



International Conference  
Nuclear Energy for New Europe

## OpenMC Analysis of TRIGA Mark II Reactor Void and Temperature Reactivity Coefficients

**Lorenzo Loi, Stefano Riva, Riccardo Boccelli, Carolina Introini, Stefano Lorenzi, Enrico Padovani, Antonio Cammi**

Politecnico di Milano  
Department of Energy  
Via Lambruschini, 4  
20156, Milano (MI), Italy

lorenzo.loi@polimi.it, stefano.riva@polimi.it, carolina.introini@polimi.it,  
antonio.cammi@polimi.it, enrico.padovani@polimi.it

### ABSTRACT

Due to the very stringent safety requirements of nuclear facilities, there is a need of developing precise and accurate computational tools for the reactor's safety analysis both during the licensing process and standard operation. Achieving this goal requires verification by other state-of-the-art neutronic codes and validation through comparison with experimental data of the simulation tools. The recent development of open-source platforms has increased the interest in adopting these technologies, which, compared to proprietary software, offer continuous exchange between developers and users and direct access to the source code. In safety analyses, studying feedback coefficients is crucial for evaluating the reactor dynamic response to control and accidental scenarios. This kind of analysis provides an in-depth understanding of reactor behaviour under different operating conditions (i.e., different power levels) and experimental settings. Existing codes are suited for commercial reactors and may not offer the capabilities for simulating future generation systems. In this framework, this paper analyses the thermal feedback coefficient and void coefficient of the TRIGA Mark II reactor using a Monte Carlo model developed with the Python-based open-source OpenMC code. The reason behind the choice of this particular reactor is twofold: first, this reactor represents a landmark in nuclear research due to its unique asymmetrical configuration and the presence of UZrH fuel, and in particular, for its passive safety feature, made possible by its highly negative feedback coefficients. Second, a large number of available experimental data are readily available. This work considers two different scenarios for the validation: the first case is the insertion of positive reactivity through a control rod extraction, allowing the temperature to increase along with the power; the second case simulates the reactivity perturbation coming from the presence of a void volume (e.g., in sub-cooled boiling regime) through the placement of a sample made by aluminium and filled by air or water in the central channel. The experimental scenarios related to the evaluation of the feedback coefficients are accurately reproduced: the tracking of the change in the criticality level ( $k$ -eigenvalue) compared to some physical quantities (i.e., the temperature or the void level) allows for the calculation of the feedback coefficients, and the results obtained from the OpenMC simulation are compared to both the experimental results as well as the outcomes from the SERPENT Monte Carlo code, showing a good agreement.

## 1 INTRODUCTION

The precise knowledge of feedback coefficients plays a key role in fission reactor dynamics: they define the reactor stability by modelling the change in reactivity that occurs when given system parameters are modified. Indeed, feedback coefficients are necessary in analyses of safety, design, during the standard operating period of fission plants and also in multi-physics (MP) applications, representing the interface between different simulation tools.

This paper focuses on the TRIGA (Training Research and Isotope production General Atomic) Mark II research reactor, located at the LENA institute (Laboratorio di Energia Nucleare Applicata) of the University of Pavia[1]. The core configuration includes 91 elements, each with  $\sim 70$  cm in length, submerged in a light water pool with a depth of around 6 m. The core is cooled by an external active system, which maintains control over the pool temperature, and it is equipped with three control rods, replicating the control functionalities found in commercial reactors. Moreover, the peculiarity of this reactor lies in its high safety, ensured by the large negative fuel feedback coefficients. One of the reasons behind the enhanced safety of the TRIGA comes from its fuel design, which has a different structure with respect to conventional  $\text{UO}_2$  used in light water reactors. In this kind of fuel, uranium atoms (U) are mixed within a zirconium-hydride ( $\text{ZrH}_x$ ) lattice, where  $x$  is the H/Zr atomic ratio (equal to either 1 or 1.6 in the case we considered). The physical processes in  $\text{UZrH}_x$  fuel are able, under accidental conditions that lead to an increase in power, to reduce the number of fissions as a result of the temperature rise. This phenomenon occurs due to the joint presence of Doppler broadening and flux hardening effects, characterising the TRIGA reactor with a negative fuel temperature coefficient  $\alpha_f$ [2, 3], larger with respect to the one found in reactors loaded with uranium dioxide. Another characteristic of the TRIGA reactor is the formation of voids close to the fuel element cladding due to the sub-cooled boiling phenomenon, which can occur in the central regions of the reactor where the power, and thus the cladding and coolant temperatures, are higher. The presence of bubbles induces a feedback effect, quantitatively characterised by the void coefficient  $\alpha_v$ [4, 5].

In the scientific research field, dedicated reactor physics software can evaluate with great accuracy the responses of systems to given perturbations, thus evaluating their feedbacks. Among them, open source codes are gaining ground in this framework since they can be adapted to the developer's requirements, being able to simulate new generation reactors with a flexibility not found when using standard proprietary codes. In particular, a lot of efforts are being put in the OpenMC code[6], an open-source software, implemented in Python/C-C++ language, extensible for high-performance calculations and for research purposes. OpenMC has several calculation capabilities, such as fixed source simulations, k-eigenvalue and depletion schemes. Also, this software is continuously updated and improved with new functionalities on a 5-month basis.

In order to assess the prediction's reliability of such software, both the comparison with experimental data (i.e., validation process) and with the outcomes of other codes (i.e., verification process) is necessary. Thus, testing these codes on well-defined benchmarks is a mandatory step. In this regard, the TRIGA Mark II reactor is well suited for validation purposes, allowing for conducting a variety of experimental measurements being characterised by its intrinsic passive safety[7].

The aim of this work is to estimate the fuel temperature and void feedback coefficients of the TRIGA Mark II reactor, adopting the the model previously developed by the author, written in the OpenMC framework and validated with respect to the control rod calibration[8]. The reactivity coefficients will be compared against both experimental data and outcomes from the state-of-the-art Monte Carlo code SERPENT.

This paper is organized as follows: Section 2 summarise the theoretical background in the feedback coefficient analysis, and focuses on the measurement methods adopted; Section 3 report the results from this work, comparing them with the SERPENT ones and from the experimental measurements; finally, Section 4 sums up the conclusions along with future improvements.

## 2 ANALYSIS OF THE FEEDBACK COEFFICIENTS

Either the multiplication factor  $k_{\text{eff}}$  as well the reactivity  $\rho = \frac{k_{\text{eff}} - 1}{k_{\text{eff}}}$  of a nuclear system depend by several quantities  $q_i$ . In order to describe the change in the system's reactivity when a perturbation in  $q_i$  occurs, a first order expansion approximation is generally used, namely:

$$\rho \approx \rho(q_1^0, \dots, q_n^0) + \sum_i (q_i - q_i^0) \frac{\partial \rho}{\partial q_i} \quad (1)$$

Where  $q_i^0$  stands for the value of  $q_i$  before the perturbation. The first order derivative of  $\rho$  with respect to the quantity  $q_i$  is defined as **feedback coefficient** ( $\alpha_i = \frac{\partial \rho}{\partial q_i}$ ), where  $q_i$  can be either the fuel temperature  $T_f$  (fuel temperature coefficient  $\alpha_f$ ) or gas volumes inside the coolant  $V_v$  (void coefficient  $\alpha_v$ ). The importance of feedback coefficients lies in reactor control: a negative coefficient will allow reactivity to decrease when in accidental situations. For example, in commercial reactors of PWR type, the fuel temperature feedback coefficient has values around  $-3 \div -1$  pcm/K. As will be explained in the next section, the TRIGA can rely on flux hardening effects which increase  $\alpha_f$  up to  $-13$  pcm/K.

### 2.1 Fuel Temperature Coefficient

#### 2.1.1 Theoretical Background

This section focuses on the two main interactions between neutrons and fuel caused by temperatures change in the TRIGA reactor. The first is the increase in capture on  $^{238}\text{U}$  due to the *Doppler effect*, which enlarges the absorption cross sections in the resonance region: its value is estimated by General Atomic to be in the order of  $-3$  pcm/K [7]. The second concerns the *flux hardening* caused by the ZrH fuel structure: the bond between zirconium and hydrogen makes the atomic lattice an Einstein solid, in which H behaves like a harmonic oscillator with allowed energies  $E_n = (n + \frac{3}{2}) h\nu$ , where  $n$  is the energy level and  $h\nu = 0.137$  eV [7, 9]. Thus, hydrogen has a dual role in this system: during scattering, energy is exchanged between the neutron and the ZrH lattice, having a ground vibration energy of 0.137 eV. Then, the fuel can behave either as a moderator for collisions with high-energy neutrons or as a source of up-scattering for lower-energy incident neutrons, increasing the particle energy in an inelastic scattering process; the latter phenomenon has increasing probability with increasing temperature, reducing the amount of thermal neutrons and hence the number of fissions. Among the two channels in which fuel temperature feedback acts, the flux hardening phenomenon is largely most pronounced with respect to the Doppler. Indeed, the thermal scattering effect is the main reason that makes TRIGA a safe reactor.

The dependency of the multiplication factor on temperature is then a linear combination between the Doppler and the flux hardening phenomena:

$$\ln k_{\text{eff}}(T) = \ln \left( \overbrace{A e^{\left(-\frac{h\nu}{k_B T}\right)} + B}^{\text{Scattering with H}} \right) + \overbrace{C\sqrt{T}}^{\text{Doppler}} \quad (2)$$

where  $k_B$  is the Boltzmann constant, and  $A$ ,  $B$  and  $C$  are constants.

Adopting the OpenMC code, several  $k_{\text{eff}}$  values has been evaluated with the Monte Carlo model of the TRIGA reactor, imposing uniform fuel temperatures ranging from 300 K to 600 K and adopting the ENDF/B-VII.1 cross section libraries. The multiplication factor trend against the temperature will be reported in Section 3.1. Adopting the formula reported in Equation 2, parameters A,B and C has been evaluated through a fitting procedure using Python. From the knowledge of  $k_{\text{eff}}^{\text{fit}}$ , both the reactivity and the fuel feedback coefficients have been evaluated. The last will be compared in Section 3.1 against SERPENT outcomes from [2] and experimental data reported in [3].

### 2.1.2 Experimental measurement ( $\alpha_f$ )

The experimental procedure for evaluating the reactivity coefficient for the fuel temperature is based on fast power transients: starting from a zero-power critical condition, the SHIM rod is extracted, inserting a positive amount of reactivity in the system and causing an increase in power. As a consequence of this increase, the fuel temperature rises, inducing the reactivity to drop and leading the system to a new equilibrium value. Since the time scale is fast (up to 250 s), the only feedback that acts during this transient on the system is the fuel temperature, neglecting the effect on the moderator temperature and density variation. This experiment was reproduced for different power levels, evaluating the  $\alpha_f$  values for temperatures between 334 K and 424 K using a DYMOLA model [3]. In the original paper, no clear indications on the uncertainty quantification were given. This work adopts a relative error for  $\alpha_f$  of 5%, according to the uncertainty of the measured power reported in the original work.

## 2.2 Void Coefficient

Following the insertion of gas volumes, coolant-neutron interactions change, as the reduction in density implies less absorption but also less moderation and more leakage. This induces an effect on the system' reactivity, quantified by the void coefficient  $\alpha_v$ . Its value can be either positive or negative, depending on which phenomenon prevails.

Due to local effects such as sub-cooled boiling, which occur if the cladding temperature exceeds the *onset of nucleate boiling* (ONB) value, void volumes can also be created in reactors where bubbling should not be present under normal operating conditions. For this reason,  $\alpha_v$ :

- Strongly depends on the reactor location: regions with a higher neutron flux (i.e., central zones) are more subjected to sub-cooled boiling to occur;
- It is nonlinear, due to proximity effects;
- It is difficult to predict, due to its stochastic nature.

### 2.2.1 Experimental measurement ( $\alpha_v$ )

At the TRIGA reactor located in Pavia, the void coefficient was measured using an indirect methodology: since the insertion of a gas volume into a water medium turns out to be difficult to setup, the complementary effect (given by the insertion of a water volume into an air medium) can be evaluated and measured. Under nominal conditions, the central channel is connected with the external air atmosphere. Through the insertion of two cylinders in the middle of the central channel, one filled with a known volume of water  $V_w$  and the other with the same volume of air, it is possible to calculate the difference in reactivity associated with these two setups. By doing so:

$$\alpha_v = \frac{\rho_w - \rho_v}{V_w} \quad (3)$$

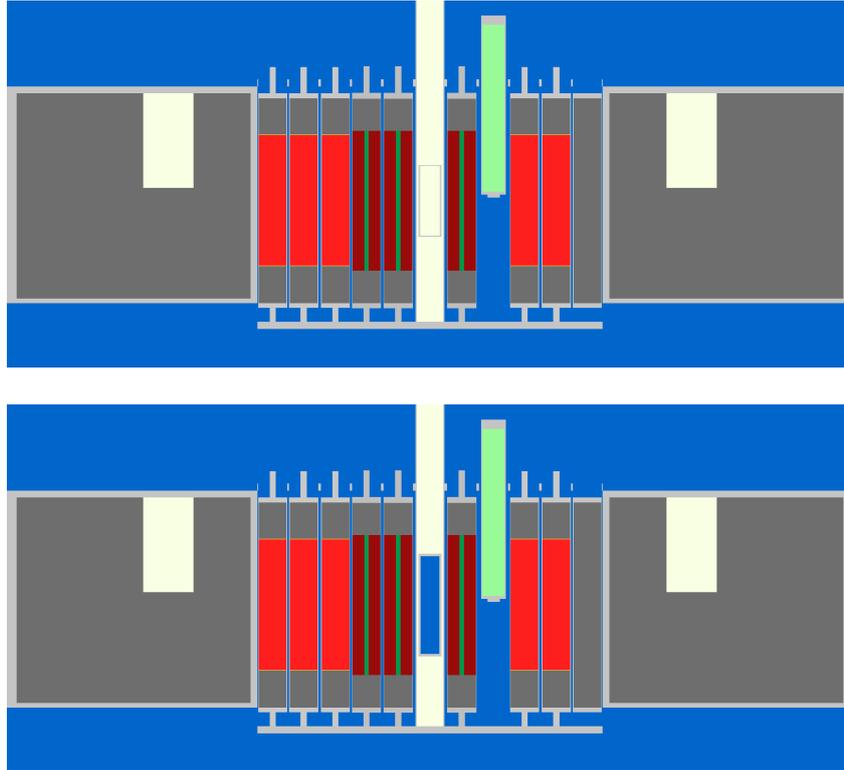


Figure 1: View of the AI-case for void coefficient calculation, placed in the central channel and filled with: air (top panel); water (bottom panel)

where  $\rho_w$  is the reactivity measured in the initial case, whereas  $\rho_v$  is the reactivity with the insertion of the void volume.

The case was modeled in Aluminium, with 120 ml of internal volume. This material was chosen due to its transparency properties in neutron interactions [2]. The two case-setups for this evaluation are reported in Figure 1.

### 3 RESULTS

The validated OpenMC model of the TRIGA reactor, described in [8], was used to calculate the fuel temperature and void feedback coefficients. These evaluations were compared with the outcomes of the state-of-the-art SERPENT model [2, 4] and with experimental data [3]. For this evaluation, OpenMC has been launched with a proper statistics<sup>1</sup> of  $n = 30000$  particles/cycle, along with  $c_a = 500$  active cycles and  $c_i = 300$  inactive cycles.

#### 3.1 Numerical Estimation: $\alpha_f$

The fuel temperature  $T_f$  has been uniformly varied in the 80 fuel rods present in the TRIGA model. The multiplication factor has been collected and reported in Figure 2, showing a decrease in the system reactivity according to the negative feedback effects (Doppler and flux hardening) previously described. The fuel temperature feedback coefficient, evaluated from the fit of the  $k_{\text{eff}}$  discrete points with Equation 2, is showed in Figure 3, along with the SERPENT

<sup>1</sup>The Monte Carlo method samples  $n$  random particles in the system subdivided in cycles. Two different stages follow each other: the first consist in apply a number of inactive cycles  $c_i$  to allow the fission source to reach convergence; the second, effectively score and record physical quantities with a proper number of active cycles  $c_a$ .

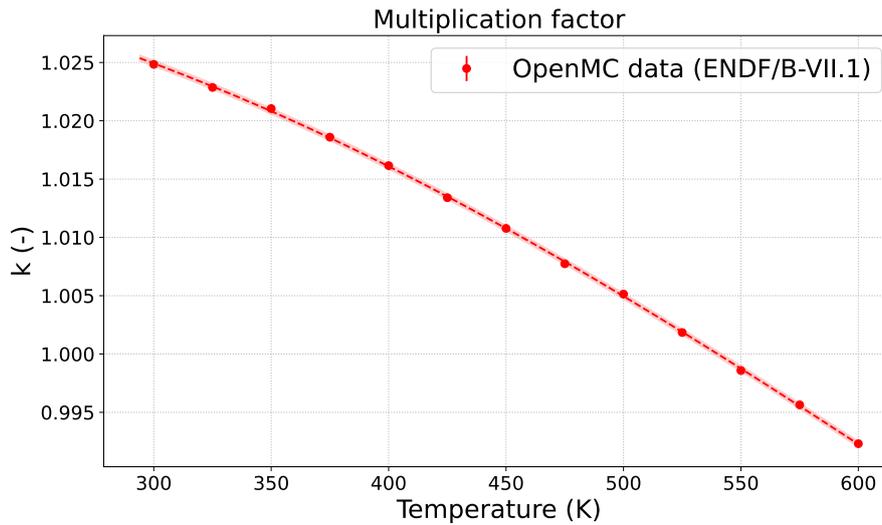


Figure 2: Multiplication factor variation against fuel temperature.

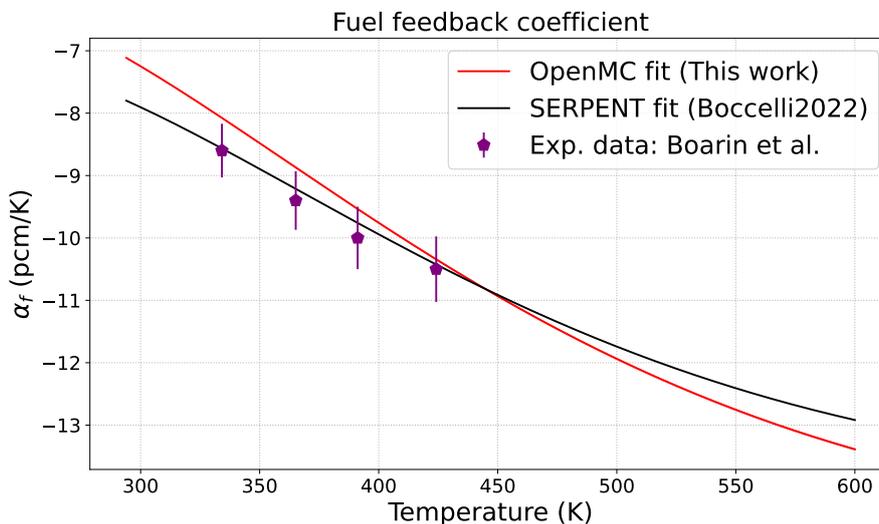


Figure 3: Fuel temperature feedback coefficient. The OpenMC results (red line) are compared with the outcomes from SERPENT (black line) and against experimental data (purple points).

predictions and the experimental measurements. It can be seen that the SERPENT results better fit the experimental data with respect to the OpenMC outcomes. This difference can be due to the thermal scattering library choice: for the SERPENT simulation, the simulation was carried out adopting the ENDF70Sab dataset; while, in OpenMC, the thermal scattering library was already embedded in the official cross section data provided by the developers, leading to a lack of information.

The slope of the OpenMC curve is larger, with a maximum deviation with respect to the SERPENT outcomes of  $-0.68$  pcm/K at 300 K. The difference turns to 0 pcm/K at 440 K and then raises to 0.47 pcm/K at 600 K. These differences, if compared with the mean value  $\langle \alpha_f \rangle = -10.63$  pcm/K appear to be little, having a maximum relative difference of 6.44%.

### 3.2 Numerical Estimation: $\alpha_v$

The void coefficient was calculated starting from the difference in reactivity if the case in the channel centerline was filled with water and with air. The comparison of  $\alpha_v$  calculated with

OpenMC and SERPENT against the experimental data is reported in Table 1. The two Monte Carlo results are in very good agreement between each other and also with the experimental data, falling within the range of  $\pm 2\sigma$  significance.

	Experimental	SERPENT	OpenMC
Void coefficient	$-0.3 \pm 0.05$	$-0.19 \pm 0.03$	$-0.21 \pm 0.056$

Table 1: Void coefficient measured in Pavia TRIGA, along with calculations made with SERPENT and OpenMC. Entries in pcm/ml.

## 4 CONCLUSIONS

This work focused on the analysis of the fuel temperature and void coefficients of the TRIGA Mark II reactor adopting the OpenMC calculation code. The evaluation of these factors plays a key role in the operational activities of the reactor, making it highly safe due to the large negative feedbacks. The Doppler effect and flux hardening allow the number of fissions to decrease as temperature increases (negative fuel temperature coefficient), while the formation of voids in the central part of the reactor, which occurs during sub-cooled boiling, decreases the moderating effect of the coolant (negative void coefficient). By evaluating the multiplication coefficient at different fuel temperatures, the temperature coefficient analysis was compared with the outcomes of the Monte Carlo SERPENT code and experimental data. The OpenMC analysis showed a steeper slope than the curve fitted with SERPENT, which is more in line with the experimental data. However, the differences between the two simulation outcomes are characterized with a maximum relative error of 6.4%, which can be considered acceptable, taking into account that the experimental data are considered to be known within a  $\pm 5\%$  standard deviation. Regarding the void feedback analysis, the difference in reactivity upon insertion of a known volume of water into the central channel was evaluated. The calculated coefficient is found to be largely in agreement with the SERPENT result and within statistical limits compared with the experimental measurement. This paper showed how OpenMC represents a reliable open-source tool for reactor physics calculations, with features comparable with the other state-of-the-art proprietary software in the framework of feedback coefficient analysis. Future works will be devoted to further analyse the fuel temperature coefficient through the imposition of a space-dependent temperature field and to explore the shadowing effect on the neutron flux given by the control rods movement.

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