Validation of the MCNP computational model for neutron flux distribution with the neutron activation analysis measurement

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Abstract. The objective of this work is to demonstrate the method for validating the predication of the calculation methods for neutron flux distribution in the irradiation tubes of TRIGA research reactor (TRR-1/M1) using the MCNP computer code model. The reaction rate using in the experiment includes ²⁷Al(n, α)²⁴Na and ¹⁹⁷Au(n, γ)¹⁹⁸Au reactions. Aluminium (99.9 wt%) and gold (0.1 wt%) foils and the gold foils covered with cadmium were irradiated in 9 locations in the core referred to as CT, C8, C12, F3, F12, F22, F29, G5, and G33. The experimental results were compared to the calculations performed using MCNP which consisted of the detailed geometrical model of the reactor core. The results from the experimental and calculated normalized reaction rates in the reactor core are in good agreement for both reactions showing that the material and geometrical properties of the reactor core are modelled very well. The results indicated that the difference between the experimental measurements and the calculation of the reactor core using the MCNP geometrical model was below 10%. In conclusion the MCNP computational model which was used to calculate the neutron flux and reaction rate distribution in the reactor core can be used for others reactor core parameters including neutron spectra calculation, dose rate calculation, power peaking factors calculation and optimization of research reactor utilization in the future with the confidence in the accuracy and reliability of the calculation.

1. Introduction
The research reactor (TRIGA- Mark III) at Thailand Institute of Nuclear Technology (TINT) referred to as TRIGA Research Reactor Modified I (TRR-1/M1) is most commonly used as neutrons sources for gem irradiation, isotope production, neutron radiography and scientific investigation using nuclear analytical techniques. Knowledge of the reactor physical parameters including neutron flux, gamma flux, neutron profiles, power profile and temperature profiles are very important to ensure safe operation, to manage for fuel loading pattern, to optimize for the fuel shuffling and to support experiment at the reactor. For the nuclear analytical techniques and neutron activation analysis (NAA), the accurate neutron spectral characteristics and neutron flux profile are crucial for the assessment of the uncertainty of the experiment and the accuracy of the method. Monte Carlo calculation with the MCNP code [1] has been validated against experimental measurements for the neutron flux and reaction rate. The computational methods, particularly geometry model of the reactor core using the

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Monte Carlo is very powerful in providing the results for the neutron flux spectrum and the reaction rate distribution. The main objective of this study is to compare between the experimental and the calculated values from a computational model. Validation is conducted to test computational model capability in predicting the measured neutron flux distribution in the reactor core and irradiation tubes of TRR-1/M1. The results from this study can be used to support for the consistency of the MCNP results with the experimental results and to improve accuracy and reliability of the NAA results.

2. Experiments and Measurements

The neutron activation analysis was used to verify the calculated neutron flux distribution in different location of the TRIGA reactor. The experiment used aluminum 99.9%wt and gold foil (disk of 0.25 cm radius and 0.0005 cm thick) which were irradiated in 9 locations in the reactor core. The positions of the foils in the reactor core during irradiation are demonstrated in figure 1. Gold foils and gold foil covered with cadmium samples were irradiated with reactor power 10 kW for 20 minutes and 40 minutes, respectively. Aluminum samples were irradiated at 500 kW for 20 minutes. After the irradiation, the gamma ray count rates were measured with high purity germanium detector (HPGe) detector for calculating the specific activities of irradiated samples.

![Figure 1. Schematic top view of TRIGA. The location of aluminium and gold foils used in the experiment are in In-core irradiation tubes (pink).](image-url)
The activation reactions which were used in the experiments are as follows:

\[ ^{27}\text{Al}(n,\alpha)^{24}\text{Na} \rightarrow ^{24}\text{Na} \xrightarrow{t_f=15\text{ hr}} ^{24}\text{Mg} + e^- + \gamma (E = 1368.6\text{ keV}) \] (1)

\[ ^{197}\text{Au}(n,\gamma)^{198}\text{Au} \rightarrow ^{198}\text{Au} \xrightarrow{t_f=2.7d} ^{198}\text{Hg} + e^- + \gamma (E = 411.8\text{ keV}) \] (2)

\(E\) is the energy of the most prominent gamma ray. The threshold for the first reaction which is illustrated in equation (1) has energy threshold at 5 MeV which is used for the fast neutron flux measurement. The cross section for the second reaction \(^{197}\text{Au}(n,\gamma)\) is the highest for the energy below 10 keV, therefore, this reaction is useful for the investigation of the thermal neutron flux \((E < 0.625\text{ eV})\) and epithermal neutron flux \((0.625\text{ eV} < E < 100\text{ keV})\). Figure 2 shows the cross section for \(^{197}\text{Au}(n,\gamma)^{198}\text{Au}\) and \(^{27}\text{Al}(n,\alpha)^{24}\text{Na}\) reactions from ENDF/B-VII nuclear data library [2].

![Figure 2. Cross sections for \(^{197}\text{Au}(n,\gamma)^{198}\text{Au}\) and \(^{27}\text{Al}(n,\alpha)^{24}\text{Na}\) reaction and Cd from ENDF/B-VII nuclear data library [2].](image)

3. MCNP Computational Method

3.1. MCNP Computer Code
The MCNP computer code was used for reaction rate and neutron flux calculation [1]. MCNP is a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport. Pointwise cross-section data typically are used, although group-wise data also are available. For neutrons, all reactions given in a particular cross-section evaluation (such as ENDF/B-VI) are accounted for. Thermal neutrons are described by both the free gas and S(\(\alpha,\beta\)) models. For photons, the code accounts for incoherent and coherent scattering, the possibility of fluorescent emission after photoelectric absorption, absorption in pair production with local emission of annihilation radiation, and bremsstrahlung.

3.2. TRR-1/M1 Computational Model
The geometrical model of TRIGA-Mark III (TRR-1/M1) reactor was modelled for accurately calculated physical parameters of the TRIGA reactor. The model is compared to the criticality benchmark model, which is described and published in the International Handbook of Evaluated Criticality Safety Experiments [3]. The simplified model can be used in calculations of the effective multiplication factor \(k_{eff}\) [4], power peaking factor [5] and reactor kinetic parameters [6]. The model of
the TRR-1/M1 simplification of the geometry is modeled by neglecting the surrounding detailed of the core to an extent that does not affect neutron flux and $k_{\text{eff}}$ significantly. MCNP calculations were performed in kmode for criticality calculations using $3 \times 10^3$ neutrons per cycle and 1000 active cycles. The standard deviations were used as uncertainties for the calculations. A criticality source (ksrc card) was utilized in this study. The initial fission neutron source distribution used the source point as the input for ksrc card. Reaction rates of $^{197}\text{Au}(n, \gamma)^{198}\text{Au}$ and $^{27}\text{Al}(n, \alpha)^{24}\text{Na}$ reactions in individual irradiation tubes are calculated by multiplying neutron flux in the irradiation tubes with corresponding cross section (figure 2). The Monte Carlo results of neutron flux are normalized per one fission neutron. Therefore the results have to be properly scaled in order to compare the neutron flux values with the measurement quantities. The absolute values of neutron flux are directly proportional to the reactor power level. The calculation results have to be scaled according to the known power level. The scaling factor is defined in the following equation:

$$\Phi = \frac{\Phi_{\text{MCNP}}}{w_{k_{\text{eff}}}}$$

(3)

where $P$ is the power level, $\bar{n}$ is the average number of neutrons per fission, $w$ is the average energy per fission and $k_{\text{eff}}$ is the effective multiplication factor determined in the MCNP run. The neutron flux parameters are referred to as thermal neutron flux, epithermal neutron flux and thermal to epithermal neutron flux ratio were calculated [7, 8].

4. Results

The MCNP calculated $^{197}\text{Au}(n, \gamma)^{198}\text{Au}$, $^{197}\text{Au}(n, \gamma)^{198}\text{Au}$ covered with cadmium and $^{27}\text{Al}(n, \alpha)^{24}\text{Na}$ reaction rates which normalized to 1200 kW power of all In-core irradiation tubes are plotted compared with the measurement of bare gold, gold covered with cadmium and aluminium. Since the Monte Carlo results of neutron flux are normalized per one fission neutron, the absolute value of neutron flux or reaction rate is directly proportional to the reactor thermal power level. The measurements and the MCNP calculations for thermal, epithermal and fast neutron flux are illustrated in figure 3, 4 and 5, respectively.

4.1. Comparison between the MCNP model and the measurements

In the MCNP simulation, the energy interval for thermal neutron is $E < 0.625$ eV and epithermal neutron is $0.625$ eV $< E < 100$ keV and fast neutron is $E > 100$ keV. The average values for thermal flux in ring C was $(2.315 \pm 0.001) \times 10^{11}$, ring F was $(1.157 \pm 0.001) \times 10^{13}$ and ring G was $(8.492 \pm 0.001) \times 10^{12}$ n-cm$^{-2}$s$^{-1}$, respectively. The average values for epithermal flux in ring C was $(2.239 \pm 0.006) \times 10^{13}$, ring F was $(8.614 \pm 0.005) \times 10^{11}$ and ring G was $(4.691 \pm 0.004) \times 10^{11}$ n-cm$^{-2}$s$^{-1}$, respectively. The average values for fast flux in ring C was $(1.069 \pm 0.002) \times 10^{13}$, ring F was $(6.520 \pm 0.002) \times 10^{12}$ and ring G was $(3.194 \pm 0.001) \times 10^{12}$ n-cm$^{-2}$s$^{-1}$, respectively. In experimental results, the average values for thermal flux in ring C was $2.494 \times 10^{13}$, ring F was $1.070 \times 10^{13}$ and ring G was $7.661 \times 10^{12}$ n-cm$^{-2}$s$^{-1}$, respectively. The average values for epithermal flux in ring C was $1.964 \times 10^{12}$, ring F was $8.411 \times 10^{11}$ and ring G was $5.878 \times 10^{11}$ n-cm$^{-2}$s$^{-1}$, respectively. The average values for fast flux in ring C was $1.253 \times 10^{13}$, ring F was $7.140 \times 10^{12}$ and ring G was $4.188 \times 10^{12}$ n-cm$^{-2}$s$^{-1}$, respectively. Figure 3 to figure 5 show comparisons of the MCNP calculations with the measurement values which show acceptable results.

4.2. The uncertainties and the discrepancies

However, it is expected that most variations in the measurement results were due to the position of the measuring point in the irradiation tubes. The discrepancies may result from the effect of fuel element burnup, the temperature effects, and the relative large uncertainty in the power calibration, which may directly affects the calculation values. The uncertainties of the calculation model may influence from the geometrical, dimension, material properties including composition and densities data, control rod positioning and the irradiation tubes positioning in the reactor core.
Figure 3. Thermal neutron flux results in 9 in-core irradiation tubes by the MCNP code and measurements.

Figure 4. Epithermal neutron flux results in 9 in-core irradiation tubes by the MCNP code and measurements.
Figure 5. Fast neutron flux results in 9 in-core irradiation tubes by the MCNP code and measurements.

5. Discussion and Conclusion

Verification of the neutron flux distribution in the incore irradiation tubes was performed by comparing the MCNP calculation and the measurement of the neutron flux was determined from the $^{27}$Al($n$, $\alpha$)$^{24}$Na and $^{197}$Au($n$, $\gamma$)$^{198}$Au reaction rates. In this study the agreement between measured and calculated values are very good within the measurement and calculation uncertainties. The results indicated that the material and the geometrical properties used in the MCNP code are modelled well. The calculated neutron flux distribution will be more accurate with refinement in the future study. For future study, in order to observe the neutron flux influence from individual structures, the detailed or refinement model should be constructed such as graphite of the thermalizing and thermal column, triangular irradiation tubes, radial and tangential beam ports. The effect of fuel element burnup model should be modelled and radioisotopes which are significantly contributed to $k_{eff}$ should be taken into account. The modification of the computational model for burnup and temperature effects should be conducted to validate the burnup and temperature effect uncertainties. The detailed sensitivity study of each parameter including xenon buildup, nitrogen dissolved, geometrical and material data (densities, compositions), the control rod position and cross section libraries which are used in the MCNP model and the effect from neighbouring irradiation should be performed to explain the systematic discrepancies between the neutron flux measurement and the MCNP calculation model. From this study, the neutron flux distribution can be utilized for spectra calculations, dose rate calculations, reaction rate calculations, power peaking factors, and kinetic parameters of the reactor core.
6. References

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