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NeuSDesc – Neutron Source Description Software Manual

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INTRODUCTION

Quasi mono-energetic neutron fields are routinely created by means of charged particle induced binary nuclear reactions. By knowing the energy loss of the ions in the target material and the double differential cross section of the particular reaction creating the neutrons, one can obtain a rather good estimate of the neutron spectrum. Since accurate modelling of neutron spectra is indeed important for a good planning as well as verification of neutron data experiments, several programs have been developed for this purpose. Example are the Drosg2000 code [1] available from the IAEA home page [2], the Target code from Physikalisch-Technische Bundesanstalt (PTB) in Germany [3][4], and the EnergySet program from the IRMM [5] available from the IRMM home page. The Drosg2000 code is based on neutron kinematics and calculates neutron fluencies for a comprehensive list of reactions, however no spectroscopic information is provided. The Target code [3][4] is a Monte Carlo code giving fluence as well as spectroscopic information and includes also several peak broadening effects discussed below. The EnergySet program is based on pure kinematics also calculating fluence as well as neutron spectrum. In contrast to the Drosg2000 and the Target codes the EnergySet program calculates data in real-time, i.e. results are momentarily calculated and displayed on the user window following user input of data. EnergySet also calculates the accelerator settings specific for the IRMM Van de Graaff accelerator which is out of the scope for this report.

The program reported herein, the Neutron Source Description - NeuSDesc, was developed on the EnergySet [5] platform. In NeuSDesc, the EnergySet real-time style presenting of calculated neutron fluence and spectrum have been kept, but also intrinsic and parasitic peak broadening effects such as energy and angular straggling of the ions in the beam, energy spread of incident ion beam, and possible non-homogeneity of the entrance foil for gas targets have been included. The NeuSDesc program makes for these calculations use of the freeware program SRIM-2008 [6] which simulates the stopping of ions in materials using Monte Carlo calculations. In addition, the NeuSDesc program includes the option of creating a neutron source description input for the MCNP [7] program, a so called SDEF card. Thus, with knowledge of the experimental set-up, the neutron spectrum for a complete neutron beam facility can be simulated which also was the main objective for the development of NeuSDesc.

The NeuSDesc software was developed using Digital Fortran, Visual Fortran Professional Edition 5.0.A, on the Microsoft Developer Studio 97 platform.

INSTALLATION OF THE SOFTWARE

The NeuSDesc program requires no installation routine, however, a number of input data text files are required to be located in the same directory as the executable file, see list below. If an input file is changed, the program has to be re-started. A detailed description of the input structure of every data file is given in the heading of the respective file:

- *StoppingData.txt*; text file containing data for calculation of the energy loss in the target material and possible entrance foil, particularly used for gas targets.
- *DoseData.txt*; text file containing the fluence-to-dose conversion function (the Siegler curve).
- *NeuSDescinp.txt*; text file containing data for customization of the program. This file is further discussed below.
- *Reactions.txt*; text file containing information about the binary reactions for neutron production included in the data base. The corresponding binary reaction data is stored in the files *react_xx.txt* where *xx* indicates (note that any filename can be used as long as it is identically listed in the *Reactions.txt* file):

  01 - ^{7}Li(p,n)^{7}Be
  02 - T(p,n)^{3}He

03 - D(d,n)^{3}He
04 - ^{7}Li(α,n)^{10}B
05 - T(d,n)^{4}He
06 - ^{7}Li(p,n)^{7}Be*
07 - ^{45}Sc(p,n)^{45}Ti
08 - D(d,pn)D

- *AngleScan.txt*; text file containing information for the angular scanning option, see below.

In order to make full use of the program, the software package SRIM-2008 [6] must be installed in a directory also given in the *NeuSDescinp.txt* input file. SRIM-2008 can be downloaded free of charge from www.srim.org.

HOW TO RUN NEUSDESC

NeuSDesc is executed by double clicking the executable file NeuSDesc.exe. The user interface is based on a standard Microsoft Windows layout, see Figure 1.

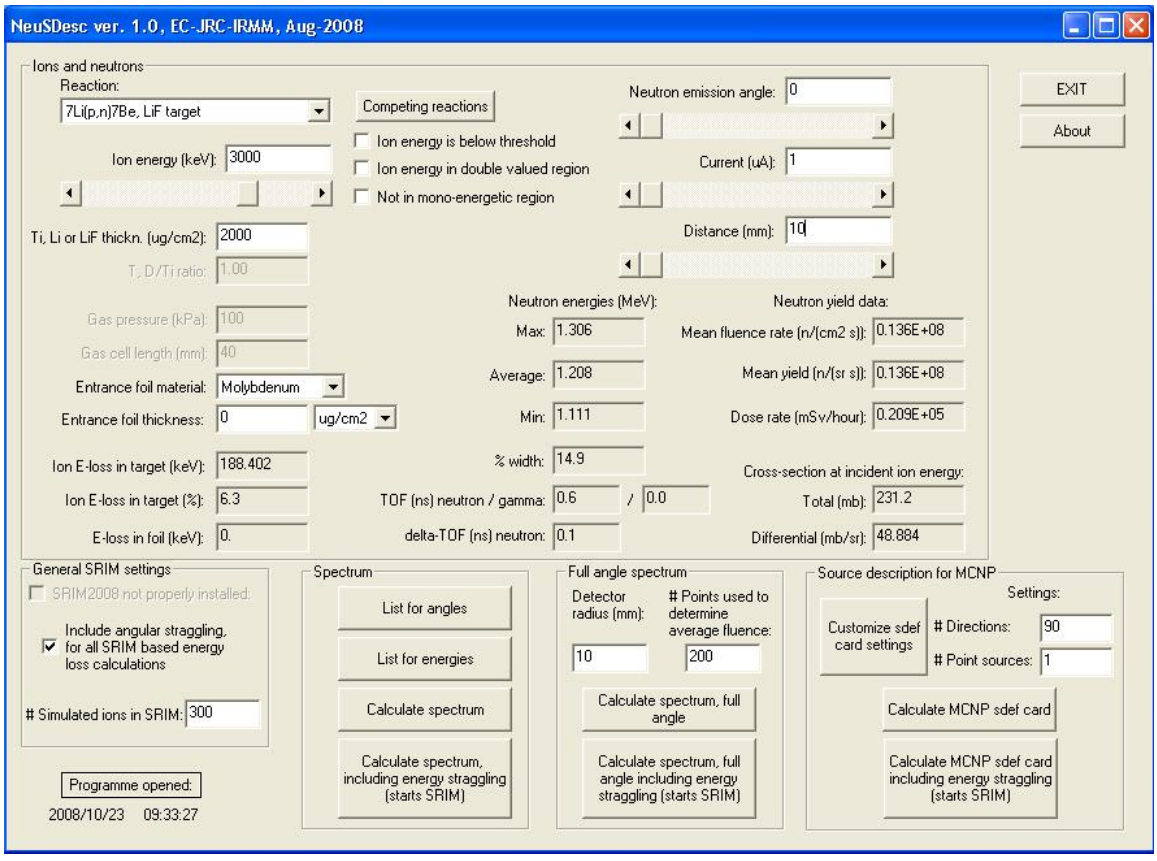

Figure 1. NeuSDesc user interface window.

In the user window input data are entered in white input boxes and calculated data are presented in the greyed boxes and in output files. In the upper part of the window ion beam, target and neutron emission parameters are defined, including:

- The nuclear reaction,
- the incident ion energy in keV,
- the ion beam current in μA,
- the thickness of the neutron producing target in μg/cm^2,
- tritium (T) or deuterium (D) atomic amount in the titanium matrix (if valid),
- pressure and length of a gas cell (when using gas targets),
- optional entrance foil material and thickness in μg/cm^2 or optionally in nm,
- neutron emission angle, and distance to measurement point in mm.

A user input of any of these parameters momentarily updates the calculated output data given in the gray fields, including:

- Ion energy loss in the target and entrance foil,
- maximum, minimum and average energy of the neutron full energy peak,
- the width of the neutron full energy peak (in percentage),
- the Time of Flight (ToF) of neutrons and gammas from neutron producing target to measurement point,
- the width of the ToF spectrum for the neutrons,
- the mean fluence rate at the measurement point,
- the mean neutron yield from the target,
- the calculated dose at the measurement point,
- the total and differential cross section for the incident ion energy.

Neutron spectral data is also momentarily updated in the text file *qplot.txt* which, thus, may be used as input for a real time graphics programme (for example Microsoft Excel). The spectrum is here calculated from pure kinematics and by slicing the target in 100 slices, see below, giving a rather crude estimation of the neutron full energy peak.

In the lower part of the user window input data and execution buttons for saving data and for more detailed calculations of neutron spectra is facilitated. The "Calculate spectrum" option saves the real-time calculated spectrum (same as in *qplot.txt*), however also including information concerning user input data. The same spectrum but including energy, angular and lateral straggling, as well as non-homogeneous entrance foil and energy spread of the incident ion beam, is saved using the "Create spectrum including energy straggling (starts SRIM)" option. This routine defines the adequate input data for SRIM-2008 from the present settings in the user window and executes the SRIM-2008 in the background. Angular straggling may optionally be included in the calculations. The number of SRIM-2008 simulations can be changed as the execution time on a standard PC can be rather long.

Based on the angles written in the *AngleScan.txt* input file the option "List for angles" outputs the fluence at all angles in the list and for the present settings in the user window. Similarly, the "List for energies" option creates a list of incident ion energies and the corresponding neutron energies and neutron fluence rates.

The "Full angle spectrum" option calculates a neutron spectrum integrated over a circular disk surface. The integration can be performed with or without energy and angular straggling (i.e. using SRIM-2008). In either case the option executes a Monte Carlo integration performed by randomizing a number of points on the surface followed by the calculation of the average neutron spectrum from

these points. For the calculation the radius of the circular disk and the number of points used to estimate the average have to be input. It should be noted that the "Full angle spectrum" option using SRIM-2008 can render a rather long execution time on a standard PC.

Creating an MCNP SDEF card

The program also includes the option to create a complete neutron source description file, i.e. an MCNP Source Definition (SDEF) card used as input file for an MCNP simulation, also here with the option of using SRIM-2008 for modelling the energy and angular straggling. The SDEF card is independent on the geometrical description in the MCNP input file. The user option "Customize sdef card settings" opens a new window, see Figure 2, where the coordinates of the neutron source (x0,y0,z0) and the direction of the incident ion beam (Vx,Vy,Vz) is defined, depending on how the geometry is described in MCNP. For the gas target description the coordinates define the position of the gas cell entrance foil. The default values are read from the *NeuSDescinp.txt* input file and can, thus, be changed. The SDEF card is defined from data in the user input window and on the two additional user inputs given in the "Source description for MCNP" window box, see Figure 1. The SDEF description is defined so as neutrons are emitted from a discrete number of points with different probabilities and in certain angle and energy intervals connected to the points. The coordinates of the points can all be the same. The result is a complete neutron source description with neutrons emitted in all angles with an appropriate weighting. Since gas targets can not, as solid targets, be considered as point sources, the gas cell may be split in a few evenly spaced geometrical points in the direction of the ion beam, on which the same angular intervals are applied. Note that the number of angular intervals, so called "directions" in the user window, see Figure 1, multiplied by the number of evenly spaced geometrical positions, so called "point sources" in the user window, is limited in MCNP to 498, which indeed normally is adequate for a good neutron source description. For each angular interval, the differential cross section is determined at the two extreme angles of the interval and a linear interpolation is used to calculate intermediate differential cross sections.

The neutron energy spectrum is determined as an average of the neutron energy spectra from three evenly spread angles within the angular interval. Each angular interval forms a stripe with a certain area on a sphere with radius r defined as:

$$r = 2 \cdot (\text{target length}) + 20 \text{ cm}$$

These areas are multiplied with the calculated neutron fluence rates at the distance r. The result is proportional to the probability of neutrons being emitted from the particular point, see Figure 3. Thus, neutrons will be simulated in all directions according to the reaction differential cross section. However, for a certain angular interval the same energy distribution is used and for gas targets neutrons are only emitted from a discrete number of positions.

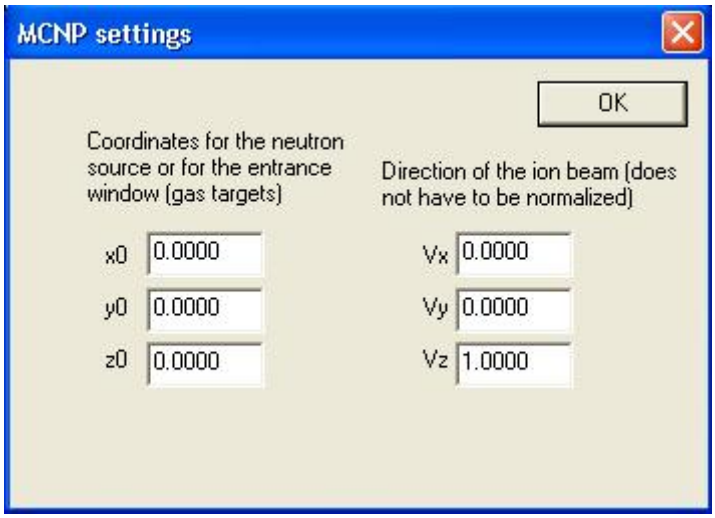

Figure 2. User window for MCNP input settings.

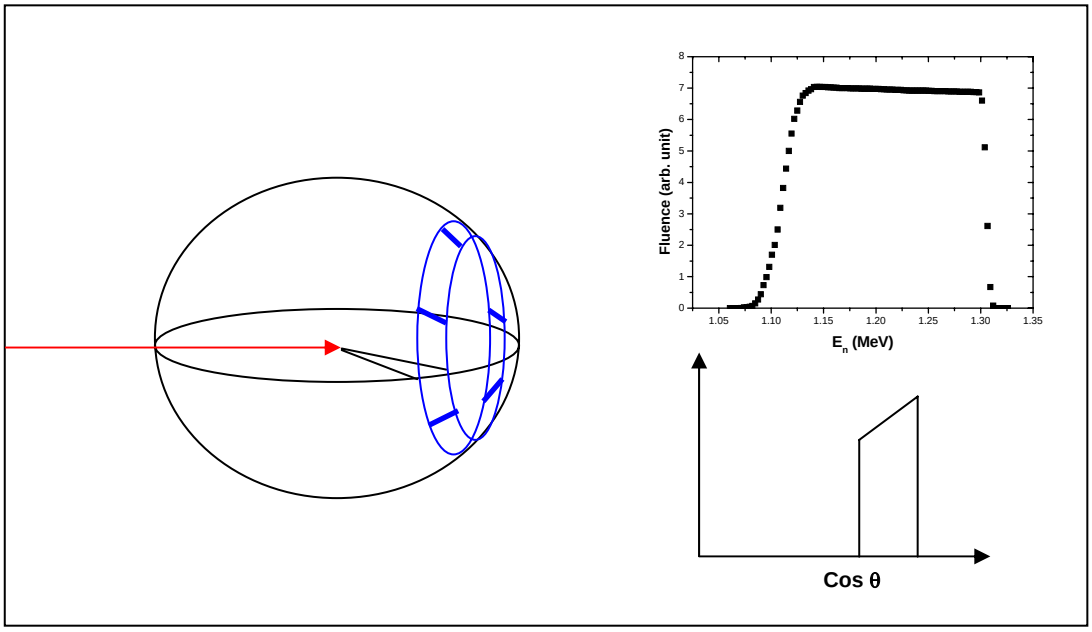

Figure 3. Visualisation of the SDEF card definition. The energy and angular distribution linked to one "point" is shown to the right. The area the angular distribution represents on a sphere is shown to the left where the incident ion is indicated by the red arrow. The probability for a neutron to be emitted from one point is calculated by multiplying the fluence yield with this area.

Competing reactions

The "Competing reactions" option opens a new window where the user may include neutron spectra from competing reactions, see Figure 4. These additional spectra are only included in the output files and no online results are provided in the main user window. The neutron spectrum may be calculated, for every reaction, from the neutrons that are emitted in the backward direction in the centre of mass (CM) system, but in forward direction in the laboratory system, the so called double valued region.

The relative weight optional input available for some competing reaction, is the weight of the competing reaction relative to the main reaction. For the deuterium content in a titanium-tritium target this implies:

$$D/T_i = (\text{relative weight}) \cdot T/T_i$$

where the *T/Ti* value is given for the main reaction in the main user window.

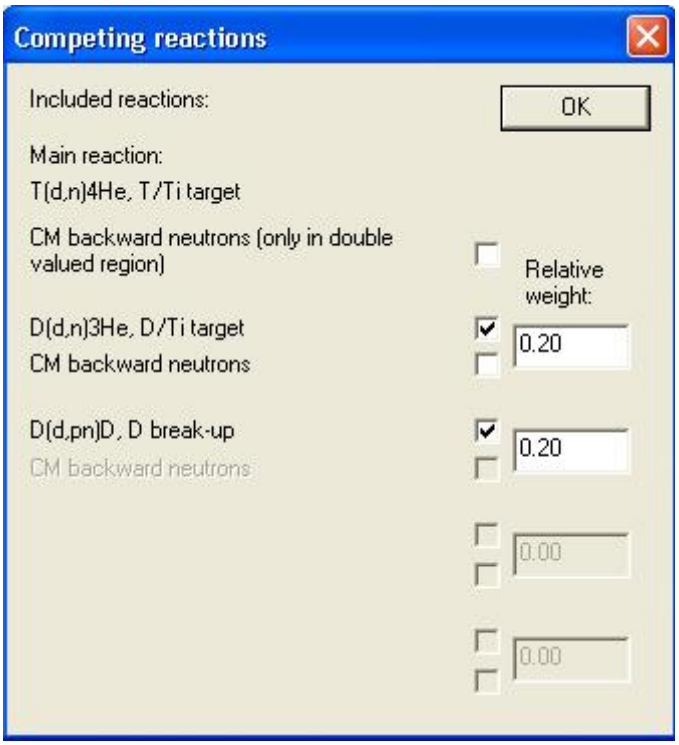

Figure 4. User input window for competing reactions.

Output files

All output data files are saved in the RESULTS folder located in the NeuSDesc main directory. As mentioned above, the program updates for graphical purposes momentarily the output file *qplot.txt*, containing the neutron spectrum calculated from pure kinematics. Spectra which are created by using the "Create spectra" options all have filenames ending with the date and time for the saving, so as not to overwrite any data. Also, a neutron spectrum is additionally automatically saved in a temporary file, *qplotx.txt*, where *x*=1,2,3 or 4, containing spectral information whenever a data file is saved. This file is, again, intended to be used for real time graphics plotting routine. The user options and corresponding files names are listed in Table 1 below.

User option	File name	Temporary file
List for angles	Angles YYYYMMDD HHMMSS.txt	
List for energies	Energy YYYYMMDD HHMMSS.txt	
Calculate spectrum	Spect YYYYMMDD HHMMSS.txt	qplot1.txt
Calculate spectrum, including energy straggling (starts SRIM)	Spect-SRIM YYYYMMDD HHMMSS.txt	qplot2.txt
Calculate spectrum, full angle	Spect-Full YYYYMMDD HHMMSS.txt	qplot3.txt
Calculate spectrum, full angle including energy straggling (starts SRIM)	Spect-Full-SRIM YYYYMMDD HHMMSS.txt	qplot4.txt
Calculate MCNP sdef card	SDEF YYYYMMDD HHMMSS.txt	
Calculate MCNP sdef card including energy straggling (starts SRIM)	SDEF-SRIM YYYYMMDD HHMMSS.txt	

Table 1. User options and corresponding generated file names

The "List for Angles" option opens the *AngleScan.txt* file for information on which angles the neutron spectrum should be calculated for. The spectra obtained are calculated using energy loss calculations from kinematics (see above). In the "List for Energies" option, neutron energy and flux is listed for ion energies up till the maximum ion energy, taken from the input file *NeuSDescInp.txt*.

All other output files with saved spectra have a similar structure. Information about the incident ion energy and target material is written in the file header followed by the neutron spectrum from the main reaction and the neutron spectra from the competitive reactions. If the low energy neutron spectrum from the double energy region is included for a certain reaction it is listed after the higher energy neutron spectrum. For each reaction the minimum, maximum, average, median and centroid energy is calculated as well as the standard deviation of the distribution. Also the total fluence and the energy bin width of the histograms are given. The last spectrum in the respective output file is the summed spectrum from all included reactions with the abscissa unit in neutrons/(s cm^2 MeV) while the integral under the curve has the unit neutron/(s cm^2). These spectra are also written in the *qplot1-4.txt* files, see table 1.

The output file including the SDEF card for MCNP calculations includes a header with information about the incident ion beam and the target characteristics. The line starting with the first SDEF definition, and all the following lines, constitutes the actual SDEF card which should be copied to the MCNP input file. Since an MCNP simulation normally gives the neutron flux per source neutron, one should multiply the result with the number of source neutrons from the neutron producing target to obtain the true flux. The total number of neutrons can be obtained by input the total cross section. However since the total cross section might change as the incident ion energy changes the NeuSDesc program calculates the neutron source strength for the current target and saves this value in the output file together with the SDEF card.

Input files and customization

All input files may be changed by the user so as to tailor the program to a certain accelerator and target, however, the structure of the file must be kept. In the *NeuSDescInp.txt* input file the following values may be changed:

- The maximum incident ion energy (for ions of charge +1).
- The beam line direction and the start coordinates for neutron production for the SDEF card definition.
- Position of the SRIM-2008 directory and the default number of SRIM-2008 simulations to run.

- Number of division of the neutron producing layer in the SRIM-2008 simulation. A higher number increases the number of points in the *EXYZ.txt* output file generated by SRIM-2008. Also increases the accuracy of the angular straggling.
- The energy FWHM of the ion beam in percent of the peak energy of the ions.
- Description of non homogeneous entrance foils for a gas targets (see below).
- The Avogadro number, amu to MeV conversion factor and atomic masses of the elements.
- SRIM-2008 input data used to create the input file for SRIM-2008.

An example of the description of the non homogeneous entrance foil in the *NeuSDescInp.txt* file is given in Figure 5. This example has 5 entries. When running the SRIM-2008 simulation the ions are started at different positions inside the entrance foil which simulates the non homogeneity. The probability of the ions being started at different fractions of the thickness of the target must be entered in the *NeuSDescInp.txt* input file. The probabilities do not have to be normalized. By using the example with 5 entries below, ions will be started with a probability 0.92 at 0.9*total length of the foil, a probability 0.95 at 0.95*total length of the foil, and so on.

```
=== Entrance foil profile ===
5
length
0.900
0.950
1.000
1.050
1.100
Probability
0.920
0.950
1.000
0.950
0.920
```

Figure 5. Entrance foil profile data from the NeuSDescInp.txt input file

In the file *Reactions.txt*, information about the reactions included in the program is given. It is not possible to remove or change the order of the default reactions. However, new reactions may be entered by the user. If a reaction is added, the given total number of reactions must be changed in the file and the following information about the new reaction must be entered (use same structure and formats as for the default reactions):

- X(ion, n)Y reaction (in text) (max 48 characters).
- Name of ion (max 24 characters).
- Net charge of ion (integer).
- Is the target a gas target (yes/no)?
- Is there a fix ratio of the "reactive material"/"matrix material" (yes/no)?
- The OH/Li, H/Ti or D/Ti ratio. (=0.0 if the target is a single element).
- The abundance (in %) of the reactive isotope (^{7}Li has 92.5 % natural abundance).
- The number of the reactive target in the stopping power data list (integer usually equal to Z), and the number of the matrix target in the stopping power list (integer). The stopping power list, *StoppingData.txt*, also includes the densities for the included materials.

- Nuclear reaction: target-Z, target-A, ion-Z, ion-A, sec-Z, sec-A, rest-Z, rest-A. (integers, sec means here the neutron).
- The reaction Q-value (MeV).
- Lower energy limit for mono-energetic neutrons (MeV) and high energy limit for mono-energetic neutrons (MeV). These values are only used for indication of parasitic peaks in the user window and do not enter in any calculations.
- File name for cross section data and the Legendre polynomials coefficients for calculation of the double differential cross section data.
- The number of competing reactions. If no competing reaction exist this should be zero and the last line of the description of the reaction.
- The reaction number of the competing reaction, amount (example fraction of D in a TiT matrix), and possibility to change amount on-line in the program (yes/no).

Once the program has been started it is still possible to customize calculations. The number of simulated ions in SRIM-2008 can be changed as well as whether angular straggling should be included in the calculations (only SRIM-2008 simulation). Note that no competitive reaction is selected by default. Also, when changing main reaction, all competitive reactions are again deselected. When changing the ion energy, the target thickness and emission angle the chosen competitive reactions do not change.

For the SDEF card calculation it is possible to change the direction of the incident ion beam and the position where the neutron production starts. If, for example, a gas target with a 3 cm long gas cell is used and the geometry in the MCNP simulation is described with the end of the gas target at coordinates (0,0,0), the start of neutron production will be at coordinate (0,0,-3) and the default value must be changed. In this example the incident beam line is assumed to be the z-direction.

NEUTRON YIELD CALCULATIONS

The calculations are based on relativistic kinematics from Refs. [8], [9] after correction of some obvious misprints. The utilized deuteron breakup model [10] uses non-relativistic kinematics. The energy loss of the incident ions is calculated by slicing the target in 100 slices and calculating the stopping in every slice using stopping powers from Refs. [11], [12]. In addition, energy and angular straggling may be included by modelling the energy loss of the ions in the neutron producing target using SRIM-2008 [6] simulations.

For the calculations of neutron energies the notations from Horstmann and Liskien [9] are used:

M_1 = rest energy of ion
M_2 = rest energy of effective target nucleus
M_3 = rest energy of neutron
M_4 = rest energy of reaction product
$Q = M_1+M_2-M_3-M_4$ = Q-value (centre-of-mass sys)
T_1 = kinetic energy of ion (lab sys)
θ_3 = emission angle of neutron (lab sys)
T_3 = kinetic energy of neutron (lab sys)
T_4 = kinetic energy of reaction product (lab sys)
θ_3^c = neutron emission angle (centre-of-mass sys)
θ_3^{max} = maximum emission angle of the neutron in the double valued energy region $T_f < T_1 < T_b$ where T_f = forward threshold energy and T_b is backward threshold energy, *i.e. 90 degrees (lab sys)*
θ_4 = angle of reaction product (lab sys)

The threshold energies for forward, T_f, and backward, T_b, directions are calculated from

$$T_f = -\frac{Q}{M_2}\left(M_1 + M_2 - \frac{Q}{2}\right)$$

$$T_b = -\frac{Q}{M_2 - M_3}\left(M_2 - M_3 + M_1 - \frac{Q}{2}\right)$$

If the ion energy, $T_1 < T_f$ no neutrons will be generated. For ion energies in the double valued energy region, i.e. if $T_f < T_1 < T_b$, the maximum angle in the lab system of the neutron in this region is given by

$$\theta_3^{\max} = \arcsin\left(\sqrt{\frac{M_2 M_4}{M_1 M_3}\left(1 - \frac{T_f}{T_1}\right)\frac{1 + \dfrac{M_2 T_1}{2M_3 M_4}\left(1 - \dfrac{T_f}{T_1}\right)}{1 + \dfrac{T_1}{2M_1}}}\right)$$

If the given neutron emission angle θ_3 is larger then the maximum angle no neutrons will be generated. The neutron energy in the laboratory system is given by

$$T_3 = \frac{M_1 M_3}{(M_1 + M_2)^2} T_1 \beta_1 \left(2\cos^2\theta_3 + z\beta_2 \pm 2\cos\theta_3\sqrt{z\beta_3 + \cos^2\theta_3}\right)$$

$\pm$ for $T_f < \mathrm{T_1} < \mathrm{T_b}$ (double valued energy region)

$+$ for $T_1 > T_b$

where

$$\beta_1 = \frac{1 + \dfrac{T_1}{2M_1}}{1 + \dfrac{2T_1}{M_1 + M_2}\left(1 - \dfrac{M_1\cos^2\theta_3}{M_1 + M_2}\right) + \dfrac{T_1^2 \sin^2\theta_3}{(M_1 + M_2)^2}}$$

$$\beta_2 = \frac{1 + \dfrac{T_1}{M_1 + M_2}}{1 + \dfrac{T_1}{2M_1}}$$

$$\beta_3 = \frac{1 + \dfrac{T_1}{M_1 + M_2}\left(1 + \dfrac{M_2 - M_3}{2M_3}\left(1 - \dfrac{T_b}{T_1}\right)\right)}{1 + \dfrac{T_1}{2M_1}}$$

$$z = \frac{(M_1 + M_2)(M_2 - M_3)}{M_1 M_3}\left(1 - \frac{T_b}{T_1}\right)$$

The neutron emission angle in the centre of mass system is given by

$$\theta_3^c = \arccos\left(\frac{-\gamma^2 k \cdot \sin^2\theta_3 \pm \cos\theta_3 \sqrt{\cos^2\theta_3 + \gamma^2\left(1-k^2\right)\sin^2\theta_3}}{\cos^2\theta_3 + \gamma^2 \sin^2\theta_3} \right)$$

$\pm$ for $T_f < \mathrm{T_1} < \mathrm{T_b}$ (double valued energy region)

$+$ for $T_1 > T_b$

where

$$\gamma = \frac{1 + \dfrac{T_1}{M_1 + M_2}}{\sqrt{1 + \dfrac{2T_1 M_2}{\left(M_1 + M_2\right)^2}}}$$

$$k = \sqrt{\frac{M_1 M_3}{M_2 M_4\left(1 - \dfrac{T_f}{T_1}\right)}} \cdot \sqrt{\frac{1 + \dfrac{T_1}{2M_1}}{1 + \dfrac{T_1 M_2}{2M_3 M_4}\left(1 - \dfrac{T_f}{T_1}\right)}} \cdot \frac{\left(1 - \dfrac{Q}{M_1 + M_2}\right)\left(1 + \dfrac{M_2 T_1\left(1 - \dfrac{T_f}{T_1}\right)}{M_3\left(M_3 + M_4\right)}\right)}{1 + \dfrac{T_1}{M_1 + M_2}}$$

The Jacobian which transforms the differential solid angle from the centre of mass system to the laboratory system is given by

$$J = \pm\gamma \cdot \frac{1 + k \cdot \cos\theta_3^c}{\left(\sin^2\theta_3^c + \gamma^2\left(k + \cos\theta_3^c\right)^2\right)^{3/2}}$$

The Jacobian takes the minus sign in the double valued region. This is actually not noted in Ref. [8] but can easily be shown.

The differential cross section is described by a series of Legendre polynomials, P_i, in the centre of mass system

$$\frac{d\sigma}{d\omega}\left(\theta_3^c\right) = \frac{\sigma_{tot}}{4\pi \cdot A_0} \cdot \sum_i A_i P_i\left(\cos\theta_3^c\right)$$

The total cross section, σ_{tot}, is linearly interpolated from tables given in Refs. [1], [2], [13], [14]. Also the A_i parameters are linear interpolations from coefficients recommended in the same reference. For the programme execution, the values are given in the input data files *react_xx.txt*.

By dividing with the Jacobian the differential cross section is transformed from the CM system to the laboratory system

$$\frac{d\sigma}{d\omega}(\theta_3) = \frac{\dfrac{d\sigma}{d\omega}(\theta_3^c)}{J}$$

The neutron yield for the particular nuclear reaction, ion energy and neutron emission angle is given by

$$Y = \frac{I}{zq}\left(1 - e^{-\frac{d\sigma}{d\omega}(\theta_3)\cdot N_t}\right) \quad \frac{neutrons}{sr\ s}$$

where I is the ion beam current, zq is the ion beam charge and N_t is the number of target nuclei/cm^2. N_t is calculated from:

$$N_t = \frac{t_r \cdot N_A}{M_r}\frac{1}{\sin\alpha}$$

where t_r and M_r are the area density (g/cm^2) and the molar mass (g/mol) respectively for the reactive material and N_a is Avogadro's constant. When the energy loss is determined by the SRIM-2008 program, the deviation, α, of the ion relative to the incident beam line is known as a function of position in the target. This corrects for the increase in material as seen by ions with increasing deviation.

The fluence rate at distance d (cm) is calculated from

$$F = \frac{Y}{d^2} \quad \frac{neutrons}{cm^2\ s}$$

For gas targets, the laboratory neutron emission angle, θ_3, as well as the distance to the target depend on the position inside the target gas cell and is recalculated for all 100 slices. For solid targets this is assumed to be the same (thin targets).

Deuteron break-up

The deuteron break-up reaction D(d,np)D appears as a competing reaction to the D(d,n)^{3}He reaction and is calculated from a model discussed in Ref. [10]. The double differential cross sections are calculated in 100 steps for neutron energies up to the maximum energy. This is done for each of the ion energies corresponding to the 100 slices the target is divided into followed by a calculation of a summed neutron spectrum. If the ion energy loss is calculated using SRIM-2008, the procedure is repeated for all ions in the simulation followed by the calculation of the average.

For the calculation of the differential cross section for a certain laboratory neutron energy and laboratory emission angle, the laboratory energy and emission angle are converted to the CM system. The double differential cross sections for forward direction in the CM system are calculated using the energy of the neutron with the highest kinetic energy. The double differential cross sections for other emission angles and energies in the CM system are calculated by multiplying the cross sections for the forward direction with a function. Finally, the CM double differential cross section is converted to the laboratory system.

Below follows a detailed explanation of the calculations. Some changes compared to Ref. [10]. have been made after discussion with N. Kornilov. Note that the model uses non-relativistic kinematics in contrast to the relativistic treatment in the rest of the program. The notations from Ref. [10] have been kept to ease comparison. For the D(d,np)D reaction one gets:

$$E^c = E - 2\sqrt{E\varepsilon_0}\cos\theta + \varepsilon_0$$

$$\cos\theta^c = \frac{\sqrt{E}\cos\theta - \sqrt{\varepsilon_0}}{\sqrt{E^c}}$$

$$\frac{d^2\sigma}{dE^c d\Omega^c} = J\frac{d^2\sigma}{dEd\Omega}$$

$$J = \sqrt{E^c / E}$$

Where the index ^{c} indicates the centre of mass (CM) system, E the neutron energy, θ the emission angle. J is the Jacobian for conversion from the Laboratory system to the CM system and

$$\varepsilon_0 = \frac{m_n m_d}{(2m_d)^2}E_0$$

Where m_n is the neutron mass, m_d is the deuteron mass and E_0 is the incident deuteron energy.
The maximum neutron energy in the laboratory system for a certain emission angle can be calculated by assuming that the proton energy is zero. The cross sections depend on the maximum neutron energy in the CM system, which is calculated from (in MeV)

$$E^c_{\max} = \frac{m_d}{2m_d}\cdot\frac{m_p + m_d}{m_n + m_p + m_d}(E_0 - E_{th}) = 0.1874\cdot(E_0 - 4.45)\cdot 2$$

$$E_{th} = \frac{2m_d}{m_d}Q$$

The double differential cross sections in the CM system are first calculated for the forward direction where the neutron spectrum is “nearly” symmetric and the average neutron energy is calculated from

$$\langle E^c \rangle = \frac{E^c_{max}}{2}$$

The following relation of the average energy and dispersion is valid the forward direction, see Ref. [10]

$$\frac{S}{\langle E^c \rangle} = 0.541 - 0.0172\cdot E_d$$

where E_d is the incident deuteron energy. The neutron spectrum, $\varphi(E^c)$, is then calculated from

$$\varphi(E^c) = \begin{cases} 6.926\cdot10^{-2}\cdot\left(\frac{\langle E^c\rangle}{S}+x\right)/\left(\frac{\langle E^c\rangle}{S}-2\right); & -\frac{\langle E^c\rangle}{S} < x < -2 \\ 0.3642 + 2.49\cdot10^{-3}\cdot x - 0.1124\cdot x^2 - 1.778\cdot10^{-3}\cdot x^3 + 9.085\cdot10^{-3}\cdot x^4; & -2 \le x \le 2 \\ 5.078\cdot10^{-2}\cdot\left(\frac{\langle E^c\rangle}{S}-x\right)/\left(\frac{\langle E^c\rangle}{S}-2\right); & 2 < x < \frac{\langle E^c\rangle}{S} \end{cases}$$

where $<E^c>$ is the mean energy and

$$x = \frac{E^c - \langle E^c \rangle}{S}$$

The spectrum is normalized by dividing with the factor

$$0.97362 + 0.0600175 \cdot \left(\frac{\langle E^c \rangle}{S} - 2 \right)$$

Since the spectrum is given using reduced x, the spectrum is transformed by dividing with *S*.
The transformed normalized spectrum is then multiplied with the differential cross section in forward direction, which in the CM system is described by

$$\frac{d\sigma}{d\Omega^c} = 7.218 \cdot \left(1 - \exp(-0.910 \cdot \alpha)\right) \cdot \alpha \quad \text{(mb/sr)}$$

where

$$\alpha = \frac{(E_d - 4.45)^2}{E_d} \quad \text{(MeV)}$$

Once the double differential cross section is obtained for the forward direction, the double differential cross section can be obtained as a function of the angle from

$$\frac{d^2\sigma}{dE^c d\Omega^c} = f(E^c, \theta^c) \cdot \frac{d^2\sigma}{dE^c d\Omega^c}\left(E^c, 0°\right),$$

where

$$f(E^c, \theta^c) = \frac{1 + \beta \cdot E^c \cos^6 \theta^c}{1 + \beta \cdot E^c}.$$

Based on a linear fit to three β values given in Ref. [10], as a function of incident deuteron energy, β is calculated from

$$\beta = -0.4878 \cdot E_d + 8.8796.$$

After transforming the double differential cross section to the laboratory system using the Jacobian, the neutron yields for the laboratory neutron energies are calculated from the amount of active material in a particular slice and the calculated cross section. The subsequent calculations are identical to the yield calculations of the main reaction.

EXAMPLES

In Figure 6 the neutron spectrum for a 2000 μg/cm^2 LiF target and an ion energy of E_p = 4 MeV at 10 cm distance and 30° emission angle is shown. The yield from the reactions ^{7}Li(p,n)^{7}Be and ^{7}Li(p,n)^{7}Be* are clearly seen. The results compare well with the results from the Target code concerning the energy straggling. However the absolute yield is slightly different and the Target code

does not include the parasitic reaction. Thus, the model for energy straggling [15]and angular straggling [16] in the Target code are consistent with the results from SRIM-2008 [6].

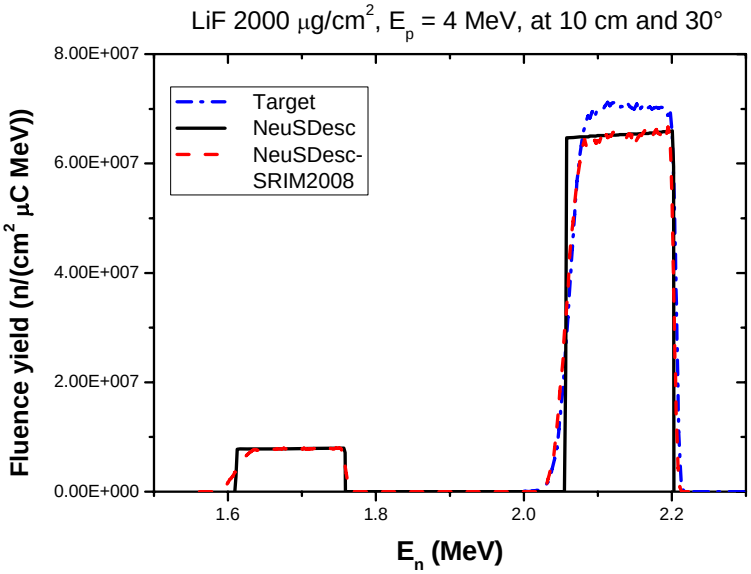

Figure 6. The neutron fluence for 4 MeV protons on a 2000 μg/cm2 LiF target at 30°, 10 cm from the target. The results are shown for the Target code as well as for the two methods of simulating the ion beam energy loss in the NeuSDesc program. The parasitic peak from the reaction ^{7}Li(p,n)^{7}Be* is clearly seen (lower energy *peak) in the NeuSDesc spectra, however, not included in the Target code calculation.*

point	X-coordinate (cm)	Y-coordinate (cm)	Z-coordinate (cm)	Δ LiF (%)	Δ D-gas (%)
1	80.30	0.00	12.72	0.139	0.271
2	44.47	0.00	47.68	-0.757	0.382
3	74.34	0.00	-39.53	0.110	0.129
4	85.79	0.00	-1.50	-0.004	0.041
5	17.19	0.00	42.56	-0.198	-0.148
6	-11.78	74.39	-40.05	-0.133	0.150
7	17.23	-88.64	31.09	-0.228	-0.131
8	-96.74	5.07	11.89	-0.141	-0.012
9	46.88	-60.01	-12.06	0.274	0.126
10	-13.43	0.00	-50.13	-0.088	0.317

Table 2. 10 randomly calculated positions in which the flux was determined with the MCNP program using the SDEF card generated by NeuSDesc. Δ is the difference in yield as calculated by MCNP and directly by NeuSDesc and given in percent for the ^{7}Li(p,n)^{7}Be and D(d,n)^{3}He reactions. Incident ion energy was in both cases 3 MeV.

The accuracy of the SDEF card describing the neutron source for MCNP was tested for a 2000 μg/cm^2 LiF target, with the reaction ^{7}Li(p,n)^{7}Be, and a 4 cm deuterium gas target with 100 kPa gas pressure and the D(d,n)^{3}He reaction. The incident ion energy was in both cases 3 MeV. The fluxes were determined in 10 random points and the coordinates of the points and the difference in flux compared to a direct determination with NeuSDesc are shown in Table 2. The fluxes are consistent in all points. The result for the MCNP is given in the unit neutrons/cm^2 normalised to one source neutron. In the output file describing the SDEF card from NeuSDesc the neutron source strength is also given. This value is multiplied with the normalised yield calculated by MCNP.

The MCNP calculated energy distribution of the neutrons 20 cm from a deuterium gas target at 90° emission angle is given in Figure 7. Also shown is the direct calculations from NeuSDesc using the "Calculate spectrum, full angle" option which integrates the flux over the surface of a disc, here with a radius of 1.4 cm. In principle the same type of integration is performed by MCNP and the two results are consistent.

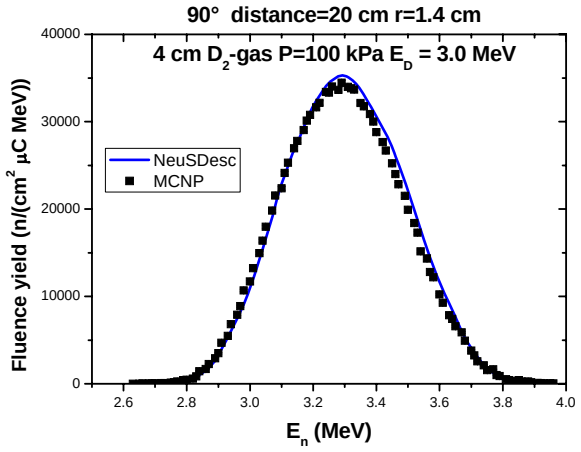

Figure 7. Neutron fluence yield calculated with MCNP using the SDEF card created by NeuSDesc, and the direct result calculated from NeuSDesc. The neutrons were calculated with the reaction D(d,n)^{3}He using a 4 cm long deuterium gas target (100 kPa) and E_d = 3.0 MeV. The fluence is calculated for a disc with radius 1.4 cm put 20 cm form the neutron source at 90° relative to the beam line.

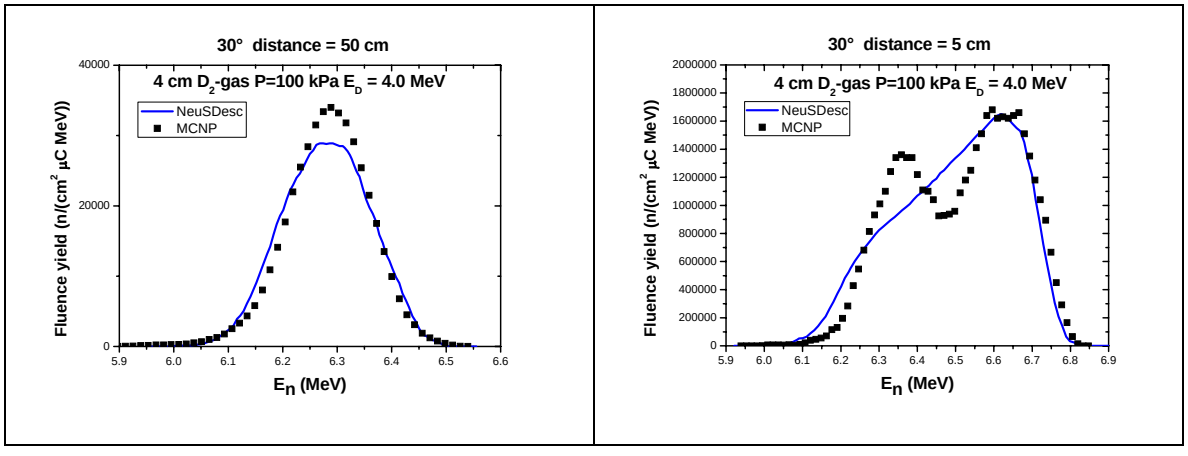

Figure 8. Illustration of the effect of using only 5 point sources compared to the 100 slices. At a distance of 50 cm a rather good agreement is obtained (left curve), while at 5 cm from the front of the target, a false spectrum is clearly obtained from the MCNP calculation (right curve).

Since the neutron source description for MCNP with the SDEF card is dividing the gas target in sections along the ion beam direction, a difference should be seen if the spectrum is determined very

close to the gas target. This is shown in Figure 8, where the spectra 50 cm away are in agreement but at 5 cm from the 4 cm long gas target are not consistent. The SDEF card used here 5 point sources and the structure of the poor resolution is clearly seen. It is not possible for the moment to use more point sources without reducing the number of angular intervals since MCNP can handle maximum 1000 cards.

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APPENDIX

SRIM energy loss treatment

NeuSDesc uses the *EXYZ* result file from the SRIM-2008 simulation. This file contains information about the intermediate energy and coordinates for the simulated ions. Since each ion has a unique energy loss also information concerning energy straggling can be calculated. In addition, the coordinates are used to calculate the deviation of the ion direction giving the possibility to estimate angular straggling. The positions in the *EXYZ.txt* file are, however, not equally spread and not randomly distributed. The result would render an artificial pattern in the calculated neutron spectrum which is avoided in NeuSDesc by using the energy loss given in the *EXYZ.txt* file only indirectly. The total energy loss for each ion is compared to the total energy loss estimated by the target slicing ion stopping calculations and a factor *f* is calculated from

$$f = \frac{\Delta E_{quick}}{\Delta E_{SRIM}} \ .$$

The factor is further on used to scale the *dE/dx* values from the target slicing ion energy calculations of the energy loss. The total energy loss for a SRIM estimation is given by

$$\Delta E_{SRIM} = \sum f \frac{dE}{dx} \Delta x \, .$$

If either the ion from the SRIM simulation or the target slicing calculation is stopped in the target material, the factor *f* is calculated from the last position of the stopped ion.

Rebinning

For some reactions the maximum neutron energy does not necessarily come from the reaction with the highest energy. This is consequence of the conversion from the CM system to the laboratory system. Also the highest energy neutrons are not always emitted in the forward direction in the laboratory system. However, for the energy binning procedure the maximum and minimum neutron energy needs to be known before calculating the neutron fluence. This is the case when the average fluence is determined for the randomized points on a disk. To find these minimum and maximum energies the program determines the spectra from the left side of the disk to the right in steps of 1 degree. A similar problem holds for the SRIM based energy loss spectra. Since many spectra are added, the minimum and maximum must be known before calculating the total spectra. Here, all spectra are calculated first and the minimum and maximum neutron energies are searched. Once these values have been found the total spectrum may be calculated after re-binning of all the calculated spectra.

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Abstract
The program *NeuSDesc* was developed at JRC-IRMM as a tool for calculating neutron fluence spectra generated by nuclear ion beams and binary nuclear reactions. The publication describes in detail how to install and use the programme, including theoretical approach and practical examples.

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