Implementation of a new energy-angular distribution of particles emitted by deuteron induced nuclear reaction in transport simulations

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Abstract. MCUNED code is an MCNPX extension able to handle evaluated nuclear data library for light ion transport simulations. In this work the MCUNED code is improved to describe more accurately the neutron emission during deuteron induced nuclear reaction. This code update consists in introducing a new methodology to take into account the angular distribution of neutron produced by deuteron breakup reaction. To carry out this work a new formulation for the angular distribution of neutrons produced by breakup reaction has been proposed. The implementation of this new methodology requires the use of extra parameters which are provided by the nuclear code TALYS and stored in the ENDF file. This new methodology shows significant improvement in comparison with the former treatment of neutron emission kinematics, these results are in good agreement with experimental data.

1. Introduction

The design of high intensity deuteron accelerator facilities like LIPAc [1] or IFMIF/DONES [2] require accurate coupled deuteron-neutron transport simulations to carry out studies related to accelerator radioprotection analysis. The analysis of neutron source induced by deuteron nuclear reaction is also a field where accurate coupled deuteron-neutron transport simulations are required.

The MCUNED [3] code has been developed as an MCNPX extension in order to supply the incapacity of MCNPX to perform deuteron transport simulation using evaluated nuclear data libraries. Exercises dedicated to validate TENDL [4] nuclear data library (the only one available for deuteron for almost all natural isotopes) against experimental results [5], have shown important discrepancy between simulation and experimental results.

These comparisons shown that at high incident deuteron energy, computed angular spectra of produced neutrons were very different from the spectra measured experimentally. Especially, the computed neutron angular distribution did not reproduce the forward peaked distribution observed experimentally. This forward peaked angular distribution is attributed to neutron produced by deuteron breakup reaction during the deuteron-target interaction, and is the principal origin of the discrepancy between experimental and simulated spectra.

In this work we address this problem by implementing a new kinematics proposed by Kalbach [6] to MCUNED, in order to reproduce the angular distribution of the emitted neutrons.

The full implementation of this new kinematics required the evaluation of additional parameters that have been included in the nuclear data library.

The comparison of experimental data with results obtained with this new methodology shows a real improvement of the calculations.

2. Neutron angular distribution in tabulated nuclear data libraries

When deuteron is used as projectile, breakup mechanism has to be taken into account as a new channel for neutron production. The angular distribution of neutrons produced by deuteron breakup is sharply peaked toward forward angles.

In the TENDL deuteron library the energy-angular distribution of the particles produced in nuclear reaction are tabulated using the Kalbach-Mann systematics [7,8]. This systematics reproduces adequately most of the energy-angular distribution of emitted particle, but in the case of the neutron angular distribution produced by deuteron induced nuclear reaction, the Kalbach-Mann systematics is not able to fit the experimental distribution because breakup mechanism is not included in the Kalbach-Mann systematics.

In reference [6], Kalbach proposed a new formulation to reproduce the energy and angular distribution of the neutrons and protons emitted in the deuteron breakup reaction. In this formulation the differential cross sections depending on the emission energy or emission angle have been established.

For the implementation of this new kinematics in MCUNED we assumed that the double differential energy-angular distribution for the particle emission after the

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deuteron breakup is the product of angular and energy differential cross sections. In the implementation only the angular distribution is taken from Kalbach works, while emission energy distribution is provided by TALYS [9] calculations.

2.1. Energy-angular distribution including breakup

A general systematics able to reproduce the energy-angular distribution of inclusive reactions, including breakup reactions, that produce neutron, could be built using both distributions presented above.

The inclusive cross section $\sigma^{incl}(d, Xn)$ is the sum of deuteron breakup cross section $\sigma^{BU}(d, n)$ and all other reaction channels $\sigma^0(d, Xn)$.

The energy-angular double differential cross section of each component is:

$$\sigma^{incl}\left(E, E', \mu\right) = \sigma^0\left(E\right) y_0\left(E\right) f_{KM}\left(E, E', \mu\right)/2\pi$$
$$+\sigma^{BU}\left(E\right) f_{BU}\left(E, E', \mu\right)/2\pi$$

Where σ^0 is the reaction cross section of all channels except breakup, y_0 the average neutron yield, f_{KM} and f_{BU} the normalized energy-angular distributions ($eV^{-1} \cdot \mu^{-1}$). The Kalbalch-Mann distribution f_{KM} is represented by the formula:

$$f_{KM}\left(E, E', \mu\right) = \frac{a S_0}{2\sinh\left(a\right)}[\cosh(a\mu) + r\sinh(a\mu)]$$

Where S_0, a and r are function of E and E'. S_0 is the neutron normalized spectrum considering all the mechanisms included in Kalbach-Mann systematics. a and r are parameters. The systematics associated to the breakup mechanism is given by the distribution:

$$f_{BU}\left(E, E', \theta\right) = K S_{BU} \exp\left(-a_{BU}\theta\right)$$

Where K is the distribution normalization constant, $S_{BU}(E, E')$ is the normalized neutron spectrum of the deuteron breakup channel and a_{BU} a tabulated parameter. This parameter is determined by an empirical formula and depends only on the projectile energy E and the type of projectile [6].

The distributions being normalized, the integrated cross section over the angles is:

$$\sigma^{incl}\left(E, E'\right)) = \sigma^0(E)y_0(E)S_0(E, E')$$
$$+\sigma^{BU}(E)S_{BU}(E, E')$$

Introducing the breakup parameter defined as:

$$r_{BU}\left(E, E'\right)) = \frac{\sigma^{BU}(E)S_{BU}(E, E')}{\sigma^{incl}(E, E')}$$

The inclusive cross section is expressed as:

$$\sigma^{incl}\left(E, E'\right)) = (1 - r_{BU})\sigma^{incl}(E, E') + r_{BU}\sigma^{incl}(E, E')$$

The first RHS term in the above equation represents the reaction cross section of all channels except breakup, and the second term the breakup channel. Reintroducing the angular dependence, the energy-angle cross section is:

$$\sigma^{incl}\left(E, E', \mu\right) = \sigma^{incl}(E)y_{incl}(E)S_{incl}\left(E, E'\right) *$$
$$\times[(1 - r_{BU})D_{KM}(\mu) + r_{BU}D_{BU}(\mu)]$$

D_{KM}, and D_{BU} are the angular parts of the distributions f_{KM} and f_{BU}.

Inclusive cross section, neutron yield and spectrum are quantities calculated so far by nuclear code like Talys to generate the transport library. The new parameter to be evaluated to take into account the kinematics of neutrons produced by breakup reaction is $r_{BU}(E, E')$. This parameter, which includes the breakup neutron spectrum, can easily be evaluated by the nuclear code at the same time as the inclusive spectrum is calculated.

2.2. Breakup reaction parameters

In the previous section two new parameters used to define the angular distribution of neutrons emitted by breakup reaction have been introduced. The parameter r_{BU} is determined by a nuclear code while the parameter a_{BU}, representing the slope of the exponential angular distribution, can be evaluated by empirical formula.

The r_{BU} parameter should be stored in the data library with the neutron yield and spectrum to be available by the transport code. Although the a_{BU} parameter can be evaluated at any step of the process (library evaluation, library processing or during transport simulation), it may be more convenient to store it together with the r_{BU} parameter, because if in the future a new angular distribution is proposed and associated parameter(s) could be evaluated by nuclear code, the structure of the data library would not change.

3. Implementation

The implementation of this new distribution for use in deuteron transport simulation will require a small extension of the ENDF format referring to energy-angle distribution, and an associated NJOY update to process this no-standard ENDF format in ACE format. Finally the MCUNED code has been also updated to take into account this new energy-angular distribution law.

3.1. ENDF modification

The value of breakup parameter r_{BU} depends on the incident and outgoing energies like the emitted particle spectrum, while a_{BU} only depends on the incident energy. The dependence of r_{BU} is the same as the dependence of parameters a and r of the Kalbach-Mann distribution, thus these new parameters can be stored in the ENDF format following the same structure as current Kalbach-Mann structure with only small modifications. In the ENDF format, the Kalbach-Mann distribution is stored in the ENDF file 6 (energy-angle distribution file) with parameters LAW = 1 (coupled energy-angular distribution) and LANG = 2 (Kalbach-Mann distribution).

The Kalbach-Mann parameters a and r are stored at the same time as the particle spectrum. Basically for each incident particle energy a data table is defined. Each line of this table corresponds to a possible energy of the outgoing particle, in this line the probability of particle emission, a and r parameters are stored.

In this law, the number of parameters that can be stored in this line is not fixed and set by the ENDF parameter NA. Thus, the new parameters defining the breakup distribution can be introduced in the ENDF format easily, simply
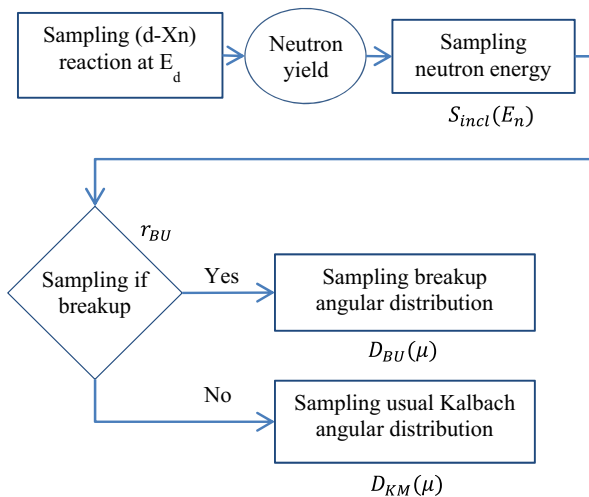
Figure 1. Breakup angular distribution sampling algorithm.

extending the number of parameters from 2 to 4 and writing the r_{BU} and a_{BU} values after r and a. ENDF LAW = 1, LANG = 2 only admits value 1 or 2 for NA, and the addition of two extra parameters convert this law in non-standard format.

Although this new definition of energy-angular distribution with breakup mechanism includes Kalbach-Mann distribution (the new distribution setting $r_{BU} = 0$ gives the usual Kalbach-Mann distribution), a new value of the parameter LANG is defined in order to keep unchanged the definition of LANG = 2 of the ENDF format. LANG = 3 is chosen to represent this new distribution including breakup mechanism, in which the number of NA parameters is 4.

In order to process correctly these non-standard ENDF files into ACE formatted files to be used with MCUNED, the NJOY ACER module has been modified.

### 3.2. Generation of deuteron library

New deuteron libraries including the new breakup parameters have been generated. For this, modifications in TALYS and TEFAL codes were necessary. The r_{BU} parameter has been evaluated with TALYS and the non-standard ENDF format including breakup parameters has been implemented in the ENDF-6 file maker code TEFAL.

Finally a complete TENDL library (based on TENDL 2014 release) including the new breakup distribution has been generated for all stable isotopes.

3.3. MCUNED modifications

In order to implement the new breakup angular distribution in MCUNED a modification of the sampling algorithm was necessary. The scheme of the algorithm is presented in Fig. 1.

During the deuteron transport process, when a nuclear interaction in sampled and a neutron is produced, the code determine, using the neutron yield value, how many neutron should be produced. Then, using the neutron spectrum, the code samples the energy of the emitted neutron. The spectrum used to evaluate the energy of the outgoing neutron is the inclusive spectrum considering all reaction channels (including breakup channel).
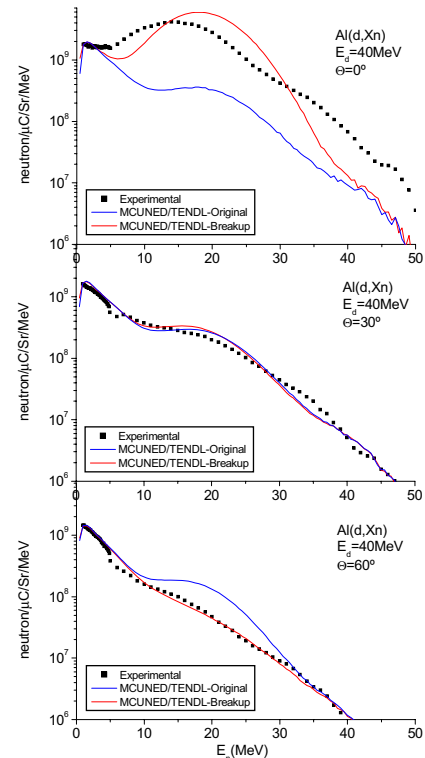
Figure 2. Neutron spectra produced by 40 MeV deuteron on thick (6 mm) Aluminium target.

The probability that the produced neutron comes from the breakup reaction is given by the parameter r_{BU}. At this stage, the value of this parameter can be determined since incident projectile and outgoing neutron energies are known. Using this probability the channel which produce the neutron is sampled and once the reaction is known the corresponding angular distribution is used to sample the direction of the emitted neutron.
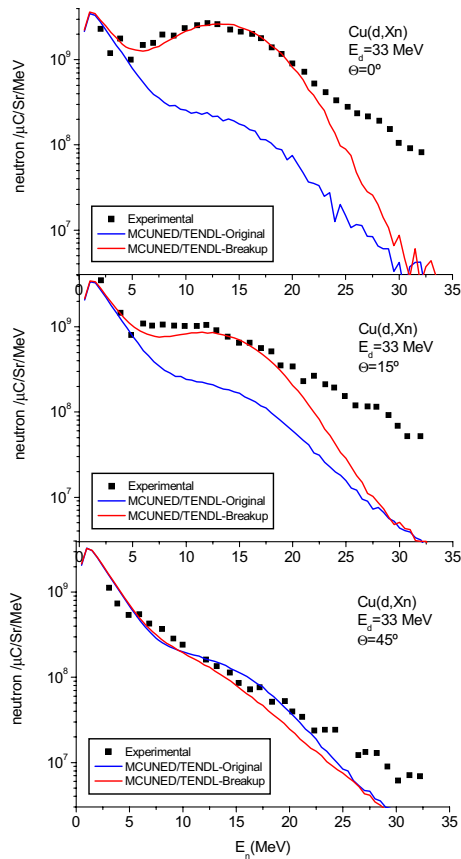
It should be noticed that in the proposed breakup systematics, the outgoing energy are given in the CM frame while the angle distribution use laboratory angle. During the transport process only energy of emitted particle has been transformed from CM to laboratory frame.

4. Results

This new methodology has been applied to reproduce previous calculations where integral experiments measuring the neutron spectrum at different emission angle were compared with MCUNED simulations [5].

Figures 2 and 3, correspond to the reproduction of integral experiment where thick aluminium and copper targets (6 and 3 mm respectively) were irradiated respectively by 40 and 33 MeV deuteron. In these figures, results obtained with the new method presented in this work are compared with experimental results and calculations performed with the former version of MCUNED.

These plots show the improvement of the new method compared to original angular distribution. The new simulations are now in much better agreement with experimental data. Copper simulation gives a better

Figure 3. : Neutron spectra produced by 33 MeV deuteron on thick (3mm) Copper target.

5. Conclusion

A methodology improving the angular distribution of neutrons emitted during deuteron transport simulation has been presented. In this approach a new angular distribution is used to reproduce the emission of neutrons produced by deuteron breakup channel. To implement this methodology, modifications on library format, library processing code and transport code were necessary. The application of this methodology shows a significant improvement of simulated spectra obtained during deuteron transport simulation in thick target. The comparisons of these simulations with experimental spectra show a good agreement.

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agreement with experimental data than simulation with aluminium target. It can be seen in the Aluminium case that the maximum due to breakup emission channel is shifted compared to experimental spectrum. This difference can be due to the evaluation of the breakup cross section and breakup spectra models included in TALYS. Recently a new breakup cross section model developed by IFIN-HH [10] is under implementation in TALYS. This new model could give mode accurate results on the position and amplitude of the breakup component and improve the agreement between simulations and experiments.