Id.: EN36

METHODOLOGY FOR THE STUDY OF BURNUP IN THE HIGH-PERFORMANCE LIGHT WATER REACTOR

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Keywords: Supercritical Water, HPLWR, Nuclear Fuel Burnup, Coupled Neutron-Thermohydraulic Calculation, Generation IV Nuclear Reactors.

ABSTRACT

Generation IV nuclear reactors are a group of conceptual designs currently under investigation. The High-Performance Light Water Reactor (HPLWR) is one of the most promising concepts among Generation IV nuclear reactors due to its high thermal efficiency and significant reduction in system components. This reactor uses water under supercritical conditions as a coolant, characterized by significant variation in its thermophysical properties near the pseudocritical line. Density, viscosity, and thermal conductivity experiment a considerable decrease near the pseudocritical point as the temperature increases. These abrupt changes in the coolant's thermophysical properties within a range of ± 25°C around the pseudocritical point represent one of the main challenges in the conceptual development of Supercritical Water Reactors (SCWR). Due to this variability, significant changes occur in energy and momentum transfer within the core channels, directly influencing heat transfer, neutron moderation, and the burnup processes of fuel elements within the reactor. For a comprehensive burnup analysis, this work develops a methodology to couple the neutronic phenomena with the changes in thermodynamic properties within the reactor channels. The methodology combines a Monte Carlo code (MCNP6) for neutronic calculations with a Computational Fluid Dynamics (CFD) code (ANSYS-CFX) for thermal-hydraulic calculations. The research evaluated the working conditions of the multiplicative properties of a typical HPLWR fuel assembly's conceptual design for six burnup values. The study allowed the analysis of several neutron parameters, such as the infinite multiplication factor, the neutron spectrum in the fuel, the behavior of the fissile inventory, and the axial distribution of the average volumetric power.

1. INTRODUCTION

One of the most viable and promising designs proposed by Generation IV International Forum to be part of the new generation of nuclear reactors is the Supercritical Water-Cooled Reactor (SCWR). The conceptual design of this reactor is based on the current Light Water Reactors (LWR). This allows the construction to be done step by step and harness the accumulated operational experience. Using supercritical water as a coolant increases thermal efficiency up to 45 %, which is a great advantage compared to thermal efficiency values registered in conventional LWRs (32-36 %)[1]. The reduction in construction and operation costs is another advantage of this design.
The High-Performance Light Water Reactor (HPLWR) is the European version of the SCWR. This reactor must operate with thermal neutron spectrum, supercritical water as coolant and enriched uranium dioxide as nuclear fuel. The operational pressure of the system is 25 MPa and the output electrical power

is about 1000 MWe. Water enters the core at an average temperature of approximately 553.15 K and reaches average values of up to 773.15 K at the outlet [2].
The use of supercritical water as a coolant and the intrinsic complexity of the core of an SCWR incorporates significant challenges in fuel burnup studies. Great changes in temperature and density of the coolant are observed while it ascends through the reactor core. This process impacts directly on neutron moderation and therefore on power profiles, neutron spectrum and fuel burnup. Coupled neutronic and thermal-hydraulic methodologies are required to evaluate the integrity and security of the reactor due to this multiphysics interaction.
Several coupling tools have been proposed and validated over the last few years. Reiss et al. (2008) presented a methodology to perform coupled calculations in the HPLWR that includes the effect of fuel burnup on power profiles and fuel temperature [3]. A similar analysis was developed by Liu and Cheng (2010) to study an SCWR with a mixed spectrum [4]. Different strategies have also been explored to perform coupled calculations in models of reactor cores. Waata (2006) applied the codes MCNP and STAFAS to develop coupled calculations in the HPLWR core. Relevant results about power and temperature profiles were obtained and discussed. Notable differences on linear axial power profiles were observed between coupled and uncoupled calculations [5]. Other codes, such as MCNPX for neutron analysis and ANSYS-CFX for thermal-hydraulic calculations, were implemented by Xi et al. (2013) and several researchers [6]. However, most recent research doesn't present a complete methodology for coupled calculations that includes the fuel burnup effect and the complexity associated with the physical process in SCWRs.
The current methodology used to analyze the fuel burnup in Pressure Water Reactors (PWRs) and Boiling Water Reactors (BWRs) is not directly applicable to SCWRs. The essence of supercritical flow introduces specific effects, such as Heat Transfer Deterioration (HTD) under pseudo-critical conditions [7,8]. This process can significantly increase the temperature reached on the cladding surface and compromise the core integrity. The goal of this research is to present and develop a methodology to perform a fuel burnup analysis in the HPLWR. The methodology must integrate a coupled neutronic and thermal-hydraulic calculation for each fuel burnup condition. This approach will allow a more accurate simulation of the HPLWR core performance during the fuel cycle and improve the reactor core's design, optimization, and safety. Although the presented methodology is implemented in the HPLWR, its use can be extended to other SCWRs, considering the new geometric specificities and selecting the appropriate physical-neutronic and thermohydraulic models.

2. METHODOLOGY

The developed methodology is recommended only for reactors where significant gradients in the coolant fluid density occur within the core. Since variations in coolant density directly affect core reactivity, impacting the axial power distribution, the proposed methodology is tailored for supercritical water-cooled reactors, where the coolant undergoes substantial changes in thermal-hydraulic properties along the height at different states with varying fuel burnup values. The main objective of this section is to explain the computational model and the integration of coupled neutronic-thermal-hydraulic calculations at each fuel burnup step, resulting in a methodology that allows the study of the SCWR channels.

2.1. Characteristics of the Fuel Assembly Computational Model.

The geometrical model developed was based on the design proposed by Hofmeister in [9] for the typical HPLWR fuel assembly. The cross-section of this design consists of an arrangement of 40 fuel elements in a square array with an outer diameter of 8 mm and a height of 4200 mm. The moderator box at the center of the array is composed of two layers of stainless steel (SS316L) combined with an inner layer of zirconium in a honeycomb structure to reduce the use of stainless steel [10]. Figure 1 shows the

various elements of the typical HPLWR fuel assembly, identifying the cooling subchannels and the different zones of the geometry. The main dimensions of the described assembly can be seen in Tab. 1.

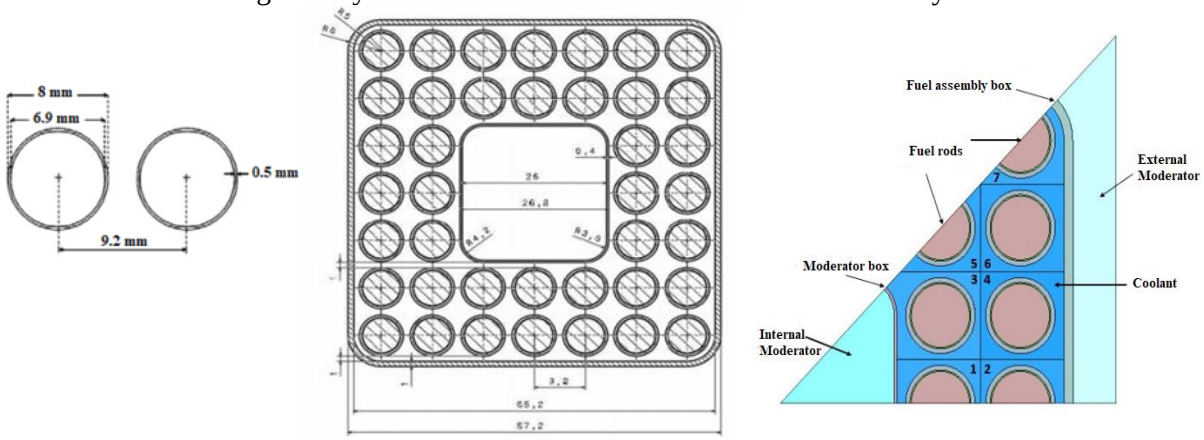


Fig. 1. Cross-section of the typical HPLWR fuel assembly, identification of geometric zones and ⅛ fuel assembly approximation model.

Tab. 1. Main dimensions of the HPLWR fuel assembly.

Outer box	**Values (mm)**	**Fuel rods**	**Values (mm)**
Width	67.2	Active height	4200
Wall thickness	1	Fuel rod outer diameter	8
Inside radius of the corner curvature	5	Cladding thickness	0.5
Gap between outer boxes	10	Fuel pellets diameter	6.9
Inner box		Gap between fuel rod and box wall	1
Width	26.8		
Wall thickness	0.3	Distance between fuel elements	9.2
Outside radius of the corner curvature	4.2		

Considering the symmetry of the fuel assembly, one-eighth of the assembly was considered for the proposed computational geometric model. For the modeling of the geometry in the MCNP6 input-file format (Fig.2), the fuel rods, cooling water, and moderators (both outer and inner) were divided into 21 cells, each 200 mm in height, in the axial direction. In each volumetric cell, the temperature and material densities are assumed to be constant in the neutronic calculations. Helium, fuel rod cladding, and moderator boxes were not partitioned. Reflective boundary conditions were applied at the external boundaries of the model in the radial direction. In the axial direction, two cells with moderator material were placed at the upper and lower boundaries to ensure proper moderation. This is associated with the analysis of a typical fuel assembly located in the central zone of the reactor, where a flat neutron flux behavior in the radial direction and higher energy release values are expected. The uranium dioxide (UO_2) in the fuel is enriched to 5% by weight in $^{235}_{92}U$ for all fuel elements, except for element number 7, which has an enrichment of 4% to counteract the excess neutron moderation occurring in that region.

The boundary conditions established for the computational model are shown in Tab. 2. For the coolant and moderators, two main boundary conditions were set: mass flow rate at the inlet and static pressure at the outlet, with a zero gradient [11]. In ANSYS-CFX, the IAPWS-IF97 library was selected, which provides a compilation of water and steam properties with temperatures ranging from 273.15 K to 1073.15 K and pressures between 100 Pa and 611 MPa.

Tab. 2. Main boundary conditions of the model for thermal-hydraulic calculations.

Parameter	Value
System Pressure	25 MPa
Inlet Temperature of the Moderator Water	553.15 K
Mass Flow Rate (Coolant)	0.167 kg/s
Mass Flow Rate (Inner Moderator)	0.01394 kg/s
Mass Flow Rate (Outer Moderator)	0.02781 kg/s

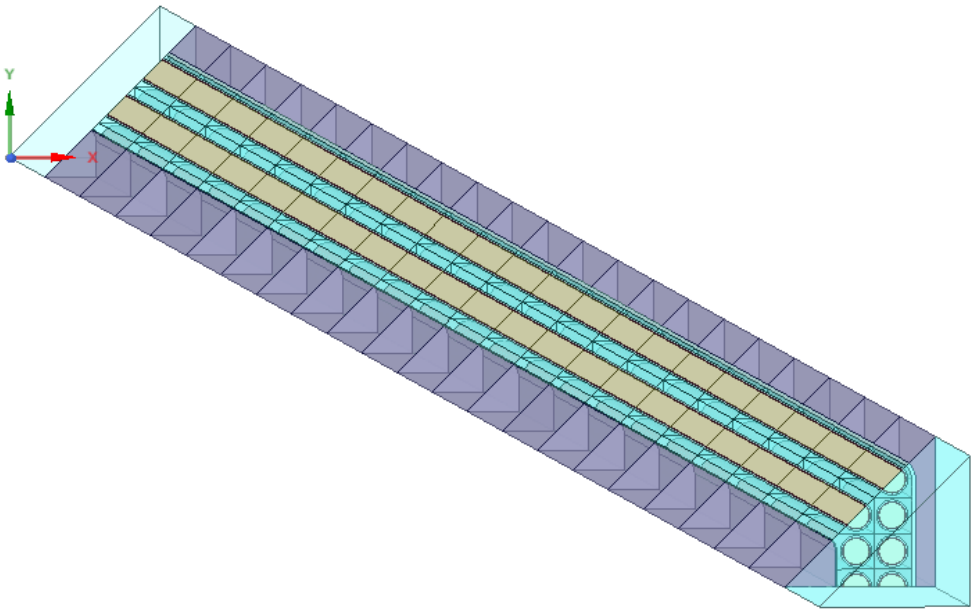


Fig. 2. 3D representation of the geometrical model for a ⅛ fuel assembly approximation used in MCNP simulations.

2.2. Iterative Burnup Method with Feedback from Coupled Neutronic-Thermal-Hydraulic Calculations.

The proposed methodology for fuel burnup analysis employs an iterative approach that integrates neutronic, thermal-hydraulic, and burnup calculations through the serial coupling of the computational codes MCNP6 and ANSYS-CFX. The iterative process provides an advanced approach by continuously feeding back results from the neutronic and thermal-hydraulic calculations, ensuring the accuracy and stability of the simulations. Fig. 3 illustrates the flowchart of the methodology used for the calculations, where Python scripts facilitated the interconnection between the different modules.
This methodology is based on the premise that the computational models studied must share geometric and physical equivalence. Initial conditions were established using the results obtained from the mesh sensitivity analysis conducted for the CFD model, where a constant volumetric heat distribution was employed in the fuel rods. These parameters are essential for setting the initial conditions of the system and preparing the model for subsequent calculations. The first step in the iterative process involves performing neutronic calculations using the MCNP6 code. This calculation provides the energy deposition values in the fuel rods, which are crucial for the next phase of the analysis. The results obtained from MCNP6 are processed with Python scripts to determine the axial distribution of the average volumetric power in each fuel rod. These values are interpolated using a sixth-degree polynomial to create a power distribution function. The power distribution function is then input as a volumetric heat source into ANSYS-CFX. In this phase, the thermal-hydraulic behavior of the reactor is simulated to obtain detailed profiles of density and temperature in the supercritical water and the fuel. The thermal-hydraulic results obtained from ANSYS-CFX, including the average temperatures and

densities of the coolant at the fuel assembly outlet, are used to update the cross-section libraries required for the next cycle of neutronic calculations.

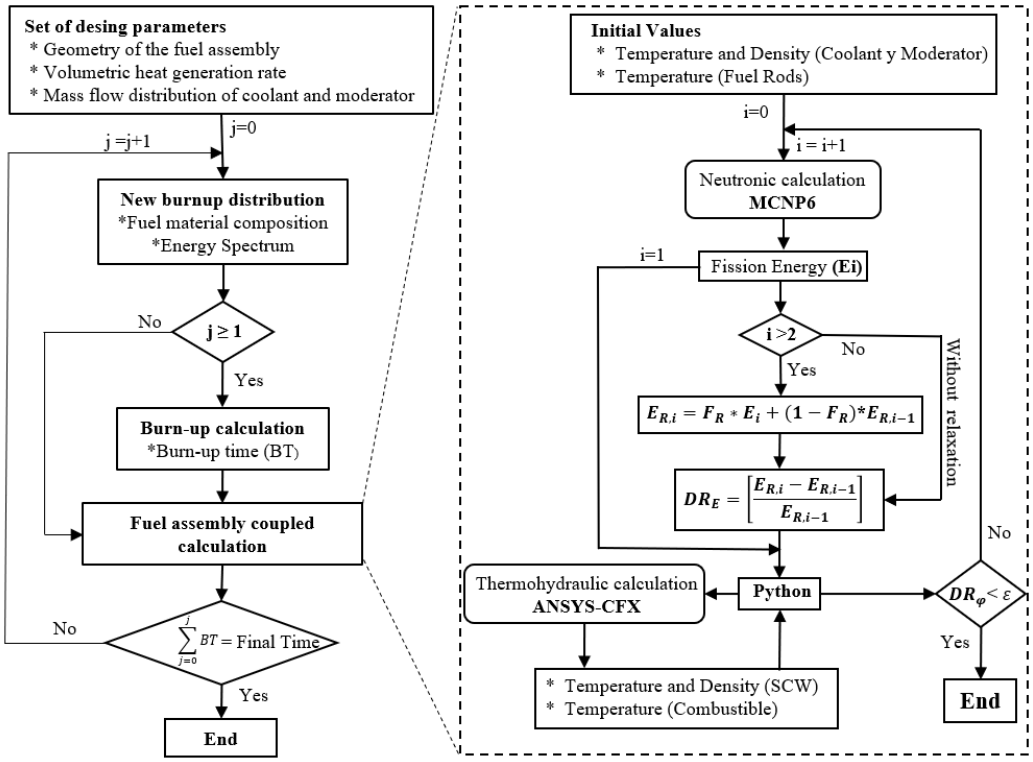


Fig. 3. Flowchart of the Coupled Neutronic-Thermal-Hydraulic Calculation.

This iterative process between MCNP6 and ANSYS-CFX is repeated until the convergence criterion is satisfied. The stopping condition for the coupled neutronic-thermal-hydraulic calculations requires that the relative deviation between the values of variables in two consecutive iterations of the analysis be less than 1% (ε=0.01). Key variables monitored include the neutron multiplication factor, the axial distribution of energy released in the fuel rods, and the axial distributions of average temperatures and densities of the moderator and coolant. The relative deviation (RD) is calculated using Eq. 1.

$$DR_\varphi = \left[\frac{\varphi_i - \varphi_{i-1}}{\varphi_{i-1}}\right] \quad \text{(Eq. 1)}$$

Where φ_i and φ_{i-1} are the values of the variable φ obtained in the current and previous iterations, respectively.

During the iterative process, oscillations in the position of the maximum power release value can occur due to variations in the density of the coolant and moderator water. To mitigate these oscillations and accelerate the convergence of the calculation, a relaxation technique is applied to the energy release values. This technique adjusts the energy produced in the fuel elements with an empirically selected relaxation factor F_R, set to 0.2 after several calculation attempts [12]. The relaxed energy $E_{R,i}$ is calculated using Eq. 2.

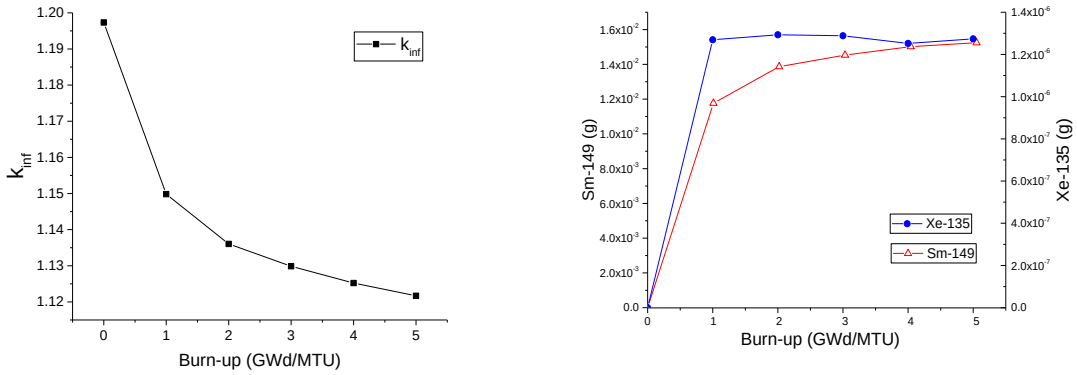
$$E_{R,i}(MeV) = F_R \cdot E_i + (1 - F_R) E_{R,i-1} \quad \text{(Eq. 2)}$$

Where $E_{R,i}$ is the energy deposited in the fuel element cells applying the relaxation technique, and E_i and $E_{R,i-1}$ are the energy deposits calculated in the current and previous iterations, respectively. Once iterative convergence of the neutronic-thermal-hydraulic calculations is achieved, the burnup is calculated using the capabilities of the MCNP6 and CINDER90 codes [13]. The time step chosen in this

work was equivalent to a burnup value of 1 GWd/MTU. Thus, for every 1 GWd/MTU, the MCNP6 input file is updated, and the iterative neutronic-thermal-hydraulic calculations are repeated until a new convergent solution is found. This study analyzes six burnup states of the reactor, ranging from startup with fresh fuel to a burnup value of 5 GWd/MTU.

3. RESULTS

Fig. 4.a shows the variation of the infinite multiplication factor (k_{inf}) as a function of fuel burnup. As observed, the value of k_{inf} significantly decreases at the beginning of the campaign. This abrupt drop is largely caused by the fission products generated during burnup, among which Xenon (^{135}Xe) and Samarium (^{149}Sm) play a significant role, as well as the reduction of Uranium-235 (^{235}U) and the radiative capture of transuranic nuclides, which will be analyzed later in this work. Subsequently, there is an approximately linear and monotonic decrease in the infinite multiplication factor until the end of the analyzed cycle due to the stabilization in the production of these poisons, as shown in figure 4.b.



(a) (b)

Fig. 4. (a) The infinite multiplication factor (k_{inf}) as a function of burnup; (b) Variation of isotope masses Xe^{135} and Sm^{149}.

The neutron spectrum in the fuel region for the initial state can be observed in Fig. 5. In this figure, two peaks in the spectrum are clearly visible, one in the thermal energy range and the other in the fast neutron range starting from 100 keV. The percentage of fissions originating from thermal, intermediate, and fast neutrons in one-eighth of the typical HPLWR fuel assembly is shown for each burnup value in Tab. 3. For all burnup steps, nuclear fuel fissions are primarily caused by neutrons with energy below 0.625 eV, with approximately 70% of fissions occurring in this energy range for the six intervals. For that reason, the studied design of the HPLWR is considered a thermal reactor.

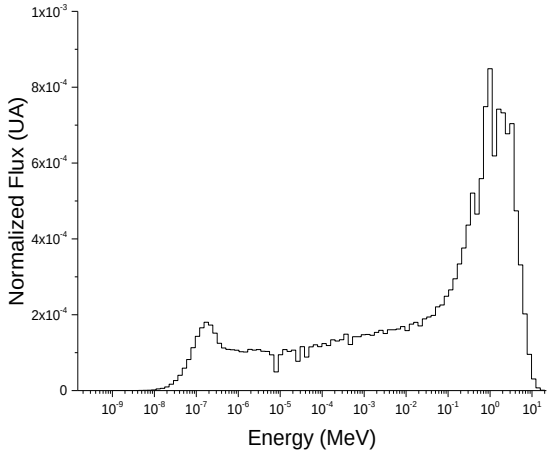


Fig. 5. Neutron spectrum for the initial state in fuel for the one-eighth model of the HPLWR.

Tab. 3. Percentage of fissions produced by neutrons in different energy ranges according to burnup.

Neutron energy	**Burnup (GWd/MTU)**					
	0	1	2	3	4	5
	Percentages of fissions caused by neutrons (%)					
0 eV - 0.625 eV	71.73	70.47	70.63	70.82	71.15	71.76
0.625 eV - 100 keV	20.21	21.07	20.91	20.66	20.35	19.82
> 100 keV	8.06	8.47	8.46	8.51	8.50	8.42

Fig. 6 shows four graphs depicting the changes in the masses of Plutonium and Uranium-235 isotopes as burnup progresses. The elements in the graphs are grouped according to their respective masses and are separated to provide a clearer understanding of their trends in each case study. The masses of the isotopes ^{238}Pu, ^{242}Pu, ^{240}Pu, and ^{241}Pu represent only 8.25% of all the formed plutonium. The mass of ^{235}U decreased by 11.5% (39.7g) in the last burnup state, while the mass of ^{239}Pu increased by only 15g. In all instances, the decrease in the mass of ^{235}U is more significant than the increase in the mass of Plutonium. This behavior is typical of light-water reactors, which, due to their thermal spectrum, have a fuel reproduction coefficient less than unity.

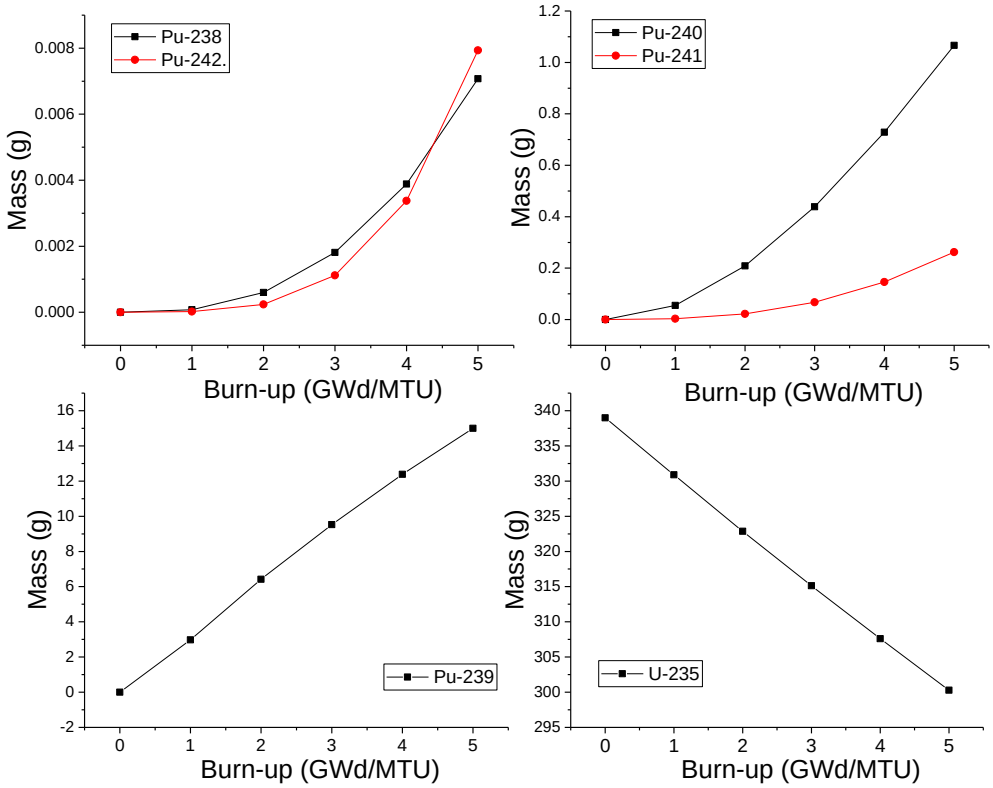


Fig. 6. Variations in the Plutonium and ^{235}U masses in one-eighth of the fuel assembly for the different burnup steps.

Fig. 7 shows the axial distribution of the average volumetric power density in one-eighth of a typical fuel assembly of an HPLWR reactor, from the initial state (0 GWd/MTU) to a burnup value of 5 GWd/MTU. At initial burnup values, the power density exhibits a significant peak within the axial height range of 0.6 to 0.8 meters. As burnup increases, a progressive decrease in power density peaks is observed in the lower section of the assembly, leading to a broadening of the peaks and an increase in power in adjacent areas. The changes observed in the axial distribution of average volumetric power density with increasing burnup can be explained by two key factors. First, as burnup progresses, the concentration of fissile isotopes like ^{235}U and ^{239}Pu gradually decreases, particularly in regions where

the neutron flux is initially higher. This reduction leads to a shift in the peak location along the axial direction. Additionally, the accumulation of fission products, some of which are strong neutron absorbers such as xenon and samarium, increases neutron absorption, resulting in a flattening of the power distribution curve over time. Consequently, the power redistributes toward the center of the assembly, smoothing the power distribution due to reduced reactivity in the lower regions and changes in the medium's thermohydraulic properties. These studies are essential for understanding the effects of burnup on power distribution within fuel elements, which could shape future operational strategies for these systems.

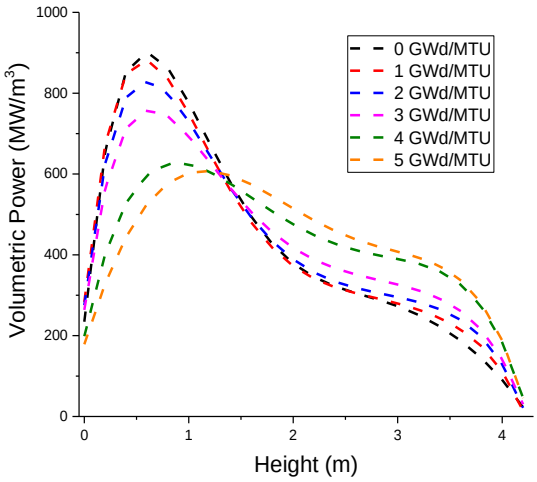


Fig. 7. Axial distribution of the average volumetric power density in the fuel assembly for each burnup step.

4. CONCLUSIONS

The operational conditions of the multiplicative properties of the conceptual design of a typical fuel assembly of the HPLWR for six burnup values were evaluated. A computational model for the coupled neutronic-thermohydraulic calculation of the HPLWR fuel assembly was developed. A relative decrease in the infinite multiplication factor of 4% was observed for 5 GWd/MTU burnup rate. The neutron spectrum exhibits two distinct peaks: the first peak reflects the moderator channel's influence, directing thermal neutrons towards the fuel, while the second, more prominent peak results from neutron emissions during uranium nucleus fission inside the fuel. This behavior is generally observed in light-water reactors with a thermal spectrum, which presents a fuel reproduction coefficient less than unity. The axial distribution of volumetric power for different fuel burnup values was analyzed. A flattening of the power peak towards the central region of the fuel assembly was observed, which significantly improves the heat transfer mechanisms in the reactor core.

ACKNOWLEDGMENTS

This project is supported by the Foundation for Supporting Science and Technology of the State of Pernambuco (FACEPE), project number: PBPG-0936-3.09/22, the Postgraduate Program in Energy and Nuclear Technologies (PROTEN) and the Northeast Regional Center for Nuclear Sciences (CRCN-NE).

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