CONY - Computer code for Neutron Yield calculations: The 7Li(p,n)7Be and 3H(d,n)4He reactions.

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CONY - Computer code for Neutron Yield calculations: The ^{7}Li(p,n)^{7}Be and ^{3}H(d,n)^{4}He reactions.

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Abstract

The neutron beam facility at NCSR "Demokritos" is driven by a 5.5 MV tandem T11/25 Van De Graff accelerator that provides continuous, high intensity ion beams. Depending on the neutron production reaction, different energy regions of neutron beams are available. Neutron fields with well defined energies are produced by means of nuclear reactions such as: ^{7}Li(p,n)^{7}Be, ^{3}H(p,n)^{3}He, ^{2}H(d,n)^{3}He and ^{3}H(d,n)^{4}He, delivering neutrons up to the energy of ~28 MeV. In order to fully characterize the neutron beam at NCSR "Demokritos", in the framework of the present work, the CONY C++ computer code has been developed. The implementation of the code for the ^{7}Li(p,n)^{7}Be and ^{3}H(d,n)^{4}He reactions is discussed. The method of calculation of differential neutron yields by thin and thick targets is described. Specifically, for the reaction ^{7}Li(p,n)^{7}Be the mathematical singularity at near threshold energies is discussed along with the method that was used as to overcome this issue. Finally, the results of the code including the double differential neutron yields, the neutron beam energy distribution at the sample position and the total neutron yields have been compared with experimental data as well as with the results of the NeuSDesc software (JRC-IRMM: Neutron Source Description).

Keywords Neutron production, Double differential yield, Tit Target

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INTRODUCTION

Two body reactions are a convenient and powerful way to produce monoenergetic neutrons. Neutron beams are used for a wide range of applications not only in Nuclear Physics and Astrophysics, but also in nuclear technology, medicine and industry.

In general, the neutron beam characterization can be realized in two ways:
a) Experimentally, by means of Time-Of-Flight measurements where the neutron field is mapped by recording the neutron time of flight (e.g nTOF CERN [1]). The implementation of the TOF technique requires a pulsed accelerator beam with specific pulse characteristics and appropriate flight path dimensions, depending on the neutron beam energies.
b)An alternative way for the neutron beam characterization is computational modeling, of the used nuclear reactions. The modeling of the nuclear reactions can be combined

with Monte Carlo calculations (e.g. GEANT4 [2]) where all the details and structural characteristics of the neutron beam facility can be taken into account.

In case where the accelerator provides only continuous beams the characterization of the neutron field can only be achieved by means of computational techniques. This is the case for the neutron beam facility at NSCR "Demokritos". For these reasons the computer code CONY (COmputer code for Neutron Yield calculations) has been developed towards to accurate characterization of the neutron beam.

The production of monoenergetic or quasi-monoenergetic neutron beams at the 5.5 MV tandem T11/25 Accelerator at the NCSR "Demokritos" is realized by means of different reactions. For low neutron beam energies between 120 and 650 keV neutrons can be produced by the endothermic reaction ^{7}Li(p,n)^{7}Be. Intermediate neutron beam energies are produced by means of the d+d reaction while higher energies between 16 and 28 MeV neutrons are produced via the ^{3}H(d,n)^{4}He reaction by using deuteron beam and TiT target [3].

For the calculation of the neutron beam energy distribution and spatial profile characterization of the beam the reaction kinematics are taken into account, the energy loss of protons or deuterons in the target material [4], the corresponding cross sections as well as the dimensions of the primary target.

These parameters are included into the CONY code that provides three different forms of the results: the differential neutron yields in the form of two-dimensional matrix (angle vs energy), the neutron beam energy distribution at the sample position and the total neutron yields for ^{7}Li(p,n)^{7}Be and ^{3}H(d,n)^{4}He reactions. In the following sections the afore mentioned components of the calculations are described. Furthermore, a mathematical singularity which appears at the calculation of energy distribution and the total neutron yield for ^{7}Li(p,n)^{7}Be reaction, is also discussed.

Neutron Yield Calculations

The ^{7}Li(p,n)^{7}Be reaction

The energy threshold for the ^{7}Li(p,n)^{7}Be is at the energy of 1.88 MeV. The number of neutrons emitted per second into solid angle dΩ by an element dx of the target bombarded by a proton beam, is given by the following equation, where i is the ion beam current, g the number of particles per microAmpere, D the atomic density and the differential cross section in the laboratory frame [5]

$$dN = igD\frac{d\sigma(E_p)}{d\Omega}dxd\Omega x \qquad (1)$$

For a given lab angle $\theta(n)$ and neutron energy E_n the elementary thickness of the target dx that is contributing to the neutron yield for each pair (θ_n, E_n) depends on the

derivative of the proton energy with respect the neutron energy as well as on the inverse stopping power of the protons into the target material. In this way the elementary target thickens dx can be calculated as follows:

$$dx = \frac{dx}{dE_p} \left| \frac{dE_p}{dE_n} \right| dE_n.$$ (2)

Accordingly, the double differential yield is related to the center-of mass system differential (p, n) cross section, the Jacobian solid angle transformation, the inverse of stopping power and the production rate as given by the next equation [6]

$$\frac{d^2 N(E_n, \theta_n)}{dE_n d\Omega} = igD \frac{d\sigma}{d\Omega'} \frac{d\Omega'}{d\Omega} \left[\frac{dE_p}{dx} \right]^{-1} \frac{dE_p}{dE_n}$$ (3)

Near threshold energy kinematics

In order to calculate the differential neutron yield near energy threshold an analytical expression for the Jacobian transformation is employed, introducing the kinematics parameters γ and ξ.

Note that when $E_p \rightarrow E_{th}$ a singularity problem appears for the calculation of the Jacobian transformation [6].

$$\frac{d\Omega'}{d\Omega} = \frac{\pm \gamma}{\xi} \left(cos\theta \pm \xi \right)^2$$ (4)

$$\gamma = \sqrt{\frac{m_p m_n}{m_{Be} \left(m_{Be} + m_n - m_p \right) \left(E_p - E_{th} \right)}}$$ (5)

$$\xi^2 = \frac{1}{\gamma^2} - \sin^2 \theta.$$ (6)

The conversion of the lab angle into the CM angle towards to the calculation of the CM differential cross section is performed according to the equations given below [6]

$$+ \rightarrow \theta' = \theta + \sin^{-1}\left(\gamma sin\theta \right)$$ (7)

$$- \rightarrow \theta' = \pi + \theta - \sin^{-1}\left(\gamma sin\theta \right).$$

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Cross Section Near Threshold

The differential cross section are provided in tabulated form by Liskien and Paulsen [7] where experimental cross sections measurements are combined with theoretical calculations. These CM cross sections are given as Legendre polynomial expansions for the energy range 1.95 to 7.0 MeV

$$\frac{d\sigma_{pn}}{d\Omega'} = \frac{d\sigma_{pn}(0^o)}{d\Omega'} \sum_{i=0}^{i=3} A_i(E_p) P_i(\cos\theta'). \quad (8)$$

The tabulated cross sections data from Liskien and Paulsen do not resolve the problem near the reaction threshold. It is necessary to use an analytical form for the CM differential cross section to determine the actual limits near threshold. Gibbons and Macklin [8] pointed out that the reaction cross section near threshold energy has the form of s-wave broad resonance centered at 1.93 MeV. The theoretical cross section has the following form

$$\frac{d\sigma_{pn}}{d\Omega'} = A \frac{x}{E_p(1+x)^2} \qquad (9)$$

where x is the ratio of the neutron to proton channel widths, that in the narrow energy range has the functional form $x = \Gamma_n / \Gamma_p \rightarrow C_0 \sqrt{1 - E_{th}/E_p}$. The constant C_0 and A (has units of cross section) are determined by Gibbons and Macklin [8].

Now using the definition of γ parameter and a combination of equations (3), (4) and (9) the following expression results. As can be seen in this equation (10) the singularity issue is resolved and the triple product can be calculated analytically.

$$\frac{d\sigma_{pn}}{d\Omega'} \frac{d\Omega'}{d\Omega} \frac{dE_p}{dE_n} = \frac{\pm A C_0 (m_{Be} + m_n)^2 (\cos\theta \pm \xi)\sqrt{m_p m_n / m_{Be}}(m_{Be} + m_n - m_p)}{(1+x)^2 [m_p m_n E_p \xi(\cos\theta \pm \xi) \pm m_{Be}(m_{Be} + m_n - m_p)E_{th}]} .(10)$$

In this way the double differential neutron yield can be calculated analytically even at near threshold energies and all the singularity issues have been removed. Having an analytical expression for the double differential neutron yield the energy distribution of the emitted neutrons for a given angular range can be calculated as follows (equation (11)). On more step of integration with respect the neutron energy and the total number of emitted neutron can also be estimated according to the equation (12).

$$\frac{dN}{dE_n}(E_n) = 2\pi \int_0^{\theta_{max}(Ep_0)} \frac{d^2N}{d\Omega dE_n}(\theta, E_n) \sin\theta d\theta \qquad (11)$$

$$N = 2\pi \int_0^{\theta_{max}} \int_{E_{n,min}}^{E_{n,max}(E_{p0})} \frac{d^2N}{d\Omega dE_n}(\theta, E_n) \sin\theta dE_n d\theta \qquad (12)$$
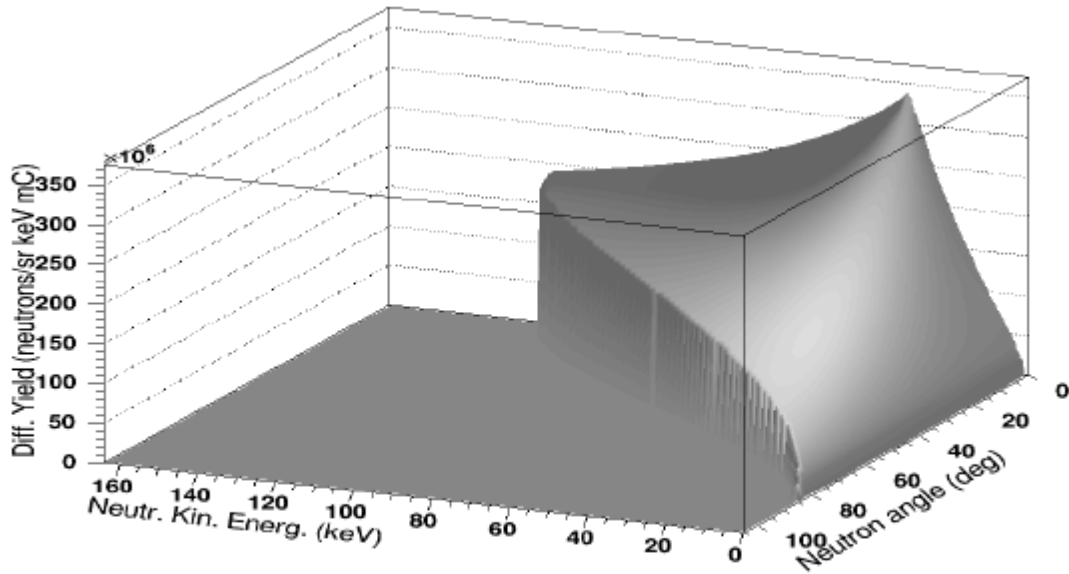

Fig.1. Differential neutron yield for ^{7}Li(p,n)^{7}Be with 7LiF target for 1920 keV protons incident energy on 10μm target thickness.

The ^{3}H(d,n)^{4}He reaction.

The Q-value of the ^{3}H(d,n)^{4}He reaction is 17.589 MeV. At NCSR "Demokritos" neutron beam facility the reaction ^{3}H(d,n)^{4}He is utilized by using a titanium tritide target with tritium atomic ratio (concentration) 1.543 tritium atoms per titanium atom [3]. The computational method of neutron yield for DT reaction is the same as before. The differential cross section is calculated from tabulated data by Liskien and Paulsen and the stopping power from Ziegler and Andersen [4]

$$\frac{d^2N(E_n, \theta_n)}{dE_n d\Omega} = igD \frac{d\sigma}{d\Omega'} \frac{d\Omega'}{d\Omega} \left[\frac{dE_d}{dx}\right]^{-1} \frac{dE_d}{dE_n}. \quad (13)$$

The Jacobian transformation and the neutron emission energy are respectively,

$$\frac{d\Omega'}{d\Omega} = \sqrt{AC} \frac{\sqrt{\frac{D}{B} - \sin^2\theta}}{\frac{E_n}{E_d + Q}} \qquad (14)$$

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$$E_n = (E_d + Q)(B + D + 2\sqrt{AC}\cos\theta) \qquad (15)$$

where A, B, C and D are kinematics parameters depending on the masses and lab emission angle [9].

RESULTS AND DISCUSSION

The CONY Computer code for Neutron Yield calculations has been developed in C++ computer language according to the equations described above. The code provides the double differential neutron yield, the neutron energy distribution and the total neutrons produced by ^{7}Li(p,n)^{7}Be and ^{3}H(d,n)^{4}He reactions. The main input parameters are the incoming ion energy (protons or deuterons), the thickness of the target and the specific geometry. The CONY code also was also compared with the Software NeuSDesc (JRC-IRMM: Neutron Source Description) [10] a well established program which provides a good estimate of the neutron energy spectrum.

Figures 2 and 3 show the neutron flux at near energy threshold and the energy distribution ^{7}Li and ^{7}LiF targets respectively. In Fig. 2 the very good agreement of CONY' s results with experimental data (Time of Flight measurements) from Karlsruhe Institute of Technology (KIT) indicates that CONY is working successfully at near threshold energies.

Also the smooth behavior of the at near threshold energies in Fig.3 (see also Fig.1) depicts the overcoming of the singularity problem. This singularity problem is unresolved in the Software NeuSDesc as can be seen in Fig. 3 [11], [12].
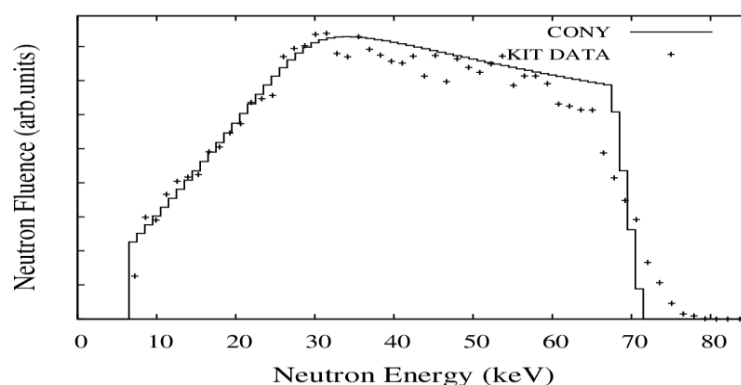

Fig.2.Experimental data from KIT. The neutron production (in arbitrary units) in comparison with CONY for ^{7}Li(p,n)^{7}Be for 1.892 MeV proton energy, thickness of natural lithium 30 μm in thickness according to the detection geometry described in [12].
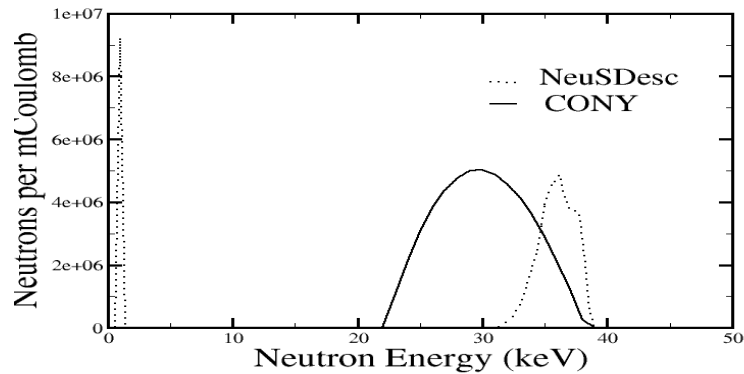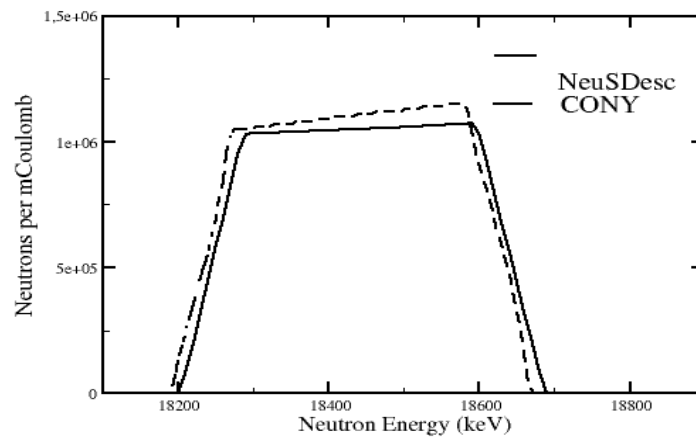
Fig.3. Neutron energy spectra for energy threshold 1.88 Mev, thickness 10μm and maximum emission angle 12 deg.

Finally, an example for energy spectrum by $^3H(d,n)^4He$ reaction and TiT target in comparison with NeuSDesc.

CONCLUSIONS

In the present work the method developed for determining thick and thin targets neutron yields for the $^7Li(p,n)^7Be$ and $^3H(d,n)^4He$ reactions. The singularity problem at near energy threshold has been overcomed by combining the kinematic equations with the parameterization of the CM differential cross section.
The CONY code was validated by comparing the calculated neutron beam energy distribution with the experimental one at different energies as well as by comparing the results of the code with the corresponding ones of the NeusDesc software.

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