

# MeV Neutron Production from Thermal Neutron Capture in $^6\text{Li}$ Simulated With Geant4

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**Abstract.** Various Li compounds are commonly used at neutron facilities as neutron absorbers. These compounds provide one of the highest ratios of neutron attenuation to  $\gamma$ -ray production. Unfortunately, the usage of these compounds can also give rise to fast neutron emission with energies up to almost 16 MeV. Historically, some details in this fast neutron production mechanism can be absent from some modeling packages under some optimization scenarios. In this work, we tested Geant4 to assess the performance of this simulation toolkit for the fast neutron generation mechanism. We compare the results of simulations performed with Geant4 to available measurements. The outcome of our study shows that results of the Geant4 simulations are in good agreement with the available measurements for  $^6\text{Li}$  fast neutron production, and suitable for neutron instrument background evaluation at spallation neutron sources.

## 1. Introduction

The long (3ms) proton pulse of the European Spallation Source (ESS) [1] gives rise to unique background challenges for the instrument suite [2, 3, 4]. In such a long pulse spallation source, one of the main instrument performance limits is that defined by the instrument background, feeding into the Signal to Noise (S/N) ratio. The instrument requirements for ESS signal to noise ratio is  $> 10^6$  [5, 6] for many instruments. Such a signal to noise ratio is achievable, but absolutely cutting edge at spallation neutron sources, and in some cases is approaching electronic noise levels.

To achieve the required performance for each instrument, full beam line simulations must be carried out while taking into account all beam line components, choppers, shutters, collimator blocks and the beam dump, with different shielding configurations.

Several different materials can be used in the beam line to shield or to attenuate the neutron background. Amongst the different possibilities, the most used are boron or lithium compounds. The main disadvantage of boron compounds is the fact that the attenuation of the neutron beam is provided through neutron capture in  $^{10}\text{B}$  which releases an alpha particle, a  $^7\text{Li}$  ion and a 0.48 MeV photon. Whilst this gamma photon is considerably easier to manage compared to those from other absorbers, such as gadolinium or cadmium, in some cases it is an unwanted background contributor.

Li compounds on the other hand provide very good attenuation for thermal neutrons with almost no  $\gamma$ -ray production. Unfortunately, Li compounds can also produce fast neutrons of



energies up to almost 16 MeV. The physics process behind this is that, after being absorbed by  ${}^6\text{Li}$ , a neutron can induce a triton and an alpha particle with a cross section of 955 barns at 0.0253 eV [7]. The triton emitted with energy of 2.73 MeV slows down in the target and interacts with Li and other constituents of the compound to produce fast neutrons and  $\gamma$ -rays. Table 1 shows a summary of the physics processes involved.

This fast neutron production mechanism may be missing from some Monte-Carlo modeling packages often used for shielding design [8], depending on the optimization being used. At ESS, one of the radiation transport codes used for instrument background and shielding optimisation is Geant4 [9]. For the reasons explained above, it is important to assess that this toolkit is able to describe the fast neutron production process. To check the capabilities of Geant4, we simulated the fast neutron production from Li compounds and compared the results to available measurements from the following paper [10]. In that work, fast neutron yields from several Li and B compounds were measured and a summary of the results can be found in Table 2.

Table 1: Fast neutron and  $\gamma$  ray producing reactions

Primary Thermal			
neutron induced reactions			
Target	Branch	+Q(MeV), E <sub>max</sub> (MeV)	Ref
<sup>6</sup> Li	→ <sup>4</sup> He + t+	4.785 · E <sub>t</sub> =2.73	[11, 12]
Secondary triton			
induced reactions at E <sub>t</sub> ≤ 2.8 MeV			
Target	Branch	+Q(MeV),	Ref
<sup>6</sup> Li	→ <sup>9</sup> Be + γ +	17.7	[11, 12, 13, 14, 15, 16]
	→ <sup>8</sup> Be + n+	16.02	
	→ 2 <sup>4</sup> He + n+	16.115	
	→ <sup>5</sup> He + <sup>4</sup> He +	15.15	

Table 2: Fast neutron yields from targets of  ${}^6\text{Li}$  compounds from thermal neutron capture from the reference paper [10] and from Geant4 simulation.

Target	${}^6\text{Li}$ abundance (%)	measured yield per $10^6$ neutrons from reference paper <sup>1</sup>	simulated yield per $10^6$ neutrons with Geant4 <sup>2</sup>
${}^6\text{Li}$	96	$84 \pm 26$	$172 \pm 13$
LiH	7.5	$201 \pm 61$	$82 \pm 9$
LiF	7.5	$178 \pm 54$	$36 \pm 6$
$\text{Li}_2\text{CO}_3$	7.5	$107 \pm 33$	$17 \pm 4$

## 2. Geant4 Simulation toolkit

Geant4 is a Monte-Carlo toolkit for the simulation of the passage of particles through matter. The toolkit is developed by a worldwide collaboration of physicists, implemented in C++ and has an open source license. The code is used across a number of different scientific fields,

<sup>1</sup> The uncertainty in the yields includes the uncertainty due to the incident flux measurement, detector efficiency and any contribution of  $\gamma$  background for more details see [10]. These uncertainty do not include any possible contributions from sample impurity.

<sup>2</sup> This yield number is obtained using the QGSP\_BERT\_HP physics list

including high-energy physics, accelerator physics and medical and space science. The physics processes offered cover a comprehensive range, from meV and extending to TeV energies, and include electromagnetic, hadronic and optical processes with a large set of long-lived particles, materials and elements. The Geant4 set of physics processes to model the behavior of particles are decoupled from each another (for the most part) and the user selects these components in custom-designed physics lists that depend on the particles, the energy range and the process which are to be simulated.

In this work, the Geant4 calculations were carried out using Geant4 version 10.0 patch 3. The physics lists used for the calculations performed in this work are the QGSP\_BERT\_HP and QGSP\_INCLXX\_HP list. These lists are recommended for shielding applications [17]. QGS stands for quark-gluon string, which describes the high-energy interactions of protons, neutrons, pions, and kaons and nuclei. The high-energy interaction creates an excited nucleus, which is passed to the precompound model (P) which models the nuclear de-excitation. The label BERT refers to the Bertini intra-nuclear cascade model [18, 19], INCL to the Liege Intranuclear Cascade model [20], and HP for the high-precision neutron package [21]. The HP package uses evaluated neutron data, named G4NDL4.4, for interactions of neutrons below 20 MeV. This data largely comes from the ENDF/B-VII.0 libraries. Additionally included in this package is thermal scattering data for neutrons below 4 eV.

The Geant4 simulations presented in this work were performed with the ESS Detector Group framework [22]. The framework is a Geant4-based Python/C++ simulation environment which contains developments useful for neutron shielding and detector calculations.

### 3. Simulation of fast neutron production from $^6\text{Li}$

To compare the Geant4 results we used a simulation setup that matches as closely as possible the geometry described in the reference paper [10], to avoid that our results could be affected by any geometrical differences. As a neutron source, we used  $10^6$  mono-energetic neutrons, with a circular beam profile of diameter 2.5 cm, and with an energy of 0.025 eV. The  $^6\text{Li}$  target intercepted the whole of the thermal neutron beam and had a thickness of 1 mm. This is considered enough for a complete attenuation of the thermal neutron beam [10]. The lithium sample was surrounded by a sensitive detector fully covering  $4\pi$  steradians, to measure the energy of the neutrons coming out from the lithium sample and to avoid any neutron losses.

The observed neutron spectrum for the two different physics lists described above is shown in Fig. 1. This spectrum has the following interesting features:

- there are several fast neutrons with energies above 14 MeV that are consistent with the production mechanism from triton secondary interactions as described above.
- the shape of the fast neutron spectrum is similar to the spectrum from available measurements. (See Fig.5. of [10])
- the neutron yields obtained in the simulation (172) for the QGSP\_BERT\_HP and (151) for the QGSP\_INCLXX\_HP are on the same order of magnitude,  $10^2$ , as the measurements from the reference paper (see Table 2).

As an additional check of the physics processes, we also studied the energy spectrum of the mother particle from which the fast neutrons are produced. The study shows that all the fast neutrons were produced by triton induced reactions. The energy distribution of the tritons that generated the fast neutrons is shown in Fig. 2. The energy spectrum is consistent with tritons being produced from interactions of a thermal neutrons with  $^6\text{Li}$  and the spectrum is almost monoenergetic due to conservation of energy and momentum. In summary, all the features illustrated above show that the primary and secondary reactions are described reasonably well in the Geant4 simulation package.

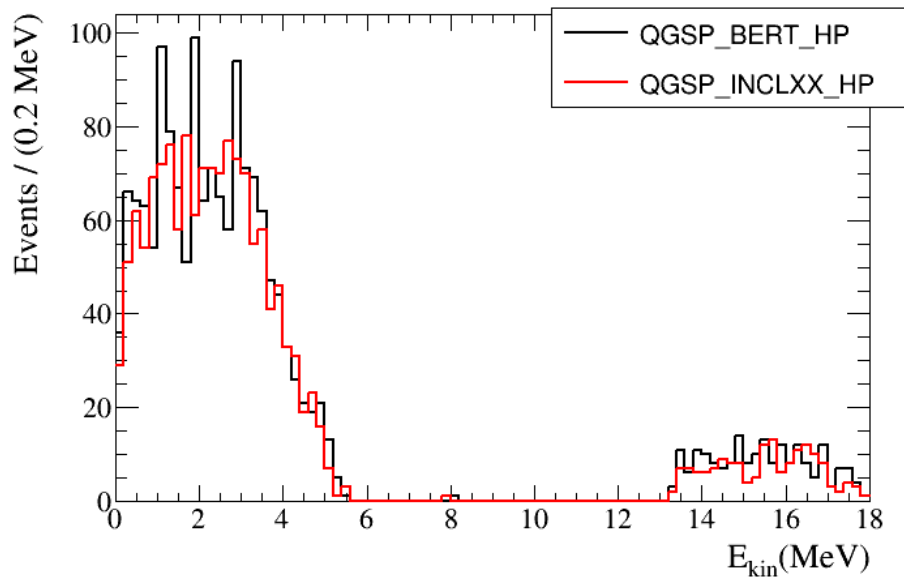


Figure 1: Energy spectrum of the fast neutrons produced by thermal neutron capture in  ${}^6\text{Li}$  for two different physics lists.

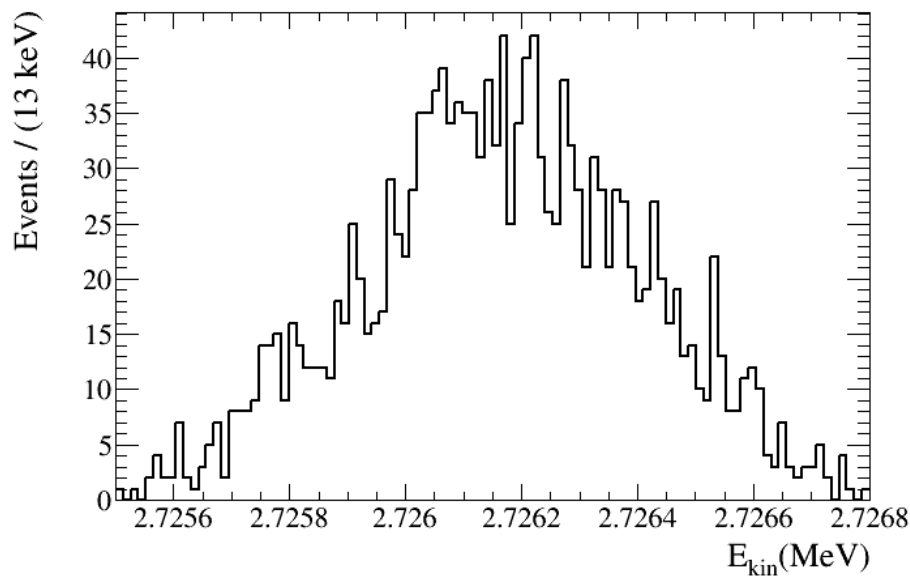


Figure 2: Energy spectrum of tritons produced by the reaction  ${}^6\text{Li}(n,t){}^4\text{He}$ .

#### 4. Lithium compound simulations

For completeness, we also tried to simulate several different Li compounds to compare with the expected yield from Table 2. The resulting spectra are shown in Fig. 3. The shape of the spectra for LiH, LiF and  $\text{Li}_2\text{CO}_3$  seems consistent with what is shown in the reference paper, but the yields are somewhat lower than expected (see Table 2). The differences between the measured and simulated spectra may be due to a number of factors. These include the lack of precise thermal neutron scattering data for some of the materials of interest; geometric and material

composition differences that are not fully documented; and the reliance on nuclear models for the charged particle interactions. This last point may be addressed with an up and coming package, titled G4ParticleHP [23], for Geant4. This package will introduce evaluated data for simulating the interactions of charged particles in Geant4. In order to further understand the origins of the differences between the measured and calculated spectra, a detailed investigation of the multi-step process would be necessary for each material.

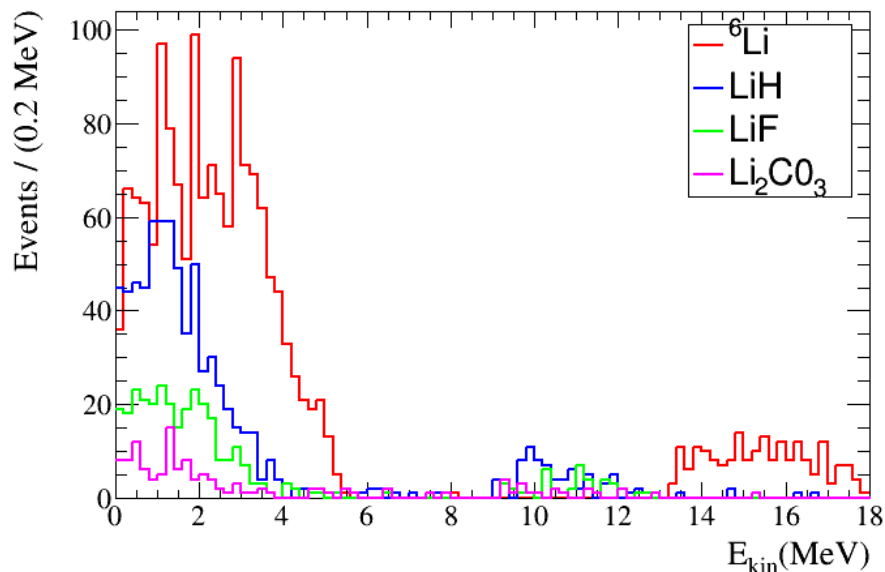


Figure 3: Energy spectrum of the fast neutrons produced by thermal neutron capture in different Lithium compounds

## 5. Conclusions

We have presented simulations of the fast neutron production channel of lithium absorption of thermal neutrons using Geant4. The simulations compare favourably with available measurements for  $^6\text{Li}$  fast neutron production in the literature. As such, we conclude that sufficient sensitivity and reliability exists in Geant4 for full beam line models of different instruments that are planned at ESS, where  $^6\text{Li}$  absorbers are the primary means of achieving efficient neutron shielding.

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