The MCNP Simulation of a PGNAA System at TRR-1/M1

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Abstract. The prompt-gamma neutron activation analysis system (PGNAA) has been installed at Thai Research Reactor-1/ Modified 1 (TRR-1/M1) since 1999. The purpose of the system is for elemental and isotopic analyses. The system mainly consists of a series of the moderator and collimator, neutron and gamma-ray shielding and the HPGe detector. In this work, the condition of the system is carried out based on the Monte Carlo method using Monte Carlo N-Particle transport code and the experiment. The flux ratios (Φ_thermal/Φ_epithermal and Φ_thermal/Φ_fast) and thermal neutron flux have been obtained. The simulated prompt gamma rays of the Portland cement sample have been carried out. The simulation provides significant contribution in upgrading the PGNAA station to be available in various applications.

1. Introduction

The prompt gamma neutron activation analysis (PGNAA) is a non-destructive technique for an elemental and isotopic analytical. The PGNAA system has been widely used for analyzing the elements. The neutron interacts with the sample and was captured with the nucleus of the sample so called a compound nucleus. The compound nucleus is formed in an excited state which then de-excites to the ground state in 10⁻¹⁴ s by released the prompt characteristic gamma ray for each element. The PGNAA technique is based on the neutron inelastic scattering (n, n'γ) and thermal neutron capture (n_th, γ) and measuring a prompt gamma spectrum which emitted from the sample.

The PGNAA have been designed based on different neutron source such as the accelerator neutron source [1-4] and reactor thermal neutron source [5-9]. The system at Thai Research Reactor 1/Modified 1 (TRR-1/M1) was designed based on the reactor thermal neutron source. It was constructed and installed since 1999 [10]. The aim is to use this technique in Thailand to analyze elements in various samples. The TRR-1/M1 is a pool type reactor with light water moderator and cooling. It is operated with the maximum power of 1.2 MW. It provides a high thermal and fast neutron flux. There are four beam experimental ports available for the utilization. One of the four is for the PGNAA system. The facility descriptions and the simulation set up of the PGNAA system at TRR-1/M1 are described in section 2.

However, the existing PGNAA system suffers from the complicate structural, neutron source and neutron and gamma background. To expand the experimental capability of the PGNAA system, the calculations using a Monte Carlo code have been obtained using the Monte Carlo N-Particle transport code (MCNP) version MCNPX [11]. The MCNP code is the most widely used for all types of particle transport, e.g. neutron, photon, electron based on the evaluated nuclear data library (ENDF/B). It has
been widely used to validate the design calculation of the PGNAA [12, 13]. The simulation and experiment results are reported in section 3. Moreover, the yield of the prompt gamma rays from Portland cement sample have been obtained and presented in this section. The conclusion is in section 4.

2. Description of the facility and MCNP model

The main components of the PGNAA system at TRR-1/M1 include a series of annular collimators, beam shutter, shielding and a high purity germanium (HPGe) detector. The layout of the system shows in figure 1. The detector and detector shielding is not taken into account in this work.

![Figure 1. Horizontal cross section view of the PGNAA facility at TRR-1/M1, showing a series of collimators, beam shutter, shielding, sample area and detector position](image)

2.1. Neutron source

The PGNAA system at TRR-1/M1 was designed for the research reactor operating at 1.2 MW with the maximum thermal neutron flux and fast neutron flux at the central of the reactor core of $3.1 \times 10^{13}$ n.cm$^{-2}$.sec$^{-1}$ and $2.3 \times 10^{13}$ n.cm$^{-2}$.sec$^{-1}$ respectively. The thermal and epithermal neutron fluxes at the sample position were measured by irradiating gold-foil (the cadmium was used to separate the activities of epithermal neutron) and found to be $4.63 \pm 2.15 \times 10^{6}$ n.cm$^{-2}$.sec$^{-1}$ and $4.43 \pm 1.13 \times 10^{5}$ n.cm$^{-2}$.sec$^{-1}$ respectively [14].

The calculated neutron source from MCNP at the reactor beam port which including thermal neutron epithermal neutron and fast neutron have been provided. The uniform neutron source is placed at the beginning of the collimator for the simulation as depicted in figure 2. The diameter of the disk source is 4 cm which almost matching that of the collimator tube.

2.2. Collimator

The collimator consists of a series of lead and boron rings and teakwood. The purpose is to reduce the fast neutron flux, maintaining the high thermal neutron flux and collimate the neutron beam to the sample. The collimator was installed with the configuration described in figure 1. The inner diameter of the entrance collimator is 13.9 cm. The entrance of the collimator connects to the reactor core at a southeast beam port of the reactor pool. The end of the collimator connects to the shutter with the inner diameter of 3.68 cm. The overall collimator length is 290 cm.

The MCNP model of the annular collimator was provided and depicted in figure 2. The shell of the collimator model consists of stainless steel, lead, teakwood and borated polyethylene. A point detector (F5) tally was used to obtain the radiation flux at the sample area. Additional, the surface-crossing (F1) mesh tally at the collimator mid-plane is used to study the neutron and photon distribution.

2.3. Shutter

The rotating shutter is placed at the end of collimator. The shutter is used to stop the beam from the collimator to the sample area. The thickness of the rectangular shutter box is 30 cm. It comprises of
borated paraffin and lead and has a hole of about 4-cm diameter. In MCNP model, the shutter was modeled at the end of the collimator.

2.4. Biological shield
The shutter and sample are surrounded by a biological shield. It is a 30-cm thick box which is filled with steel shots and paraffin. It is mounted to the reactor wall and aimed to reduce background gamma and neutron radiation levels around the facility. Paraffin is used for the neutron moderator and steel shots are used for the thermal neutron capture and absorb prompt gamma and gamma rays from other structure. Sample was held at 45° angle to the beam and to the detector. The sample holder was held vertically from the 24 cm × 24 cm hold on the top side of the biological shield. The biological shield was modeled in this calculation.

![Figure 2. The collimator arrangement](image)

3. Results and discussions

3.1. The collimator characterization
In this section, the transmission of neutron from the reactor core to the biological shielding through the collimator was calculated. The mesh tally results of neutron and photon flux through the collimator and biological shield have been obtained and plotted with the geometry as shown in figure 3(a) and figure 3(b) respectively. The results show that the neutrons have been collimated by the collimator and transferred to the biological shield. Nevertheless, the results show that the biological shielding is not sufficiently thick enough that high neutron and photon fluxes leak out through the shielding.

![Figure 3. Mesh tally results from MCNP simulation of (a) neutron and (b) photon distribution in collimator and biological shielding](image)
The neutron and photon fluxes per source neutron at the collimator mid-plane are presented in figure 4. The neutron flux is constant through the collimator and biological shielding. About three orders of magnitude of neutron flux reduce at the end of the biological shield. In addition, the gamma fluxes produced by the interaction of neutron with the collimator and surrounding structure in the system have been obtained.

The neutron spectra per source neutron at the sample position have been calculated. It consists of the thermal neutron, epithermal neutron and fast neutron fluxes. The neutron flux ratios ($\Phi_{\text{thermal}}/\Phi_{\text{epithermal}}$ and $\Phi_{\text{thermal}}/\Phi_{\text{fast}}$) have been conducted. The ratio of $\Phi_{\text{thermal}}/\Phi_{\text{epithermal}}$ is equal to 10.15 while $\Phi_{\text{thermal}}/\Phi_{\text{fast}}$ is equal to 5.11. The thermal neutron flux was $3.55 \times 10^7$ n.cm$^{-2}$.sec$^{-1}$ which higher than the experimental results by a factor of seven [14]. The in-scattering neutrons in collimator at sample position have been obtained as shown in figure 5. The 1.88 percent of in-scattering neutron in the collimator is found.

**Figure 4.** The mid-plane collimator neutron flux per source neutron (red line) and photon flux per source neutron (blue dash)

**Figure 5.** Total neutron spectrum per source neutron (blue line) and in-scattering neutron spectrum per source neutron (red dash) at the sample area
3.2. Beam characterization

3.2.1. Neutron. In this section the neutron beam shape was characterized by the experiment and simulation. In the experimental set up, the neutron radiograph imaging plates were used to measure the neutron while the shutter opened and closed. The imaging plates were placed perpendicular to the neutron beam from the collimator at sample position at 20 cm from the shutter. The results were used to determine the dimension and shape of neutron beam. The image and profile of measured neutron beam shape while the shutter opened show in figure 6(a). The results show that the neutrons beam relatively distribute in a Gaussian function over 2-cm diameter, approximately. The outer beam is not symmetrical, it distributes more toward to the right side. The beam size is 6-cm diameter approximately. The image and profile of neutron distribution at the sample position while the shutter was closed are presented in figure 6(b). The intensity of the neutron at the center of the beam is higher than the outside the beam by a factor of 1.2 approximately.

For the simulation using MCNP code, the results of the neutron beam distribution and profile show in figure 7. The beam distributes with a Gaussian function over 6-cm diameter approximately.

**Figure 6.** The image and profile of the neutron beam at the sample position: (a) opened shutter and (b) closed shutter

**Figure 7.** The distribution and profile of the neutron beam at the sample position using the MCNP simulation
3.2.2. Gamma. In the experimental set up, the gamma ray was determined using the sensitive gamma radiograph imaging plates while the beam shutter opened and closed as neutron beam. The image and profile of measured gamma ray while the shutter opened show in figure 8(a). The results show the non-symmetrical. The flux is high on the left side. This is similar to the results while the shutter closed in figure 8(b) which the distribution shows a high flux on the left side of the beam due to the non-symmetrical of the shutter.

In the simulation, the gamma ray was calculated to determine the effectiveness of the neutron to the surrounding structure. The 0.47 MeV and 7.6 MeV peak of gamma ray produced from boron and iron are found as presented in figure 9(a).

![Figure 8. The image and profile of the gamma rays at the sample position: (a) opened shutter and (b) closed shutter](image)

3.3. Simulation of the Prompt gamma ray yield of Portland cement sample

In this section, the yields of prompt gamma rays from the cylinder Portland cement sample have been calculated. The sample model held at 45° angle to the beam at distance 20 cm from the beam shutter with the thickness of 1 cm and radius of 6 cm. The chemical composition of the Portland cement is given in table 1.

| Compound | Composition weight (%) |
|----------|------------------------|
| SiO₂     | 20.52                  |
| Al₂O₃    | 5.64                   |
| Fe₂O₃    | 3.80                   |
| CaO      | 64.35                  |
| MgO      | 2.11                   |
| SO₃      | 2.10                   |
| K₂O      | 0.36                   |
| Na₂O     | 0.19                   |

Table 1. The chemical composition of Portland cement [4]

The energies of the prompt gamma ray have been carried out by subtracting background radiation and presented in figure 9(b). The 2.23 MeV photon peak is found due to the neutron capture reaction (n,γ) of the neutron in the polyethylene shielding. Moreover, the 3.55 MeV and 4.95 MeV of the prompt gamma rays due to capture the thermal neutron in silicon in the cement sample are observed.
The 7.63 MeV and 7.64 MeV of the prompt gamma rays due to the thermal neutron capture reactions of the iron in cement sample are found.

![Figure 9.](image)

**Figure 9.** (a) Background gamma ray spectrum per source neutron and (b) the prompt gamma ray spectrum per source neutron of the Portland cement without the background radiation

### 4. Conclusion

The MCNP model of the PGNAA system at TRR-1/M1 have been set up. The simulation results show that the neutrons are well collimated through the collimator. At the sample position, the number of $\Phi_{\text{thermal}}/\Phi_{\text{epithermal}}$ and $\Phi_{\text{thermal}}/\Phi_{\text{fast}}$ have been obtained. The calculated thermal neutron flux at the sample position is higher than the measured one by a factor of seven. However, to improve the results, the detector efficiency will be considered. The neutron beam shape at the sample position is characterized by both experimental set up and calculation. The disagreement between the experiment and simulation are found. The non-symmetrical shape shows in the experimental result while the simulation result is well symmetry. The improvement of the MCNP model is needed by taken the surrounding structure in the reactor hall into account. In addition, the prompt gamma ray spectrum from a sample of Portland cement is calculated. The results provide an information in order to fabricate the experimental set up. For the future work, the detector, detector shielding and sample size will model and optimize using the MCNP simulation. Since, there is a plan to upgrade the PGNAA system in 2016-2017, thus the simulation results will provide significant contribution in upgrading the system. The improvement of the facility will be a great asset to be available in various applications.

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