of neutrons in heterogenous materials and deep penetration problems such as in the Neutron Capture Therapies (NCTs) design, in special for us the Boron Neutron Capture Therapy (BNCT) (Barth, 2003; Barth et al., 2005).

The "BNCT-UNIFRA/UFSM Project" (Orengo et al., 2004, 2005) will establish the BNCT in the south region of Brazil. This project is developed by two universities: the Federal University of Santa Maria (UFSM) and Franciscan University (UNIFRA).

In the next experimental stage of the BNCT Project, based on *D–T* reaction, various materials (Anderson, 1976; Lou, 2003; Martín and Abrahantes, 2004) will be tested both for attenuation and collimate neutrons. Also the energy deposition and radiation damage to human tissues will be obtained through calculation of neutrons and associated photons transport.

In this context, experiments with neutron generators play a important role (Blue and Yanch, 2003; Martín and Abrahantes, 2004; Cerullo et al., 2004; Allen et al., 1999; Giusti, 2004). The neutron generators yielding 14 MeV neutrons will be tested in the BNCT Project. To study 14 MeV neutron transport in benchmark experiments (Nakamura et al., 1983; Oyama et al., 1993) an external neutron source is used, the *D–T* reaction, the same that probably will be used in the first tests in the BNCT Project and that currently takes place in particle accelerators. In this work this kind of experiment has been adapted to the neutron generator of the UFSM, where the deuterons have 120 keV as maximum kinetic energy impacting on a *TiT* target yielding 14 MeV neutrons from the *D–T* reaction. Based on this reaction we developed a theoretical model to simulate the neutron source term as input data for solution of the neutron transport equation, such as ANISN (Engle, 1967), DORT-TORT (DORT-TORT, 1980), and in the future also to GEANT4 Monte Carlo code (GEANT4, 2007).

2. The theory

2.1. The neutron angular and energetic distribution for the D–T reaction

In the *D–T* reaction,

$$ {}^{3}_{1}\mathrm{H} + {}^{2}_{1}\mathrm{H} \quad \rightarrow \quad {}^{4}_{2}\mathrm{He} + n + Q, \tag{1}$$

the Q value is ≅17,570 MeV. The neutron energy is function both of the deuteron energy and neutron emission angle relative to the direction of the incident deuteron. The neutron angular and energetic distribution also depends of the kinematic and differential cross section for this reaction.

Considering a deuteron beam bombarding a *TiT* target, the probability (dP) for one deuteron of energy E to react, while traveling a distance dx in a target containing N_t atoms of tritium/cm^3, is given by:

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$$dP(E,\psi) = N_t \frac{\sigma(E,\psi)dE}{\left(\frac{dE}{dx}\right)} W, \tag{2}$$

where $\sigma(E,\psi)$ is the microscopic cross section for the D–T reaction as function of the deuteron energy and angle ψ for the neutron produced; (dE/dx) is the stopping power for deuterons in the target material and, W is an angular distribution function that supplies the multiple scattering contribution of the deuteron within target.

To obtain an effective expression to compute the neutron angular and energetic distribution it is necessary to study which model is more suitable for each element of the Eq. (2), $\sigma(E,\psi)$, W and (dE/dx).

2.2. The D–T cross section calculation

For deuteron energy less than 300 keV, the center-of-mass cross section is known to be isotropic (Benveniste et al., 1960; Argo et al., 1952). Therefore, the value of $\sigma(E,\psi)$ can be calculated from some reported values (Fewell, 1968; Conner et al., 1952; Argo et al., 1952) of $\sigma(E)$ and through the analysis of the interaction between deuteron and tritium. The resultant expression for $\sigma(E,\psi)$ will be given by:

$$\sigma(E,\psi) = \frac{\sigma(E)}{4\pi} \frac{(\gamma^2 + 2\gamma\cos\theta + 1)^{\frac{3}{2}}}{(1+\gamma\cos\theta)} \tag{3}$$

where the available values for $\sigma(E)$ are in barns. The relation between the laboratory scattering angle (ψ) and center-of-mass angle (θ), is given by:

$$\cos\psi = \frac{\gamma + \cos\theta}{\sqrt{\gamma^2 + 2\gamma\cos\theta + 1}},$$

with

$$\gamma = \sqrt{\frac{M_n M_D}{M_\alpha M_T}\left(\frac{M_n + M_\alpha}{M_D + M_T}\right)\frac{E}{E + Q\left(1 + \frac{M_D}{M_T}\right)}},$$

where M_n, M_D, M_α and M_T are, respectively, mass of neutron, deuteron, alpha particle and tritium.

2.3. The angular distribution function W

The distribution of deuterons after multiple scattering is simulated by the function $W(\eta|z)$, reported by Snyder and Scott (Poss et al., 1952) with the approximation for small scattering angles ($\sin\theta \approx \theta, \cos\theta \approx 1$). $W(\eta|z)$ is the angular distribution function for the projected angle η between the initial particle direction and the particle direction at the end of the track for various values of z (z = distance traversed by a particle in units of the mean free path, λ, for a single scattering).

The function $W(\eta|z)$ is approximated by the following angular distribution function (Poss et al., 1952) used to represent the deuteron multiple scattering on the *TiT* target:

$$W(\eta|z) = b^{\frac{1}{2}} - b\eta(E), \tag{4}$$

where $\eta(E)$ is the angle η between the initial particle direction and the particle direction at the end of the track for various values of z, and b is an experimental parameter. The linear approach for $W(\eta|z)$ has the effect to cut the tail and increase the width of the distribution. The parameters b and $\eta(E)$, linearly approximated (Poss et al., 1952), to be used in this work are:

$$b = 9.33 \quad \text{and} \quad \eta(E) = 0.002790909E - 0.01020522.$$

2.4. A stopping power model

Targets used for the D–T reaction are generally made of a copper metalic plate in which a fine layer of titanium is deposited as a sponge form where the tritium is ocluded.

The deuterons kinetic energy is lost in a continuous process by successive collisions of the D^+ ion with the target material. This loss of energy is described by the stopping power function (dE/dx).

The difficulty to obtain experimental values of the dE/dx for *TiT* target, led us to consider the use of the Bragg–Kleeman law (Knoll, 1989; Marmier and Sheldon, 1985), which asserts that the lost energy by a particle in a compound material is the sum of the losses for each compound separately. For the *TiT* target this approximation can be written by (Benveniste et al., 1960):

$$\left(\frac{dE}{dx}\right)_{TiT_N} = \frac{48}{48+3N}\left(\frac{dE}{dx}\right)_{Ti} + \frac{3N}{48+3N}\left(\frac{dE}{dx}\right)_{T}, \tag{5}$$

where N is the average number of the atoms of tritium per atom of titanium, and $\left(\frac{dE}{dx}\right)_{Ti}$ is the stopping power of the deuteron in titanium, and $\left(\frac{dE}{dx}\right)_{T}$ is the stopping power of the deuteron in tritium.

Normally, N varies between 1.0 and 1.8, given the lack of a better value $N = 1.75$ was adopted. N is actually variable with the target lifetime and therefore this calculation should be periodically repeated. The stopping power value both for titanium and tritium were obtained from the literature in the range from 10 to 200 keV (Fewell, 1968).

3. A general expression for the neutrons distribution

The TiT_N target was considered thick enough to stop all incident deuterons, therefore the probability of the D–T reaction to occur, is finite, for energy values between 0 and the maximum value for the deuteron energy, E_D. Using the models described above, for $\sigma(E)$, W and (dE/dx), a general expression for Eq. (2) is obtained to represent the neutron angular and energetic distribution:

$$dP(E,\psi) = dE\,d\Omega(\psi)\frac{N_t}{\left(\frac{dE}{dx}\right)_{TiT_N}} \frac{\sigma(E)}{4\pi} \frac{(\gamma^2 + 2\gamma\cos\theta + 1)^{\frac{3}{2}}}{(1+\gamma\cos\theta)} W(\eta|z), \tag{6}$$

where the relation between θ and ψ is given by:

$$\theta = \arcsin\{\sin\psi[\gamma\cos\psi + ((1-\gamma^2) + \gamma^2\cos^2\psi)^{\frac{1}{2}}]\}.$$

The expression for the neutron energy is obtained through the kinetics of the D–T reaction:

$$E_n = \frac{M_D M_n}{(M_D + M_T)^2}\left(\cos\psi + \frac{\sqrt{1-\gamma^2\sin^2\psi}}{\gamma}\right)E. \tag{7}$$

The probability of one neutron to be emitted between ψ_1 and ψ_2 angles, with energy between E_1 and E_2, due to the reaction of one deuteron, with energy E_D, in a thick TiT_N target is given by:

$$P(\psi_1 - \psi_2, E_1 - E_2) = \frac{N_t}{2}\int_{\psi_1}^{\psi_2} \sin\psi \int_{E_b}^{E_s} \frac{\sigma(E)}{\left(\frac{dE}{dx}\right)_{TiT_N}} \times \frac{(\gamma^2 + 2\gamma\cos\theta + 1)^{\frac{3}{2}}}{(1+\gamma\cos\theta)} W(\eta|z)\,dE\,d\psi, \tag{8}$$

where $d\Omega(\psi) = 2\pi\sin\psi d\psi$, and the intervals E_b e E_s is the energy interval for the deuterons, within of the intervals of angle and energy considered.

4. Results

The integration in Eq. (8) is performed by numerical methods for different energy and angular intervals using the code FONTEN (Orengo, 1997) for this purpose. To test the efficiency and stability of this code two well known results (Coelho, 1985; Santoro et al., 1981) were used, comparing the neutron angular distribution for the same angular interval and the neutron energy dependence with the laboratory angle ψ.