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GEANT4 SIMULATIONS OF PROTON-INDUCED SPALLATION FOR APPLICATIONS IN ADSR SYSTEMS

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Abstract

In order to assess the feasibility of spallation driven fission and transmutation, we have simulated proton induced neutron production using GEANT4, initially benchmarking our simulations against published experimental neutron spectra produced from a thick lead target bombarded with 0.5 and 1.5 GeV protons. The Bertini and INCL models available in GEANT4, coupled with the high precision (HP) neutron model, are found to adequately reproduce the published experimental data. Given the confidence in the GEANT4 simulations provided by this benchmarking, we have then proceeded to simulate neutron production as a function of target geometry and hence to some preliminary studies of neutron production in an ADSR with the geometry similar to that of the proposed Belgian MYRRHA project. This paper presents the results of our GEANT4 benchmarking and simulations.

INTRODUCTION

Spallation is exploited as a reliable technique for the production of high intensity neutron fluxes. Spallation sources generally use high intensity proton beams with energies of typically 1-2 GeV and a geometrically and materially optimised target. Spallation reactions can be simulated by Monte-Carlo based transport codes. In principal, the simulation codes record as many particle histories and probabilistic interactions as possible with the simulated events determined by sampling associated probability distributions. GEANT4, a Monte-Carlo based transport code developed by CERN, provides an extensive set of hadronic physics models for energies up to 10 - 15 GeV, both for the intranuclear cascade region and for modelling of evaporation [1]. These features enable the programme to describe the spallation process. We have evaluated the suitability of the GEANT4 code in simulating the spallation process by benchmarking GEANT4 results against published experimental observations [2] for various spallation target geometries. Having confirmed the suitability of GEANT4 for such simulations our subsequent goal is to optimise the target geometry for optimal neutron yield. Additionally, we have also generated the neutron energy spectrum resulting from embedding a spallation target within an assembly of thorium fuel rods and reflectors with a geometry similar to that of the proposed ADSR project MYRRHA [4,5].

Reference [2] provides the validation study of MCNP-4A code against experimental data taken from KEK, Japan. The experiment was designed to measure neutron spectra for a thick lead target bombarded with 0.5 and 1.5 GeV proton beams. The experiment was originally carried out at KEK in an attempt to resolve the discrepancy of neutron spectra between their calculated results and an experiment results in lead and tungsten targets 500 MeV protons. For these experiments the chosen target material was lead. The geometry is shown in Figure 1.

![Figure 1: Experimental arrangement, taken from [2].](image)

In the KEK study, a 12 GeV proton synchrotron supplied a stream of proton beams onto the spallation target after passing through a bending magnet. This process configured proton beams with a unique momentum suitable for the thick spallation target.

GEANT4 SIMULATION GEOMETRY

For our simulations the geometry was chosen to be as similar as possible to the configurations used in the experiments [2]. The spallation target was placed at the centre of a simulated space with detectors placed at 15, 30, 60, 90, 120 and 150 degrees with respect to the target and incoming proton beam; in most cases these were at a distance of 1 metre, though the detector at 15 degrees was placed at 1.5 metres [2]. GEANT4 provides numerous hadronic physics models describing particle interactions.

The physics lists used in this study were QGSP_BERT_HP which uses the Bertini intranuclear cascade model to describe the inelastic interactions of protons and neutrons, QGSP_BIC_HP which uses the Binary Cascade model, and QGSP_INCLXX_HP which uses the Liège model. All three physics lists were coupled with a high precision (HP) neutron model which uses evaluated neutron data libraries for neutron cross-sections below 20 MeV [5]. These physics lists were chosen because they are capable of predicting neutron production with a precise range of neutron energies, and they are the recommended physics models for simulating the neutron spallation processes [6, 7].

The area of “detectors” were set to 12.7 × 12.7 cm², the same size as the NE213 scintillator used in the KEK experiment.

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RESULTS OF THE SIMULATIONS

Figure 2 and 3 show the neutron spectra measured at various angles. It can be seen that there is a good agreement between the GEANT4 results and the experimental data. Furthermore, the GEANT4 simulations are closely comparable to those obtained from the earlier MCNP-4A simulations in [2].

In terms of the relative accuracy of the three physics models we have used, the QGSP_INCLXX_HP physics list produced the closest results to the experimental results, followed by the Bertini, whilst the Binary Intranuclear Cascade (BIC) proved to be the least accurate. The results from INCL at 0.5 GeV proton beam energy showed a match to the experimental results at every angle. The Bertini model also produced accurate results at between 0 and 10 MeV neutron energy (see Figure 2). At 1.5 GeV, INCL produced the most accurate outcome in relation to the experimental results in the neutron energy range between 0-10 MeV and 100-1000 MeV. However, the Bertini model produced better results than the INCL at the range between 10-100 MeV.

MYRRHA THORIUM FUEL STUDY

The above simulations indicate that GEANT4 is capable of modelling spallation neutron reactions in an energy regime useful for exploitation in an ADSR. We therefore carried out a preliminary simulation of neutron distributions in a thorium fuelled ADSR. MYRRHA (the multipurpose hybrid research reactor for high-tech applications) was chosen as an appropriate design geometry for the simulated ADSR. MYRRHA is a flexible fast spectrum research reactor (50-100 MWth), which is being designed to operate in sub-critical and critical modes [3]. The MYRRHA design proposes the use of a 600 MeV proton accelerator, a spallation target and a multiplying core with uranium based MOX fuel. The core area is cooled by liquid lead-bismuth [8], which also provides the spallation target material [9].

For the purpose of this study, we have replaced the reactor fuel by fertile thorium, a material which is currently attracting considerable interest as both a potential fuel and a matrix for transmutation of nuclear waste. In order to understand the effect of the reflector, the simulations were carried out with the shielding assemblies removed.

Table 1: Core specification Used in the Simulation

<table>
<thead>
<tr>
<th>Area</th>
<th>Material</th>
<th>Size (cm²)</th>
<th>Number place</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spallation target</td>
<td>PbBi</td>
<td>97.55 × 30</td>
<td>1</td>
</tr>
<tr>
<td>Fuel</td>
<td>Thorium</td>
<td>97.55 × 140</td>
<td>76</td>
</tr>
<tr>
<td>Reflector</td>
<td>PbBi</td>
<td>97.55 × 140</td>
<td>36</td>
</tr>
<tr>
<td>Shielding</td>
<td>Zirconia Y-TZP</td>
<td>97.55 × 140</td>
<td>42</td>
</tr>
</tbody>
</table>

The results of the GEANT4 simulations, figures 5 and 6, show the energy spectra of neutrons travelling from one region to another in the core. Each region was measured from the centre of the core on the size of a fuel assembly (i.e. region-1 97.55 cm, region-2 195.1 cm etc.). Figure 5 shows the number of outer going neutrons per proton. In the figure, the neutron spectrum for the region 1 to 2 shows the highest number of neutrons per proton. This result indicated that this region contributed to neu-

Figure 4: GEANT4 MYRRHA core configuration (Blue, spallation target, yellow thorium fuel, reflectors green, shields cyan).

Figure 5: Neutron flux at 0.5 GeV proton beam energy using GEANT4, with the experimental data taken from [2].

Figure 6: Neutron flux at 1.5 GeV proton beam energy using GEANT4, with the experimental data taken from [2].
tron production significantly. The number of neutrons produced from the spallation target is 16.68 neutrons per incident proton.

![Graph](image1)

Figure 5: Number of outer going neutrons into each region in the core as a function of neutron energy.

In Figure 6, the highest number of neutron back-scattered was recorded from the region 1 to the spallation target. The figure also shows that the neutron energy spectrum representing region 5 to region 4 is lower than in other regions.

![Graph](image2)

Figure 6: Number of neutrons back-scattered into each region in the core as a function of neutron energy.

Comparing neutron energy spectra between the reflector and the non-reflector as shown in Figure 7, the reflectors decrease the number of neutrons per proton in high neutron energy. The figure also indicates that the maximum neutron energy of the non-reflector result was recorded at 33.5 MeV while the highest neutron energy for the reflector was at 17.5 MeV. Regarding the number of neutrons escaping from the core per proton, there is no significant difference between the reflector and the non-reflector at the neutron energy range of 0-2 MeV. This result indicates that the nuclei of the reflector material (i.e. LBE) were not effective for stopping neutrons escaping from the reflector.

![Graph](image3)

Figure 7: Number of neutron escaped from the core as a function of neutron energy.

Comparing neutron energy spectra between the reflector and the non-reflector as shown in Figure 7, the reflectors decrease the number of neutrons per proton in high neutron energy. The figure also indicates that the maximum neutron energy of the non-reflector result was recorded at 33.5 MeV while the highest neutron energy for the reflector was at 17.5 MeV. Regarding the number of neutrons escaping from the core per proton, there is no significant difference between the reflector and the non-reflector at the neutron energy range of 0-2 MeV. This result indicates that the nuclei of the reflector material (i.e. LBE) were not effective for stopping neutrons escaping from the reflector.

**CONCLUSION**

We have shown that GEANT4 simulations of experimental spallation neutron production, at least as accurate if not more than MCNPX. The QGSP_INCLXX_HP physics list appears to reproduce the experimental results most closely.

For MYRRHA configuration study, it is conclusive that reflectors showed a significant effect to reduce the neutrons escaping from the core. However, the number of escaping neutrons per proton from the core was still at the high level. This suggests that extra shielding area is necessary for increasing neutron flux inside the core which reflects the rate of thorium-uranium conversion.

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**REFERENCES**