Validation of Geant4 simulation tool for low energy proton induced reactions

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Abstract. With the development of high-intensity accelerators, it is now envisaged to build compact high-intensity neutron sources for various applications. At the CEA Saclay, we have started a project to promote such technology based on the existing 100 mA IPHI proton injector. We are focusing our interest on low-energy proton-induced reactions (less than 20 MeV) to provide an economical way to produce neutrons and also to limit the radiological constraints. Optimization studies of the target-moderator assembly require validated simulation tools in order to maximize the neutron flux. In this document, the development status of the GEANT4-based simulation tool is presented, as well as its validation by comparison with gold foil activation measurements on the IPHI proton injector. The experimental setup and the simulation procedure are described. A good agreement is obtained between experimental data and simulation results when considering angular distribution of primary neutrons provided by Howard and Yanch’s measurements.

1. Introduction. The coupling of high-intensity accelerator technology and the concept of compact neutron source permits to envisage a large panel of applications, such as solid state physics studies with neutron scattering experiments, nuclear data measurements for nuclear industry, neutron radiography for industry materials qualification and also medical purposes like isotope production and neutron-capture therapy. Nevertheless, when dealing with high-intensity proton beams, many challenges appear. First from the accelerator side, strong space charges can induce emittance growth, beam halo and beam losses that have to be controlled. Then from the target/moderator side, heat removal is the main challenge for the target and the limiting parameter for beam intensity. At CEA Saclay, in France, we have started a project to promote such technology based on the existing 100 mA IPHI proton injector developed at IRFU within a CEA – CERN – CNRS collaboration [1]. We are focusing our interest on low-energy proton-induced reactions (less than 20 MeV) on beryllium (Be), aiming to provide an economical way to produce neutrons and also to limit radiological constraints. As most applications need moderated neutrons (less than 100 meV), the moderator/reflector assembly has to be optimized, in order to slow down primary fast-neutrons and to maximize the neutron flux on the sample, by using validated and predictive Monte-Carlo simulation tools (Geant4 version 10.02 [3]). In the following parts, we will present the development status of the GEANT4-based simulation tool and its validation by comparison with gold foil activation measurements.

2. Experimental validations of GEANT4 code. It is well-known that the efficiency of a moderator depends on the large neutron elastic cross sections of its constituents, a reduced neutron capture cross...
section and a large energy loss per collision for the scattered neutrons. For neutron energies at a few MeV, hydrogenous materials are the best suited moderator, slowing down neutrons in a few collisions (about 20). With its high hydrogen concentration and easy shaping, polyethylene (PE) was considered as a potential material for a neutron moderator. In this section, we describe an experimental validation of simulation neutron transport based on a simple geometry of PE moderator.

2.1 Experimental setup. To validate the simulation tool in terms of neutron transportation and moderation in PE moderator, we have performed an experiment using the high-intensity proton injector (IPHI) which was installed at CEA-Saclay. It consists of a proton source emitting 100 keV protons (the SILHI source) [1]. The protons are then accelerated in a Radio Frequency Quadrupole up to an energy of 3 MeV. The accelerator was designed to operate in continuous mode with proton currents up to 100 mA, corresponding to a maximum power of 300 kW. For tests, the accelerator was operated in pulsed mode with pulses of length 100 µs and a repetition rate of 1 Hz to minimize the number of fast neutron produced and be able to perform time-of-flight measurements. Figure 1 shows the scheme of the experimental setup with a simple moderator made of polyethylene. The proton beam was impinging on a thin beryllium target of thickness 0.5 mm. The support was air cooled to remove the heat deposit, limited to a maximum of 10 W for this test. The proton beam size was limited to 16 mm in diameter. The proton current incident on the target ranged from 2.6 to 3.1 µA.

![Figure 1: Scheme of the experimental set-up.](image)

The beryllium target was located close to the centre of a polyethylene (PE) moderator box (300x300x400 mm³) (see Figure 2). A 20 mm diameter hole was drilled through the moderator at 38 degree with proton beam axis (see Figure 2). To measure the neutron flux inside the moderator, 0.112 g gold foils, in the form of 6 mm diameter discs, were set at two positions inside the moderator (at 70 mm and 210 mm from the intersection of the proton beam axis with the neutron guide one). The foils were then irradiated for durations ranging from 15 to 22 minutes and a proton beam current of about 3 µA. ¹⁹⁸Au isotopes were formed from neutron capture on ¹⁹⁷Au and decayed by the emission of gamma-rays. The measuring of these latter leads to the number of ¹⁹⁸Au isotopes present in the foil after activation.
2.2 GEANT4 simulations. In the simulations of the experiment, we compared the effect of the energy and angular distributions by defining the neutron source term at the target position either from nuclear data using the particlehp package (ENDF/B-VII nuclear data library [4]) or from the energy and angular distributions measured by Howard and Yanch [5] at 3.7 MeV or the angular distribution measured by Marion [6] at 3.06 MeV combined with the energy distribution of Howard and Yanch at 3.0 MeV (see details in [2] and [7]). The lack of experimental data for 3 MeV proton beam does not allow a direct comparison with simulations, as only the total neutron yield and the angular distribution are available. The experimental distributions were normalized to the total neutron yield measured by Porges et al. [8] at 3.05 MeV, i.e. 3.0x10^{11} n/mA. For the particlehp calculation, the calculated neutron yield gives 2.19x10^{11} n/mA, i.e. 27% less than the experimental data. The neutron transport was realized using the neutron-data library G4NDL4.5 based on the evaluated ENDF/B-VII nuclear data library [4]. The thermal scattering library was also included for neutron energies less than 4 eV, to take into account for molecular effects. The density of PE was set to 0.94 g/cm³.

Gold foil activations were calculated along the cylinder hole with Geant4 and compared with experimental data (see Figure 3). The density of the gold discs was set to 19.320 g/cm³. The calculation using the angular distribution of Marion shows an underestimation for the whole range of measurements (roughly a factor 2) whereas using Howard and Yanch’s data a better agreement with experimental data is found but still below those ones. For this latter, an underestimation of about 30% is found close to the target while the discrepancy reduces to about 20% close to the exit hole. It clearly shows the effect of the angular distribution as data from Howard and Yanch are mainly focused in the forward direction whereas Marion’s one present a maximum near 120°. One may point out that the experimental uncertainties are of 20%, leading to a fair agreement in between experimental data and simulation results. However, a determination of angular distribution and neutron yield at 3 MeV could confirm the results and lead to useful information for moderator geometry optimization.

From these results we can extrapolate the thermal neutron flux for an installation based on 100 mA and 20 MeV protons on beryllium target. A gain in the neutron yield of a factor 200 can be achieved by increasing the proton energy from 3 MeV to 20 MeV (see details in [2]). The flux of the simple PE moderator would be of about 5.7x10^9 n/cm²/s (in pulsed mode with a typical duty cycle of the order of 4%) at a distance of 4 meters and a pinhole of size 5x5cm², the geometry corresponding to an L/D radio of about 80 as routinely used on the radiography station G45 at the Orphée reactor. With an optimized moderator-reflector geometry, a flux of about 1.0x10^7 n/cm²/s should be achievable. For neutron imaging applications, the ICON@SINQ beamline [10] provides a flux of about 1.3x10^7 n/cm²/s and the IMAGINE station at Laboratoire Léon Brillouin [11] provides a flux of about 1.0x10^7 n/cm²/s. These latter flux values are obtained for high L/D collimation ratio of 350. However, for industrial screening applications, low L/D ratios (~80) are not detrimental to the spatial resolution of the measurements. In absolute values, an imaging station on a pulsed compact source would be about 20 times less bright for high L/D ratios than a continuous source. This is due to the fact that
radiography techniques cannot benefit from the neutron pulse time structure. On the other hand, these figures suggest that techniques which can benefit from the time structure should be as efficient on a compact neutron source as on a medium power reactor or a continuous spallation source.

![Comparison of gold activation as a function of distance from $^9$Be target.](image)

3. Conclusion. A good agreement was observed between experimental data and simulation results for the transportation and the moderation of low-energy neutrons in polyethylene moderator. This permits to validate the transportation and the moderation process performed in GEANT4 using G4NDL library. Simulations put into light a wide influence of the angular distribution of emitted neutrons in the $^9$Be(p,n) reaction on the thermal neutron distribution inside the moderator. New measurements will be performed to confirm the angular distribution of the emitted neutrons for 3 MeV protons.

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