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OpenMC Model Validation of the TRIGA Mark II Reactor

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ABSTRACT

The development of open-source applications in the nuclear field has recently attracted interest from the scientific community, due to the potential mutual support useful both in the research field and in the analysis of new nuclear reactor concepts. This kind of tool allows developers to adapt the code according to their own needs, which is not generally feasible with proprietary software, designed for traditional commercial reactors and used as a black-box from the user's point of view. In this framework, the OpenMC neutronic simulation tool, based on the Monte Carlo method and implemented in the accessible and easy-to-learn Python language, provides a wide range of computational capabilities, including fixed source, criticality, and burnup simulations. Verifying the reliability of open source software requires comparison processes with other already existing codes, as well as benchmarks with measurement campaigns. The TRIGA Mark II research reactor is primarily used for neutron activation analysis, education and training, making it an extensive tool for the benchmark of numerical models due to the large amount of available experimental data collected in the past years by Politecnico di Milano. In this paper, the OpenMC model validation of the current configuration of the reactor TRIGA Mark II is proposed by first comparing the control rod worth values of the three reactor control rods (REG, TRANS, SHIM); then, the experimental calibration curves of the three rods were compared with both the OpenMC and the SERPENT predictions, taking into account both the statistical error and the measurement uncertainty, aiming to demonstrate the reliability of the OpenMC code on a real reactor test-case in comparison to the widely-used SERPENT software.

1 INTRODUCTION

In recent years, the development of open-source applications in the nuclear field has gained significant attention within the scientific community, as open-source codes offer a collaborative platform that supports researchers and facilitates the analysis of novel nuclear reactor concepts and the collaboration between research groups. Unlike proprietary software designed for commercial reactors, whose code is not readily accessible by end-users, open-source tools provide developers with the flexibility to adapt and customise the code according to their specific needs. Among the various open-source tools, the OpenMC [1] neutronic simulation tool stands out as a promising and powerful computational code: built on the Monte Carlo method and implemented in the accessible and easy-to-learn Python language, OpenMC offers a wide range of capabilities, including fixed source, criticality, and burnup simulations. To ensure the reliability of OS software, a rigorous verification and validation process is needed, which includes both verification against existing state-of-the-art proprietary codes and validation against experimental measurements. In particular, the latter must be performed not only against laboratory test cases but also against real-world nuclear facilities.

The TRIGA (Training Research and Isotope production General Atomics) Mark II reactor is a particular type of research nuclear reactor widely used in various applications, including radioisotope production, non-destructive testing, fundamental material research, and educational training. In the context of code validation, the TRIGA Mark II research reactor emerges as a valuable resource for validating numerical models. Relative to this work and neutronics codes, the TRIGA Mark II reactor located at the LENA (Laboratorio Energia Nucleare Applicata) institute in Pavia, has been used to validate several neutronics models: for example, [2, 3] benchmarked an MCNP model of the first TRIGA configuration; [4] studied the burnup and the core reconfiguration with MCNP; [5] studied the new core configuration with SERPENT.

The aim of this work is to present the TRIGA Mark II reactor model in the open-source framework OpenMC and validate its neutronic capabilities by comparing key quantities such as the control rod worth, core excess reactivity and calibration curves predicted by the Monte Carlo software against experimental data. The objective of this work is two-fold: i) demonstrating the reliability of the OpenMC code in simulating a real-world reactor; ii) comparing its performance against the state-of-the-art SERPENT software to verify if an open-source approach, with all of its advantages, can be a valid alternative to proprietary codes such as SERPENT.

This paper is organized as follows: Section 2 provides an overview of the adopted methodology within the OpenMC framework. Section 3 describes the modelled TRIGA reactor with its design features. Section 4.2 presents first the selected figures of merit and then the numerical results obtained using OpenMC, comparing them with experimental data and SERPENT results. Finally, Section 5 summarises the findings and proposes perspectives for future research.

2 METHODOLOGY

The simulation of neutron interactions is approached with the Monte Carlo method: by sampling random particles, reactions in the system are scored and recorded (scattering, absorption, fission etc.) to understand the system's physical behaviour. To tackle the stochastic effects, the simulated particles will be sampled in two subsequent stages: the first will apply a certain number of inactive cycles in order to allow the fission source to reach convergence; the second will effectively score and record quantities with a proper number of active cycles.

2.1 Modelling Framework

OpenMC [1] is a simulation tool for evaluating the interactions of neutrons and photons with matter by exploiting the Monte Carlo method. It is an open-source software implemented in Python/C-C++ language, making it an easily accessible tool by the worldwide scientific community, available for free and extensible for high-performance calculations and for research purposes including the study of novel reactor concepts with unique features. Despite being a relatively new code, OpenMC has several calculation capabilities, such as fixed source simulations, k-eigenvalue and depletion calculations. In addition, OpenMC is actively developed and improved with new functionalities on a 5-month basis. Also, the code is able to build models, either by using a constructive solid geometry or a CAD representation. Finally, it is also designed as an extensible code for multi-physics coupling applications[6].

The code structure adopts the Extensible Markup Language (XML) for what concern the user input files, with the advantage to have the input model pre-processed in a nested and organized form (useful for debugging purposes), so that the same model written by two different persons will have the exact same input files down to the line order. In order to launch a simulation, there are some mandatory files needed by OpenMC, listed below and shown in Figure 1.

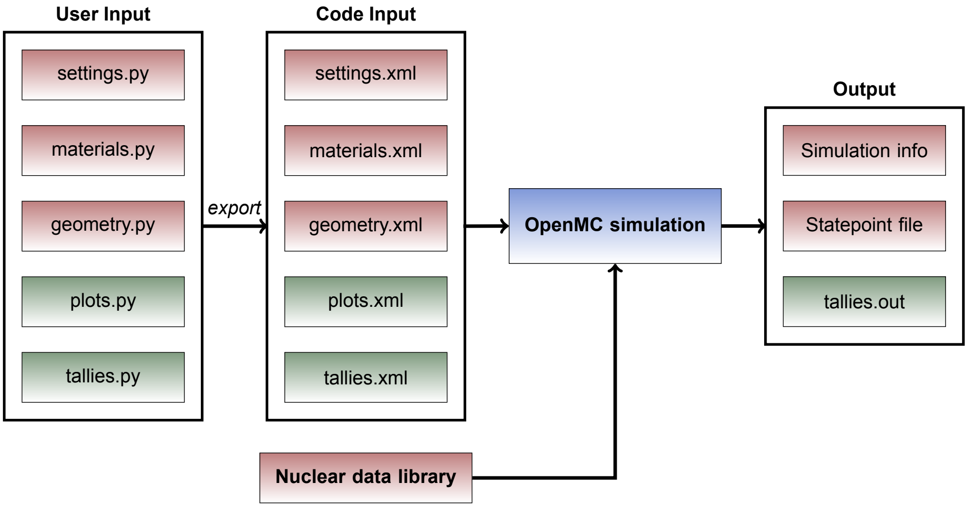


Figure 1: Scheme for the input files in an OpenMC simulation. Red blocks represent optional files, and green blocks represent mandatory files.

1. **settings.xml**: describes all simulation parameters, e.g., how many particles to run, the starting source, the temperature treatment and other options that can be turned on or off;
2. **materials.xml**: describes the composition of all materials in the model by their densities and their constituent nuclides (either in atomic fraction '*ao*' or weight fraction '*wo*'). Natural elements are automatically expanded into individual nuclides by their natural abundance;
3. **geometry.xml**: describes the model geometry using constructive solid geometry primitives (surfaces, cells, universes, lattices) and assigns materials to cells. The material volumes are built as the intersection of infinite *regions*; each region is defined as the positive or negative side of surfaces (user-defined). By doing so, fuel rods will be defined as the intersection of the inner region from a cylindrical surface, and the upper and lower region from planar surfaces. This peculiarity allows curved surfaces (such as spheres and cylinders) to be modelled exactly with no error due to mesh discretization.

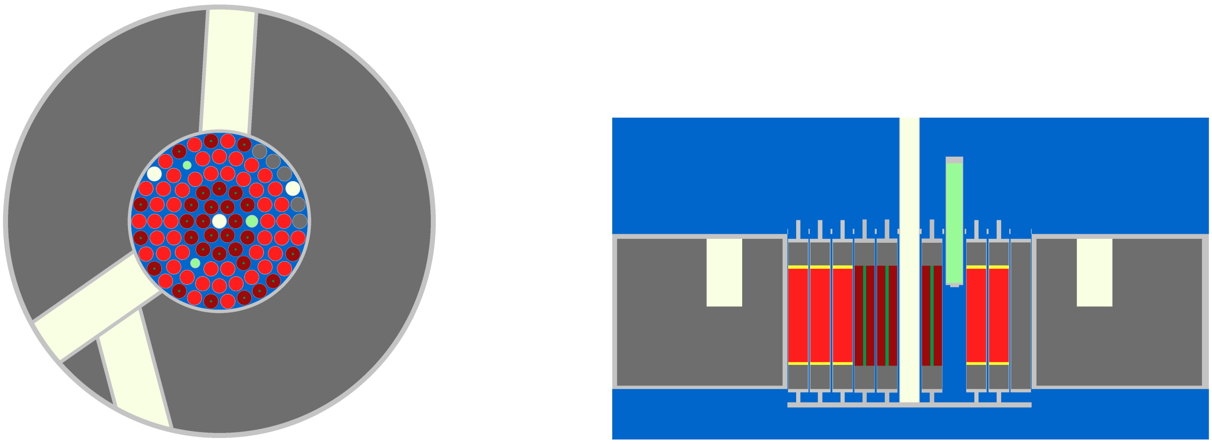
Some optional XML files are allowed:

1. **tallies.xml**: specifies what physical quantities the user wants to tally during the simulation (e.g., neutron spatial flux, deposited heat, thermal neutron spectrum etc.);
2. **plot.xml**: describes the parameters for 2D or 3D plots when OpenMC is run in plotting mode;

The software input can be written in the Python language and then exported to XML format by specific built-in functions. In this way it is possible, for example, to exploit the full potential of a programming language for defining iterated geometries.

3 TRIGA AND MODEL DESCRIPTION

The current reactor core configuration includes 91 vertically oriented elements, each approximately 70 cm in length, submerged in a light water pool with a depth of around 6 m. The



(a) (b)

Figure 2: 2a: XY view of TRIGA reactor; 2b: XZ view of TRIGA reactor. The different elements can be identified by their colour: Fuel-101 (light red), Fuel-103 (dark red), Zirconium rod (dark green), Samarium disk (yellow), Cladding (light grey), Graphite (dark grey), Air (light yellow), Water (blue). The samarium disk is not in scale with the other reactor elements for visualisation purposes.

core features stainless steel cladding for the central rings, while the outer rings utilise elements with aluminium cladding. The fuel rods consist of a homogeneous mixture of Uranium (8 wt%, enriched to 20 wt% in ^{235}U) and Zirconium Hydride (ZrH), which provides internal moderation. Natural circulation facilitates the primary cooling process, transferring heat from the fuel cladding to the water within the pool. An external active cooling system maintains control over the pool temperature. Equipped with three control rods, the TRIGA reactor replicates the functionalities found in commercial reactors. The transient (TRANS) rod, composed of borated graphite, is pneumatically inserted or fully withdrawn to achieve emergency shutdown via SCRAM. During normal operations, it remains outside the core. The other two rods, composed of boron carbide and activated using a rack, allow power adjustments. The SHIM rod facilitates coarse regulation and primarily compensates for the effects of neutron poison fission products, such as xenon and samarium. Due to this role, the SHIM rod possesses higher reactivity storage. Finally, the regulating (REG) rod allows for fine adjustments in response to small and rapid reactivity changes. Figure 2 shows the simulated TRIGA geometry. The reactor composition has been faithfully reproduced in the OpenMC framework based on the most recent configuration:

- 50 rods of Fuel-101 (light red) made with a thin Samarium disk (yellow) between the Aluminium cladding;
- 29 rods of Fuel-103 (dark red), having a thin Zirconium rod (dark green) in the centre and with Stainless Steel cladding;
- 5 Graphite (dark grey) dummy elements;
- 3 empty channels (light yellow), which are the central channel and the source channels;
- 3 Control Rods (light green): SHIM (ring C), TRANS (ring D) and REG (ring E);

4 NUMERICAL RESULTS

4.1 Figure of Merits

The validation of the OpenMC model is carried out by comparing key reactor neutronics quantities against experimental data and other values computed with the SERPENT Monte Carlo code. Both software adopts the ENDF/B-VII.1 nuclear data library. The central FoM in this analysis is the multiplication factor k_{eff}, evaluated by the k-eigenvalue method, which solves the stationary Boltzmann equation and identifies the k_{eff} as the ratio within the neutron population in successive generation cycles[7]. This quantity reflects the ability of a fissile system to multiply its neutron population by a factor k_{eff} within each generation. If $k_{\text{eff}} > 1$, the system is supercritical; if $k_{\text{eff}} < 1$, the system is sub-critical; if $k_{\text{eff}} = 1$, the system is critical. Knowing k_{eff}, the *reactivity* can be computed as the unitary deviation of the multiplication from the critical case:

$$\rho = \frac{k_{\text{eff}} - 1}{k_{\text{eff}}}. \tag{1}$$

Reactivity can be expressed in dollar units by knowing the fraction of delayed neutron β, as $\rho\ (\$) = \rho/\beta$, as will be done in this work. The delayed neutron fraction assumes different values for different reactor families; for the TRIGA Mark II, the previous analysis showed a value of $\beta = 730 \cdot 10^{-5}$.

For the TRIGA Mark II research reactor, the three control rods allow modification of the multiplication factor of the system. Their movement can be directly linked to a reactivity change, quantifiable and comparable with simulation predictions. As such, the analysis will be devoted to comparing the corresponding reactivity values associated with well-defined control rod configurations, and for this reason, the following FoMs have been chosen.

4.1.1 Control rod worth

The *control rod (CR) worth* represents an FoM useful for a preliminary comparison during the verification process of the OpenMC model. This quantity is defined as the reactivity that a control rod can insert in the system if it were totally extracted from the core. The correct prediction of this value reflects the ability of the code to correctly describe the single rod global effect. Also, it is a simple quantity to evaluate, since it only needs two k_{eff} values, namely the one with the rod totally inserted and the one with the rod totally withdrawn. Thus, the CR worth of the i-th rod, $\rho_{i,W} = \bar{\rho}_{i,W} \pm \sigma_{i,W}$, will be the difference between the reactivity in a configuration where the rod is fully extracted and the reactivity in a configuration with the rod fully inserted:

$$\bar{\rho}_{i,W} = \bar{\rho}_{i,out} - \bar{\rho}_{i,in} \qquad \sigma_{i,W} = \sqrt{\sigma^2_{\rho_i,in} + \sigma^2_{\rho_i,out}} \tag{2}$$

To assess if the calculated CR worth value is in statistical agreement with respect to the measurements, a pull analysis has been performed, not reported here for the sake of brevity.

4.1.2 Core reactivity excess

The *core reactivity excess (CRE)* is defined as the surplus of positive reactivity stored in the core when the system is critical. This value depends on several factors, such as the power level, the fuel depletion and the poisoning. This work considers as a starting point an experimentally critical rod configuration at zero power, with fresh fuel and without poisoning. The considered rod positions in the critical configuration are[1]:

[1]The reference framework for the control rod positions is +0.0 cm when fully inserted.

- REG at +0.27 cm,
- SHIM at +19.27 cm,
- TRANS fully extracted.

The core reactivity excess is evaluated compared to the multiplication factor associated to the configuration where all the rods are extracted. Compared to the CR worth, the CRE is able to reflect the capability of the code in predicting the core reactivity value, considering the combined effect of the three control rods.

4.1.3 Calibration curve

The ability of the control rods to absorb neutrons depends on their position within the core in a non-linear way. From the reactor operator's point of view, the knowledge of the rod absorption level in each location is fundamental, and thus the correct estimation of the calibration curve is of paramount importance. The calibration curve is a map between the integral reactivity and the height of the rods in the reactor. The reactor period method was adopted to experimentally measure the calibration curves of REG, SHIM and TRANS. These experimental curves will be compared with the prediction of OpenMC and SERPENT, exploring the local comparison capabilities of the two codes. The rod extraction transient will be replicated as follows: for each rod position, the k_{eff} estimated by the Monte Carlo code will be recorded, along with the relative reactivity calculated with Equation 1: this way, a map between the rod position and the reactivity can be retrieved.

4.2 Results

The Figure of Merit previously described has been evaluated with the OpenMC code with statistics of n_0 = 600000 neutrons/cycle, 200 active cycles and 100 inactive. Table 1 reports the CR worth for the REG, SHIM and TRANS rod and the CRE evaluated with the codes OpenMC and SERPENT, along with the experimentally measured values. The reported uncertainties are measure errors for experimental data; statistical errors for Monte Carlo results. It is important to highlight that the CR worth evaluation of the i-th rod lacks information on the positions of the remaining control rods during the procedure. This adds to the system an extra uncertainty related to the *shadowing effect*: indeed, the mutual position of one rod influences the absorbing capability of the others [8]. For this analysis, the TRANS rod was considered fully extracted for the evaluation of the REG and SHIM CR worth. This setup reflects the real reactor operation, with the TRANS rod completely withdrawn to allow the SCRAM of the reactor in case of emergency; then, for computing the REG worth, the SHIM was fixed at half-height of its full-inserted configuration. Conversely, for the SHIM worth, the REG was fixed at half-height of its fully inserted configuration.

Table 1: REG, SHIM, TRANS control rod worth and core excess reactivity comparison between experimental data, OpenMC and SERPENT calculations, reported in dollars ($). The reported uncertainties are the measurement errors for the experimental data and the contribution of the stochastic transport for the Monte Carlo results.

	REG	**SHIM**	**TRANS**	**Core excess**
Experimental	1.261 $\pm$ 0.068	3.11 $\pm$ 0.18	2.21 $\pm$ 0.33	2.49 $\pm$ 0.03
SERPENT	1.33 $\pm$ 0.07	3.34 $\pm$ 0.07	2.25 $\pm$ 0.07	2.75 $\pm$ 0.07
OpenMC	1.247 $\pm$ 0.047	3.31 $\pm$ 0.047	2.20 $\pm$ 0.048	2.85 $\pm$ 0.047

Figures 3,4 and 5 show the calibration curves for the three control rods: the REG curve evaluated with OpenMC exhibit a very similar fit of the experimental data with respect to the

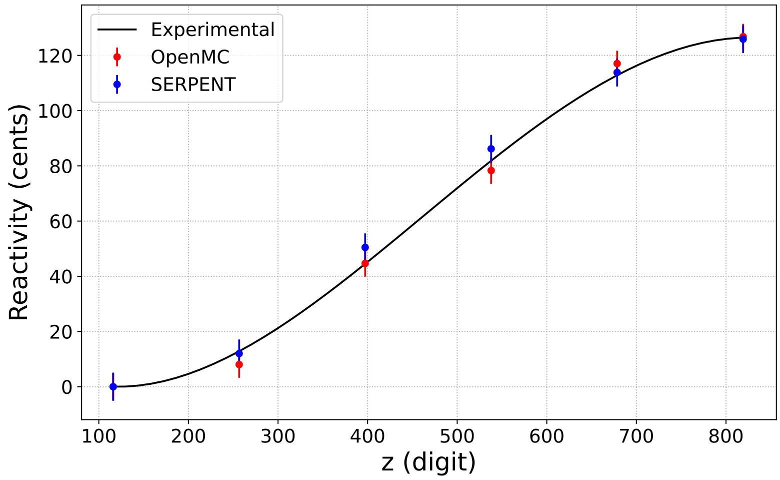


Figure 3: REG calibration curve. Comparison between OpenMC and SERPENT outcomes against experimental data.

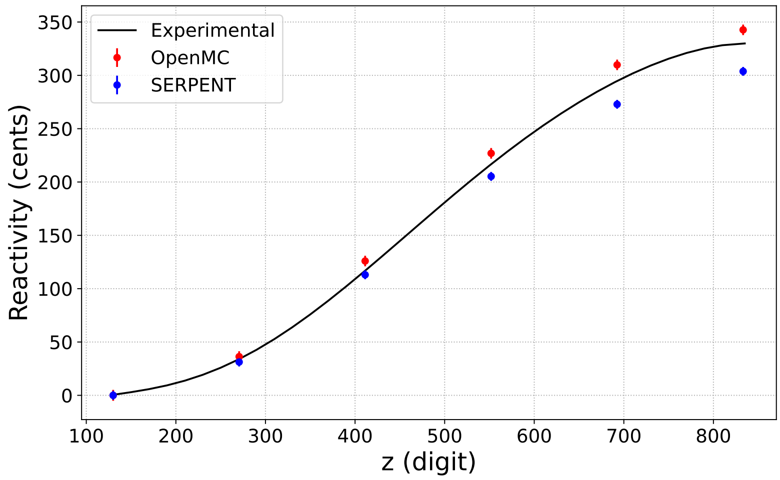


Figure 4: SHIM calibration curve. Comparison between OpenMC and SERPENT outcomes against experimental data.

SERPENT calculations, and the same trend can be seen in the TRANS curve. The SHIM calibration curve is slightly overestimated by OpenMC and is underestimated by SERPENT with respect to the experimental data. Among the two simulation results, the former is better than the latter in predicting the SHIM curve. The slight differences between the two Monte Carlo results can be addressed to the lack of the delta-tracking in the OpenMC code, which are accentuated in the vicinity of local absorbers (like the control rods).

5 CONCLUSIONS

This work focused on the verification and validation of the OpenMC model of the TRIGA Mark II reactor, testing the reliability of open-source software compared to experimental data and proprietary codes. In this kind of system, the movement of the control rods allows to experimentally induce measurable reactivity changes, making it possible the comparison between simulated and measured quantities. In particular, the control rod worth, the core excess reactivity and the calibration curves of the three control rods (REG, SHIM and TRANS) have been evaluated with the OpenMC code. The analysis of the REG and TRANS control rod worth

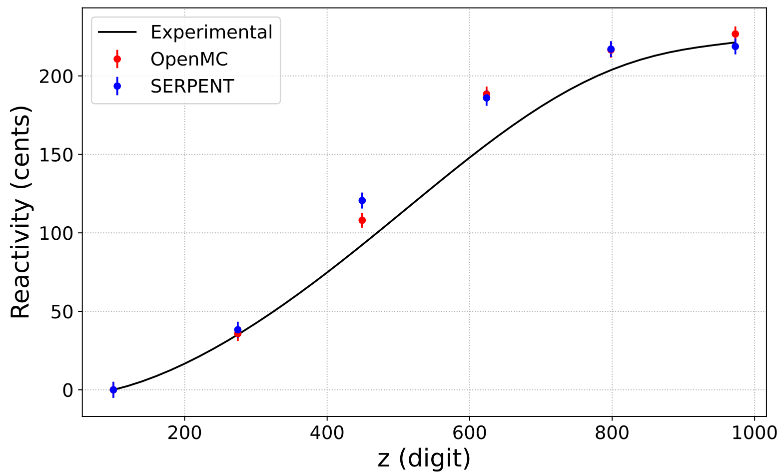


Figure 5: TRANS calibration curve. Comparison between OpenMC and SERPENT outcomes against experimental data.

showed good agreement with the experimental data, whereas the SHIM and the core excess reactivity are more in line with the results of the SERPENT Monte Carlo code. For the calibration curve, the OpenMC predictions show either a similar agreement with SERPENT and the experimental data (REG, TRANS) or even a better prediction with respect to the SERPENT results for the SHIM rod. From the results of this paper, OpenMC showed to be a valid open-source tool for reactor physics calculations, comparable with other state-of-the-art proprietary software. Future works will be devoted to validating the burnup capabilities of OpenMC and to implementing a multi-physics framework to take into account temperature effects on the reactor behaviour.

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