

Upgrades to the Monte Carlo Computational Model of the JSI TRIGA Research Reactor

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ABSTRACT

The Monte Carlo computational model of the JSI TRIGA research reactor was upgraded by adding 3D fuel burnup and temperature distribution. The effect of fuel burnup and fuel temperature on the effective multiplication factor has been evaluated at -4324 pcm, -1120 pcm respectively. Changes of neutron spectrum in TRIGA measuring position MP17 were investigated and 3 % increase was observed when burnup was included. Based on the obtained results, fuel burnup and temperature distribution were added to the existing model. Calculations of reaction rates of ${}^{197}Au(n,\gamma){}^{198}Au$ and ${}^{27}Al(n,\alpha){}^{24}Na$ reactions in the reactor core were compared to experimental data. The agreement improved by 6 % in the calculation/experiment ratio when compared to the existing model with fresh fuel at room temperature. The improvement is a combination of changes in the neutron spectra as well as the normalization factor.

1 INTRODUCTION

The TRIGA Research Reactor at the "Jožef Stefan" Institute is one of the most utilized research reactors from the standpoint of student and nuclear staff education and training and due to the ability to perform versatile experiments in the fields of nuclear physics, reactor physics, material irradiations, medical physics, etc. [1]. The main reason of such utilization is the availability of well characterized neutron and gamma fields in every part of the reactor core and its surroundings [2, 3, 4, 5]. This was achieved in last 20 years by multiple experimental campaigns supported by Monte Carlo calculations.

The basis of reactor simulations is having a detailed computational model. For the JSI TRIGA reactor the model in the Monte Carlo neutron transport code MCNP [6] has been developed in 2006 and significantly upgraded and refined since. It was validated against benchmark experiments [7, 8] and used to support multiple experimental campaigns. The model includes detailed geometry of the reactor core with its surrounding with fresh fuel isotopic composition at room temperature. Such description was sufficient for the calculation of neutron spectra, reaction rate profiles and gamma field. However, it was reported [3, 4] that by using this model the calculated effective multiplication factor was higher than critical, which resulted in small discrepancies when comparing absolute values of physical parameters such as axial neutron flux. Our goal was to investigate the reasons for this discrepancy by analysing different processes in the reactor core that have not yet been simulated and to use the knowledge to improve the model for further use.

In the first part of the paper the current status of the computational model is presented. The second and the main part presents the analysis of the effect of fuel burnup, fuel temperature distribution and HZr thermal scattering cross sections. In the last part, the improvements to the model are presented by comparing simulations and measurements of neutron activation analysis experiment.

2 JSI TRIGA MARK II RESEARCH REACTOR

The JSI TRIGA MARK II research reactor is a pool type reactor which has been in operation since 31st of May 1966. The reactor has a circular lattice with 91 fuel element locations arranged in 6 concentric rings as presented in the right part of Fig. 1. Fuel elements are made of a U-Zr-H mixture (12 wt. % of 19.75 % enriched uranium) with a central Zr rod. The core is equipped with four control rods, three of which are equipped with a fuelled follower, while the "transient" (P) one has an air follower. Several irradiation channels are inserted in different parts of the reactor, such as the central channel, triangular channel, and several channels in the outermost ring.

In the last couple decades, the reactor has mostly been used for training of student and nuclear staff and for research in the fields of reactor physics, material irradiations, medical physics, etc. One of the main reasons for such good utilization is in the characterization of the reactor core's physical parameters, which is a process that has been ongoing since the start of operation with higher focus in the last decade. Successive characterization is a result of different experimental campaigns and the availability of a detailed computational model for computer simulations.

2.1 Status of the Computational Model in the MCNP code

The JSI TRIGA computational model in the MCNP code was first constructed in 2006 by L. Snoj and R. Jeraj [9]. In 2012 it was upgraded by Ž. Štancar [3], who modelled detailed geometry of fuel elements' top and bottom parts as well as detailed support grids. The latest detailed model is presented in Fig. 1. The model was later validated using the JSI TRIGA benchmark experiment, included in the International Physics Experimental Evaluation Project Handbook [8]. Fission rate axial profile was compared to absolute values measured using miniature fission chambers. The normalization of calculated results to reactor power was carried out using a normalisation factor K, which represents the neutron source strength (i.e. neutrons per second) of the system during the experiment [4, 10]:

$$\mathbf{R} = \mathbf{K} \cdot R_{mc}; \quad K = \frac{P_{reactor} \bar{\nu}}{w_f k_{eff}}, \tag{1}$$

where R is the absolute reaction rate, R_{mc} is the Monte Carlo calculated reaction rate $P_{reactor}$ is the reactor thermal power, \bar{v} is the average number of neutrons released per fission, w_f is the average deposited energy per fission event and k_{eff} is the calculated effective multiplication factor of the computational model. The values of \bar{v} and w_f are constants and $P_{reactor}$ is determined with high accuracy, however values of the calculated effective multiplication factor are dependent on the computational model and were reportedly higher than those of a critical system. We performed MCNP simulations for core configuration No. 235 that was in operation in November 2018, presented on left side of Fig. 1., and determined the $k_{eff} = 5930 \ pcm \ \pm 560 \ pcm$. The stated uncertainty is the uncertainty of the benchmark experiment [8]. In the next section the source of this discrepancy is analysed.



Figure 1: Schematic presentation of the JSI TRIGA research reactor 3D computational model (left) and schematic of core configuration No. 235 (right)

3 EFFECTS ON CALCULATED CORE REACTIVITY

The improvement of the JSI TRIGA research reactor computational model was conducted in such a way that in the first step we evaluated the effect of modelling additional physical processes (fuel burnup, temperature, etc.) on the reactor core physical parameters such as core excess reactivity and neutron spectrum. We identified and analysed two different possible sources for core reactivity discrepancy: Fuel element burnup and fuel temperature.

3.1 Fuel element burnup

The reactor has been in operation for more than 55 years, during which all changes of the reactor power and core configuration have been recorded in reactor logbooks. Recently, we have started to thoroughly analyse the complete operating history of the reactor and perform burnup calculations. The methodology is presented in [11]. The state-of-the-art Serpent-2 Monte Carlo neutron transport and burnup code [12] was used to determine the fuel element burnup in November 2018 for core configuration No. 235. The calculated effect of fuel burnup on TRIGA k_{eff} was $\Delta \rho = -3742 \pm 100 \text{ pcm}$. The stated uncertainty is due to the modelling of the reactor operating history. The initial calculations did not include the axially dependent burnup because the original methodology was developed for 2D calculations. We updated the methodology to allow 3D burnup calculations over the entire operating history. With the updated burnup calculations, we determined the effect on k_{eff} to be $\Delta \rho = -4324 \pm 100 \text{ pcm}$. Accounting for the axial fuel burnup distribution reduced the calculated reactivity by an additional 582 pcm. The calculated burnup for fuel elements used in core conf. No. 235 is shown along with its effect on core reactivity in Fig. 2.

306.3

20.0 20 TRIGA k_{eff} 17.5 15 [pcm] 5930 pcm -3742 pcm -4324 pcm 6000 15.0 uel element burnup (SERPENT) 10 12.5 5 4000 Л cm] 10.0 7.5 2D fuel el. 1000 burnup in 2018 -105.0 3D fuel el. Initial model -152.5 (axial division) discrepancy -20 0.0 -20 -1010 20

306.4

Figure 2: Calculated fuel element burnup of the JSI TRIGA reactor for core conf. No. 235 with the Serpent-2 code [12] and the burnup effect on the effective multiplication factor of the core.

3.2 Fuel temperature distribution

[cm]

Due to the variety of the TRIGA operation the temperature distribution among reactor components and the coolant is highly dependent on type of operation and the power of the reactor. Three different cases of temperature distributions can be assumed. First one, representing the conditions of the benchmark experiment, is operation at low reactor power $P_{reactor} \approx 100$ W, where the assumption can be made that all components and materials, including the fuel, are at room temperature. The second is the pulse mode operation [13], where the reactor power reaches up to $P_{reactor} \approx 1 \text{ GW}$ and the fuel temperature up to $T_{fuel} \approx 500 \text{ K}$. In this case adiabatic model is assumed where only the fuel temperature is increased while all other materials are at room temperature. The last case, important from the standpoint of supporting experimental campaigns, is the standard steady-state operation at max power of $P_{reactor} = 250$ kW. The temperature is in equilibrium, where water flowing through the core due to the natural convection is used to cool the reactor. In theory, coupling of thermal-hydraulics and neutron transport is needed to determine in detail the temperature distribution of all materials and coolant. However, for the TRIGA reactor it was shown in [14] that the coupling is weak and that coolant temperature and density have a small influence on power density distribution. However, the temperature of the fuel, acting as moderator due to hydrogen in H-Zr-U mixture, has a prompt and large effect on core reactivity.

Knowing this, we focused our analysis on two effects on core reactivity due to increasing temperature. The first one is the change of neutron spectrum due to Doppler broadening and neutron spectrum shift. The second one is the fuel element expansion.. For the first analysis we first assumed homogeneous temperature profile for all fuel elements. Only temperature of fuel was changed, while the temperature of surrounding water and its density was constant. For all the cases temperature profile in the fuel itself was homogeneous. We performed calculations at $T_{fuel} = 373$ K and $T_{fuel} = 473$ K and determined reactivity effect of $\Delta \rho = -1000$ pcm and $\Delta \rho = -1200$ pcm, respectively. The model was improved by considering a more detailed temperature distribution among fuel elements. Using the existing MCNP model, we calculated the fission rate distribution and used it to determine the specific power per fuel element P_{el} , assuming the reactor is operating at $P_{reactor} = 250$ kW. Knowing P_{el} , we determined the temperature distribution among fuel elements $T_{fuel,el}$ using the following empirical relation from the deterministic TRIGLAV code[15]:

$$T_{fuel,el} = T_{fuel}(P_{el}) = a_1 P_{el} + a_2 P_{el}^2 + a_3 P_{el}^3 + T_{water},$$
⁽²⁾

 $\langle \mathbf{n} \rangle$

where $a_1 = 67.18 \ K/kW$, $a_2 = -8.381 \ K/kW^2$, $a_3 = 0.3843 \ K/kW^3$ and T_{water} represents the temperature of surrounding coolant. Cross sections were generated using NJOY 2016 [16] at temperatures 400 K and 500 K and cross section mixing was used to determine cross sections that represent temperatures between. We calculated the core reactivity decreases by 1120 ± 25 *pcm.* The calculated fuel temperature profile is presented on the left side of Figure 3, and the summary results of the reactivity effect due to fuel temperature is presented on the right side of Figure 3.



Figure 3: Fuel temperature distribution in the JSI TRIGA reactor (left), calculated using Eq. 2, and the temperature effect on the effective multiplication factor of the core.

In the scope of this analysis, only fuel temperature was changed, however other processes that occur with the temperature increase are to be modelled in the future. One such process is the expansion/contraction of fuel and stainless steel (SS) cladding during reactor operation at higher power. Preliminary analysis was performed, where the fuel meat and SS cladding dimensions were changed based on the linear expansion law so that the material mass remained constant. We isolated the effect of fuel meat and SS cladding expansion. It was found that expansion of fuel meat has no appreciable effect on core reactivity, while the expansion of SS cladding had a minor effect on reactivity in the order of *100 pcm*. However, no final conclusions on the fuel expansion effect can be made at this point and further analysis is needed. Consequently, the changed dimensions during higher temperature are not included in the upgraded model. During the analysis we identified multiple possible improvements for future modelling of fuel temperature effects. A further step is to model the temperature distribution within the fuel elements and consider the fuel expansion on higher temperatures. The latter is more important in pulse experiments as the fuel reaches higher temperatures.

3.3 Burnup and temperature effects on neutron spectra

For both cases of adding fuel burnup and fuel temperature to the computational model, we studied the effect of those changes on neutron spectra in one of the measuring positions MP17, located between ring B and C (second and third ring). Neutron flux was calculated in 640-energy group structure and tallied throughout the whole length of the aluminium rod, used for neutron activation measurements. For the case of fuel burnup, increase of thermal part of the spectrum in the order of 3 % was observed for the case of burned fuel. Change of fast part of the spectrum was negligible. For the case of fuel temperature, a shift to the higher energies of the thermal peak of the spectrum was observed. From this a conclusion can be made that by

considering fuel burnup and fuel temperature, thermal part of the neutron spectrum increases and slightly shifts to higher energies. The results are presented on Fig. 4.



Figure 4: Calculated absolute difference in neutron lethargy spectrum in measuring position MP17 for the case of adding fuel burnup (top graph) and fuel temperature (bottom graph) to the computational model.

4 IMPROVEMENTS TO THE COMPUTATIONAL MODEL

Based on the analysis presented in Section 3., we concluded that fuel burnup and temperature distribution need to be added to the existing computational model. A script was developed that takes as an input the existing MCNP model, fuel isotope inventory, fuel temperature distribution and core configuration, and creates a runnable input. In order to test the input, we analysed neutron activation analysis measurements performed in November 2018 on core configuration No. 235. We studied axial distribution of two reactions: ${}^{197}Au(n,\gamma){}^{198}Au$ and ${}^{27}Al(n,\alpha){}^{24}Na$. Comparison between measurements and calculations was evaluated with average ratio of calculations vs measurements, defined as:

$$\frac{C}{E} = \frac{1}{N_{measure}} \sum_{i=1}^{N_{measure}} \frac{RR_{i, calculations}}{RR_{i, measurements}},$$
(3)

where RR_i presents the calculated on measured reaction rate for individual reaction type, *i* the axial locations where the measurements were performed, and total $N_{measure}$ total number of measurements performed.

Comparison between measurements and calculations using the initial MCNP model with fresh fuel and room temperature showed good agreement with calculation vs experiment ratio (C/E) of 0.92 ($^{197}Au(n,\gamma)^{198}Au$) and 0.86 ($^{27}Al(n,\alpha)^{24}Na$). Using the upgraded MCNP

model the agreement improved to C/E of 0.99 (^{197}Au) and 0.92 (^{27}Al). In addition, relative comparison between both calculations was performed. The axial distribution did not change when 3D burnup and fuel temperature were included. The results are presented in Fig. 5. And Tab. 1.



Figure 5: Comparison of measured and calculated reaction rates for ${}^{197}Au(n,\gamma){}^{198}Au$ and ${}^{27}Al(n,\alpha){}^{24}Na$ reactions for neutron activation analysis experiment conducted on JSI TRIGA reactor core No. 235 in November 2018. Improved MCNP model with fuel burnup and temperature is compared to initial with fresh fuel and room temperature.

Table 1: Comparison of Calculations/Experiments ratio for experimental validation with neutron activation measurements. Parameter C/E, defined in Eq. 3, represents an average over all axial positions where measurements were performed.

Calculations / Experiments (C/E)	MCNP model with fresh fuel and room temperature	Improved MCNP model with 3D burnup and fuel temperature
$^{197}Au(n,\gamma)^{198}Au$	C/E = 0.92	C/E = 0.99 (8 % increase)
$^{27}Al(n,\alpha)^{24}Na$	C/E = 0.86	C/E = 0.92 (7 % increase)

5 CONCLUSION

The effects of fuel burnup, fuel temperature distribution and HZr thermal scattering cross sections on the JSI TRIGA reactor physical parameters have been analysed. This was done to determine the core reactivity effect and explain the overestimation of calculated effective multiplication factor of the core. The effect of fuel burnup and fuel temperature distribution was -4324 pcm, -1120 pcm. Together both effects resulted in explanation of the observed discrepancy (5444 pcm \pm 560 pcm) within 1 σ of the benchmark experiment. The model was improved by adding detailed 3D fuel burnup distribution and temperature distribution. Using

the improved model, the calculations of ${}^{197}Au(n,\gamma){}^{198}Au$ and ${}^{27}Al(n,\alpha){}^{24}Na$ neutron activation reactions were compared to the axial measurements. For each reaction the calculations/experiments ratio improved from 0.92 to 0.99 and 0.86 to 0.92, respectively. The improvement was due to the change of neutron spectrum (increasing of the thermal peak) and the change of normalization factor. It can be concluded that initial implementation of fuel burnup and fuel temperature was successful and that further work is to be done to improve the model.

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REFERENCES

- [1] Snoj, L. and Smodiš, B., 2011. 45 years of TRIGA Mark II in Slovenia. In *Proc. International Conference Nuclear Energy for New Europe 2011.*
- [2] Štancar, Ž., et al., 2018. Computational validation of the fission rate distribution experimental benchmark at the JSI TRIGA Mark II research reactor using the Monte Carlo method. *Annals of Nuclear Energy*, 112, pp.94-108.
- [3] V. Radulović, Ž. Štancar, L. Snoj, A. Trkov. "Validation of absolute axial neutron flux distribution calculations with MCNP with 197Au(n,γ)198Au reaction rate distribution measurements at the JSI TRIGA Mark II reactor" Appl. Radiat. Isot., 84 (2014), pp. 57-65
- [4] Goričanec, T., et al. 2018. Evaluation of neutron flux and fission rate distributions inside the JSI TRIGA Mark II reactor using multiple in-core fission chambers. *Annals of Nuclear Energy*, 111, pp.407-440.
- [5] Ambrožič, K., et al., 2020. JSI TRIGA neutron and gamma field characterization by TLD measurements. In *EPJ Web of Conferences* (Vol. 225, p. 04034). EDP Sciences.
- [6] C.J. Werner, et al.,,"MCNP6.2 Release Notes", LA-UR-18-20808 (2018).
- [7] Mele, I., Ravnik, M. and Trkov, A., 1994. TRIGA Mark II benchmark experiment, Part I: Steadystate operation. *Nuclear Technology*, *105*(1), pp.37-51.
- [8] Štancar, Ž., et al. Reaction Rate Distribution Experiments at the Slovenian JSI TRIGA Mark II Research Reactor, TRIGA-FUND-RESR-002. In: International Handbook of Evaluated Reactor Physics Benchmark Experiments. NEA/NSC/DOC(2006)1. OECD NEA, Paris.
- [9] Snoj, Luka, et al.. "Calculation of power density with MCNP in TRIGA reactor." (2006).
- [10] G. Žerovnik, M. Podvratnik, L. Snoj On normalization of fluxes and reaction rates in MCNP criticality calculations Ann. Nucl. Energy, 63 (2014), pp. 126-128
- [11] Pungerčič, A., Čalič, D. and Snoj, L., 2020. Computational burnup analysis of the TRIGA Mark II research reactor fuel. *Progress in Nuclear Energy*, *130*, p.103536.
- [12] Leppänen, J., et al., 2015. The Serpent Monte Carlo code: Status, development and applications in 2013. *Annals of Nuclear Energy*, 82, pp.142-150.
- [13] Vavtar, I. and Snoj, L., 2021. Evaluation of Approximations in Reactor Pulse. In *EPJ Web of Conferences* (Vol. 247, p. 08006). EDP Sciences.
- [14] Henry, R., 2017. *Neutronic and thermal-hydraulics coupling for simulations of the TRIGA Mark II reactor* (Doctoral dissertation, Univerza v Ljubljani, Fakulteta za matematiko in fiziko).
- [15] Peršič, A., et al., 2017. TRIGLAV: A program package for TRIGA reactor calculations. *Nuclear Engineering and Design*, *318*, pp.24-34.
- [16] Macfarlane, R., et al. The NJOY Nuclear Data Processing System, Version 2016. United States: N. p., 2017. Web. doi:10.2172/1338791.
- [17] Brown, D.A., et al., 2018. ENDF/B-VIII. 0: the 8th major release of the nuclear reaction data library with CIELO-project cross sections, new standards and thermal scattering data. *Nuclear Data Sheets*, 148, pp.1-142.