Implementation in transport simulation of angular distribution of nucleon emission from breakup reaction

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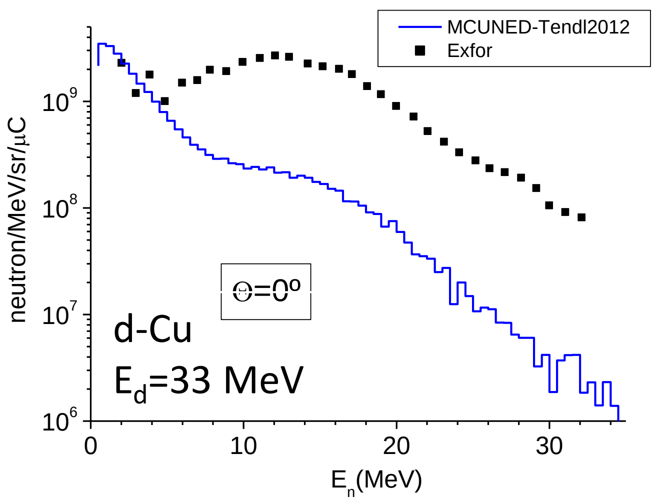
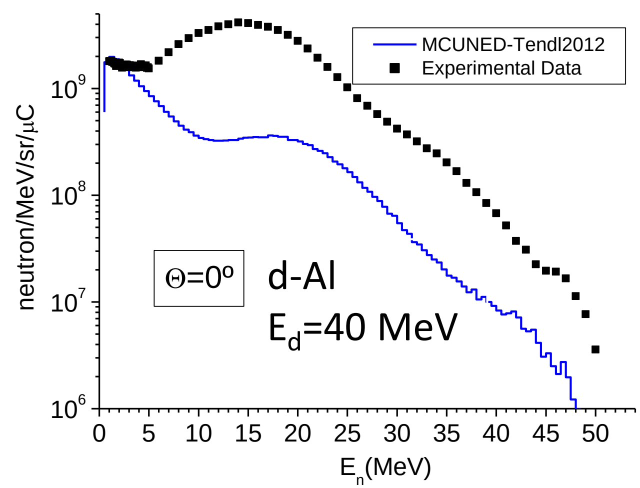
Introduction

- Previous work (F4E-SGA-168.01 task 2.2) highlighted that angular distribution of inclusive neutron spectra produced by deuteron induced nuclear reaction were not reproduced satisfactorily by simulations.
- It was pointed out that Kalbach angular distribution was not able to reproduce forward peak nucleon emission from breakup reaction channel.





- In this work a new methodology is proposed to improve the behaviour of neutron angular distribution produced by deuteron induced nuclear reaction.

Energy-angle distribution

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- ENDF format for double differential cross section :

$$\sigma(E, E', \mu) = \sigma(E)\, y_i(E)\, f_i(E, E', \mu)/2\pi$$

$\sigma(E)$: Total reaction cross section

$y_i(E)$: Particle yield

$f_i(E, E', \mu)$: Normalized distribution ($eV^{-1}.\mu^{-1}$)

- Each reaction channel can be described by a specific distribution function f_i

Continuum Energy-angle distribution (ENDF LAW=1)

- Law used to describe particles emitted in multi-body reactions, combinations of several reactions or reactions at high energies where many channels are normally open.

- Usually, in ions-induced reactions, Kalbach systematics is used to represent the distribution function of emitted particle.

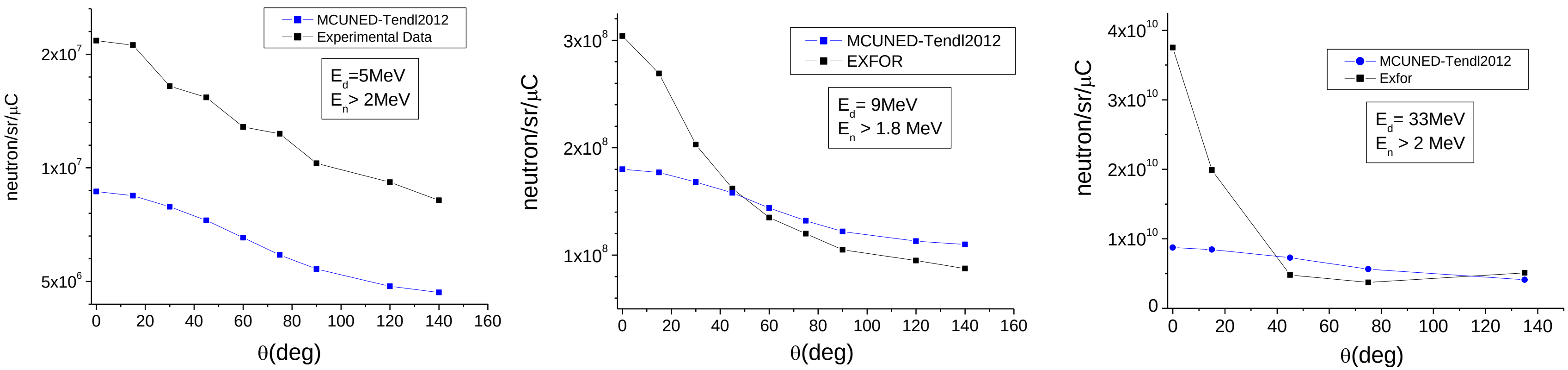
$$f_i\ (E, E', \mu) = \frac{a\ S_0}{2\sinh(a)} [\cosh(a\mu) + r\sinh(a\mu)]$$

S_0, a, r are function of E and E'

- $S_0(E')$ is the normalized spectra of the outgoing particle
- $D(\mu) = \frac{a}{2\sinh(a)} [\cosh(a\mu) + r\sinh(a\ \mu)]$ is the normalized angular distribution

Kalbach angular distribution

- When deuteron breakup channel has significant contribution to the total neutron production, Kalbach function is no longer capable to reproduce angular distribution.



d-Cu

Angular distribution of particles emitted from breakup reaction

➢ An angular distribution function has been proposed by Kalbach in 2nd FENDL-3 RCM report to reproduce the emission of particle produced by breakup reaction.

$$D_{BU}(\theta) = Ke^{-a_{BU}\theta}$$

K : normalization constant (rad^{-1})
a_{BU} : breakup angular distribution slope parameter (rad^{-1})

$$a_{BU} = \begin{cases} 4\,A_b + Z_b - 2 + 0.029E + \dfrac{7.6}{A_a}\left[1 + \exp\left(\dfrac{12\,S_{ab} - E}{0.84\,S_{ab}}\right)\right]^{-1} & for\;\; A_b = A_a - 1 \\ 4.7 + A_b & for\;\; A_b < A_a - 1 \end{cases}$$

C. Kalback, *“Complete Phenomenological Model for Projectile-Breakup Reactions”, Report to 2nd RCM of FENDL-3 CRP, (2010)*

New methodology

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- To include this new angular distribution into a new global distribution, breakup reaction channel has been separated from other reaction channels.

$$\sigma^{all}\,(d,Xn) = \sigma^{0}\,(d,Xn) + \sigma^{BU}\,(d,n)$$

$$\sigma^{0}\,(d,Xn) = \sigma^{0}(E)\; y^{0}(E)\; S_{0}(E,E')D_{0}(\mu)$$

Usual Kalbach angular distribution

$$\sigma^{BU}\,(d,Xn) = \sigma^{BU}(E)S_{BU}(E,E')D_{BU}(\mu)$$

New Kalbach breakup angular distribution

Breakup parameter

- Considering angle integrated cross section

$$\sigma^{all}(E,E') = \sigma^0(E)\, y^0(E)\, S_0(E,E') + \sigma^{BU}(E) S_{BU}(E,E')$$

New parameter r_{BU}

$$r_{BU}(E,E') = \frac{\sigma^{BU}(E,E')}{\sigma^{all}(E,E')} = \frac{\sigma^{BU}}{\sigma^{all}(d,Xn)}$$ breakup parameter

$$\sigma^{all}(E,E') = \underbrace{\big(1 - r_{BU}(E,E')\big)\sigma^{all}(E,E')}_{\sigma^0(E,E')} + \underbrace{r_{BU}(E,E')\sigma^{all}(E,E')}_{\sigma^{BU}(E,E')}$$

Global energy-angle distribution

- Introducing the angular dependence:

$$\sigma^{all}\,(E,E',\mu) = \sigma^{all}(E)\,y^{all}(E)\,S_{all}(E,E')[(1-r_{BU})D_0(\mu)\;+r_{BU}D_{BU}(\mu)\,]$$

- The breakup angular distribution introduced in the formulation two extra parameters r_{BU} and a_{BU}. Other parameters S, a, r, remains unchanged.

  - The parameter r_{BU} can be determined with nuclear code like Talys
  - The parameter a_{BU} is determined with empirical formula.

Kalbach parameters in ENDF format

- Kalbach distribution law is coded in ENDF format with LAW=1 and LANG=2
- For each projectile energy E, parameters S(E'), r(E') and a(E') are stored in the table.
- ENDF LAW=1 format allows defining the number of angular parameters with the parameter NA.
- For usual Kalbach distribution NA can be 1 or 2 whether *a* parameter is provided or not.

E'	S	r	E'	S	r
0.000000+0	4.076872-7	9.999770-1	1.476337+3	4.085957-7	9.999550-1
3.444785+3	4.112590-7	9.998880-1	7.381683+3	4.156399-7	9.997780-1
1.476337+4	4.243479-7	9.995660-1	3.444785+4	4.504510-7	9.989780-1
7.381683+4	4.938927-7	9.984040-1	1.476337+5	5.778256-7	9.994620-1
2.460561+5	6.546563-7	9.998190-1	3.444786+5	7.180461-7	9.999100-1
4.429010+5	7.623190-7	9.999630-1	5.413234+5	7.834186-7	9.999810-1

Kalbach distribution parameters
NA = 1

New parameters for breakup reaction in ENDF format

- New parameters including breakup can be added with the same format.
- A new LANG = 3 has to be define to identify the new distribution law.

LAW=1 LANG=3 NA=2

E'	S	r	r_{BU}		
0.000000+0	4.076872-7	9.999770-1	9.996130-1	1.476337+3	4.085957-7
9.999550-1	9.994450-1	3.444785+3	4.112590-7	9.998880-1	9.990990-1
7.381683+3	4.156399-7	9.997780-1	9.986940-1	1.476337+4	4.243479-7
9.995660-1	9.980940-1	3.444785+4	4.504510-7	9.989780-1	9.968390-1
7.381683+4	4.938927-7	9.984040-1	9.956430-1	1.476337+5	5.778256-7
9.994620-1	9.959430-1	2.460561+5	6.546563-7	9.998190-1	9.957200-1

a_{BU} parameter is evaluated in transport code with empirical formula

Breakup library generation and processing

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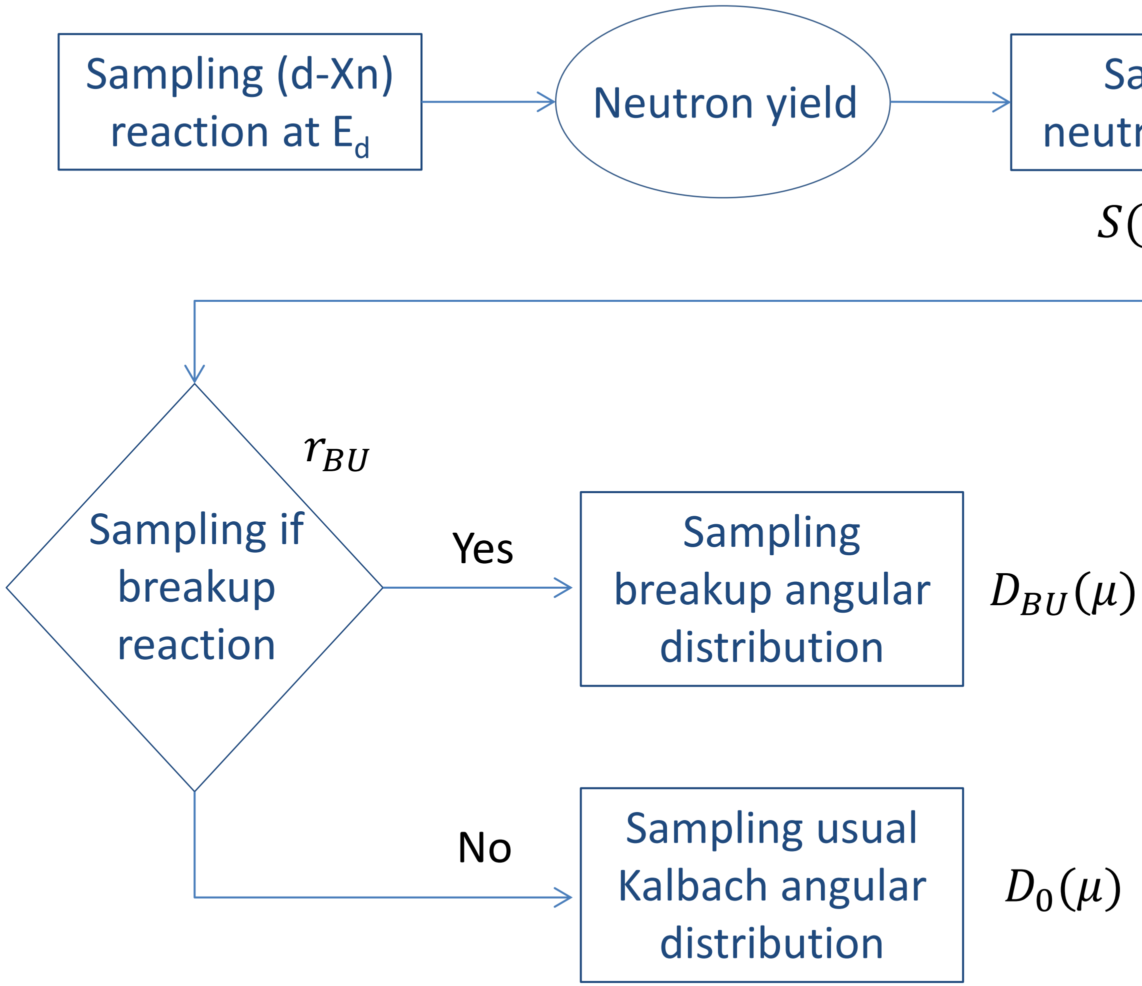
- New formatted library has been generated with TALYS-TEFAL codes.
- Modifications in both codes have been implemented in order to evaluate the r_{BU} parameter and provide the new formatted ENDF library
- A new library based on TENDL 2014 has been generated for all stable isotopes
- NJOY ACER module has been modified to process the new formatted library

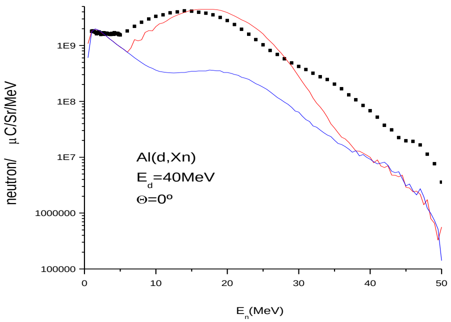
Application to transport simulation

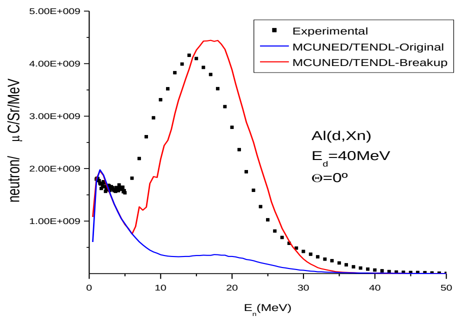
- MCUNED code has been modified in order to handle new formatted library and reproduce the breakup angular distribution during the transport process

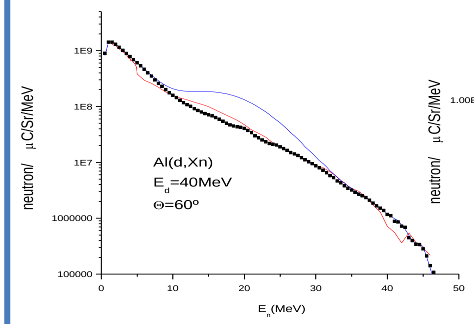


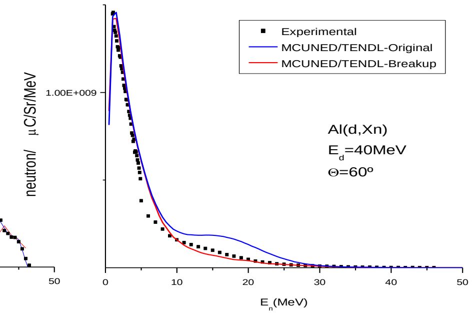
Results

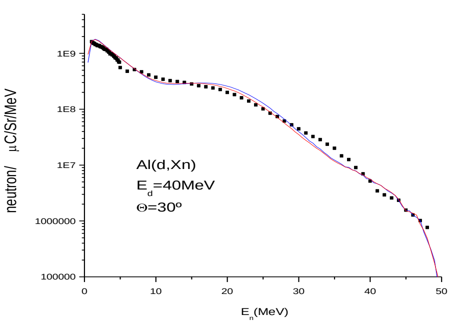
- Simulation of 40 MeV deuteron on Aluminum target

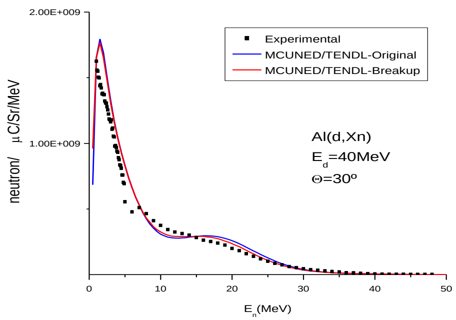


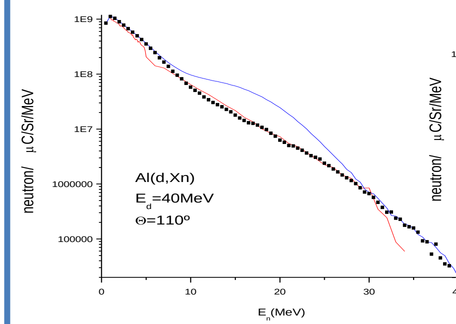


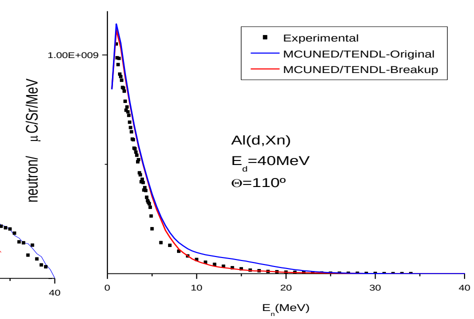






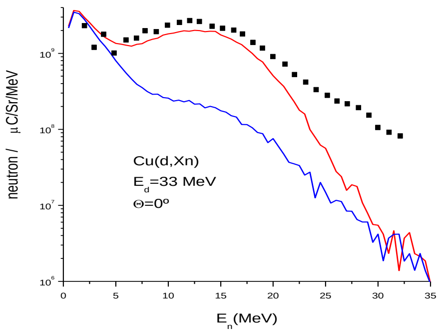


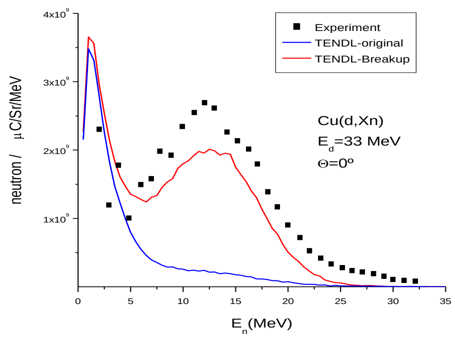


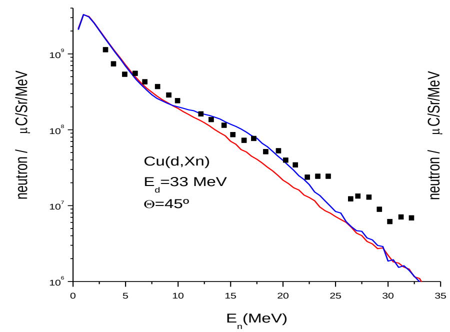


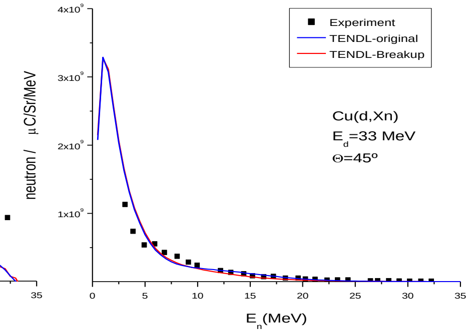
Results

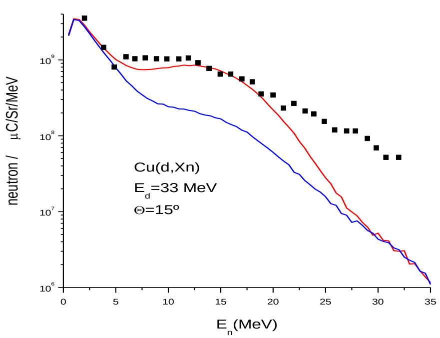
- Simulation of 33 MeV deuteron on Copper target

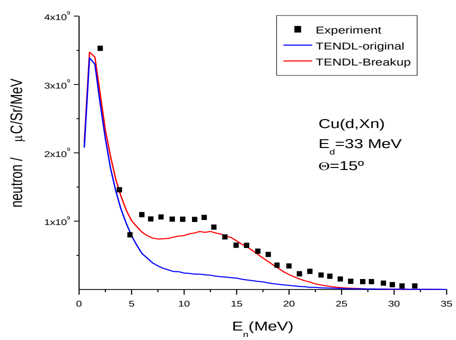


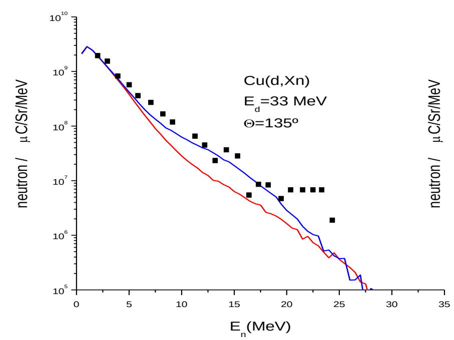


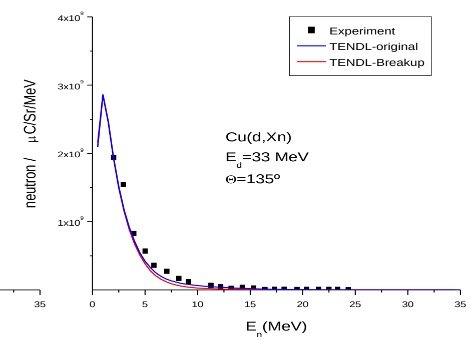












Summary

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- A new methodology has been proposed to represent more accurately the angular distribution of inclusive neutron spectra produced by deuteron induced nuclear reaction.

- This methodology requires only two extra parameters:
    - One to be evaluated by nuclear code and stored in the data file
    - One evaluated with empirical formula.

- Generation of new libraries and code modifications have been performed.

- Results show a great improvement with respect to former simulations and give a good agreement with experimental data.

Acknowledgment

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Thank you for your attention