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NEUTRONIC AND THERMAL-HYDRAULIC CALCULATIONS FOR THE AP-1000 NPP WITH THE MCNP6 AND SERPENT CODES

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ABSTRACT

The AP-1000 is an evolutionary PWR reactor designed as an evolution of the AP-600 project. The reactor is already pre-licensed by NRC, and is considered to have achieved high standards of safety, possible short construction time and good economic competitiveness. The core is a 17x17 typical assembly using Zirlo as cladding, 3 different enrichment regions, and is controlled by boron, control banks, and burnable poison. The expected fuel final burnup is 62 MWD/ton U and a cycle of 18 months. In this paper we present results for neutronic and thermal-hydraulic calculations for the AP-1000. We use the MCNP6 and SERPENT codes to calculate the first cycle of operation. The calculated parameters are keff at BOL and EOL and its variation with burnup and neutron flux, and reactivity coefficients. The production of transuranic elements such as Pu-239 and Pu-241, and burning fuel are calculated over time. In the work a complete reactor was burned for 450 days with no control elements, boron or burnable poison were considered, these results were compared with data provided by the Westinghouse. The results are compared with those reported in the literature. A simple thermal hydraulic analysis allows verification of thermal limits such as fuel and cladding temperatures, and MDNB.

1. INTRODUCTION

In 1999 the Nuclear Regulatory Commission (NRC) granted a project certificate to the AP600, the only reactor with the passive safety technology licensed on the West and Asia [1]. The AP600 project was intended to present a good price-performance ratio and to meet the requirements of the USA's power plants [2]. It was not able to be competitive in USA's energy market because of its cost estimated between 41 to 46 $/MWh. To circumvent this difficulty, the AP1000 project was undertook to gain economies of scale and incorporate a series of design improvements. The cost of the AP1000 is more, between 30 and 35 $/MWh. due to a.

The AP1000 is a pressurized water reactor (PWR) with an evolutionary design derived from AP600.The AP1000 design improvements include 60 % fewer valves, 75 % fewer pipes, 35 % less control cables, 35 % fewer pumps and 50 % less volume of seismic structures. The simplified design of the AP1000 met all the requirements for Advanced Light Water Reactor (ALWR) established by the NRC and Electric Power Research Institute (EPRI).

This study aims to validate the AP100 model developed at the Universidade Federal do ABC. It utilizes the MCNP6 codes [3] and SERPENT code [4], and data provided by Westinghouse AP1000 Design Control Document [2]. The model will be used as reference for future reactor physics studies considering Thorium MOX fuels in PWRs. The AP1000 project was chosen because of its advanced design and available data in the open literature.

2. BRIEF DESCRIPTION OF THE AP1000 REACTOR

The reactor cooling system (RCS) is composed of two coolant loops each containing a steam generator and two coolant pumps. The system also includes a pressurizer, valves, interconnecting piping and instrumentation for operation and safety systems. Figure 1 shows a schematic of the reactor cooling system.

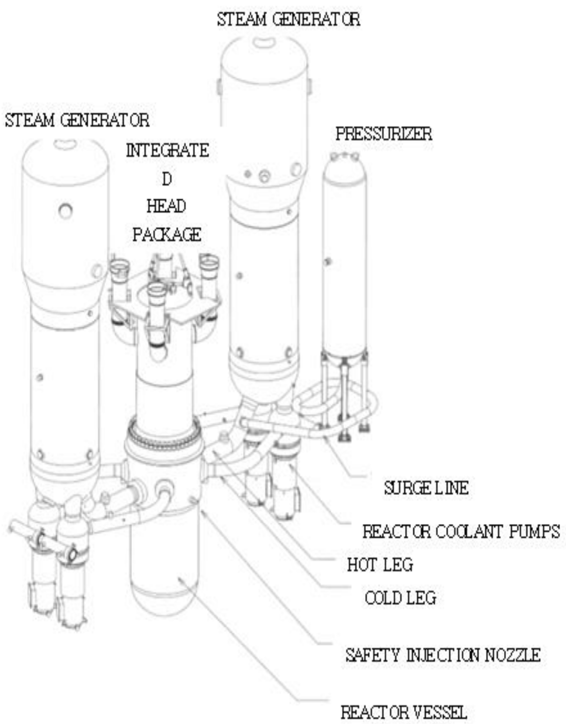

Figure 1: AP1000 Reactor Coolant System schematic [2].

The reactor coolant system is located in the reactor containment and the safety systems are located in the containment and auxiliary buildings. The containment and auxiliary buildings are built to meet seismic requirements.

The reactor contains fuel assemblies, internal structural parts and control elements. The fuel assemblies have different fuel enrichments. The reactor internals provide mechanical structure and direct the coolant to pass through the fuel assemblies. The coolant acts as moderator and is composed of light water at a pressure of 2,250 psia. The fuel assemblies, internals and coolant are contained within a pressure vessel with thick walls. A fuel assembly contains 264 fuel rods distributed in a square 17x17 array as shown in the Figure 2. The fuel enrichments are 2.35 w/o, 3.40 w/o and 4.45 w/o.

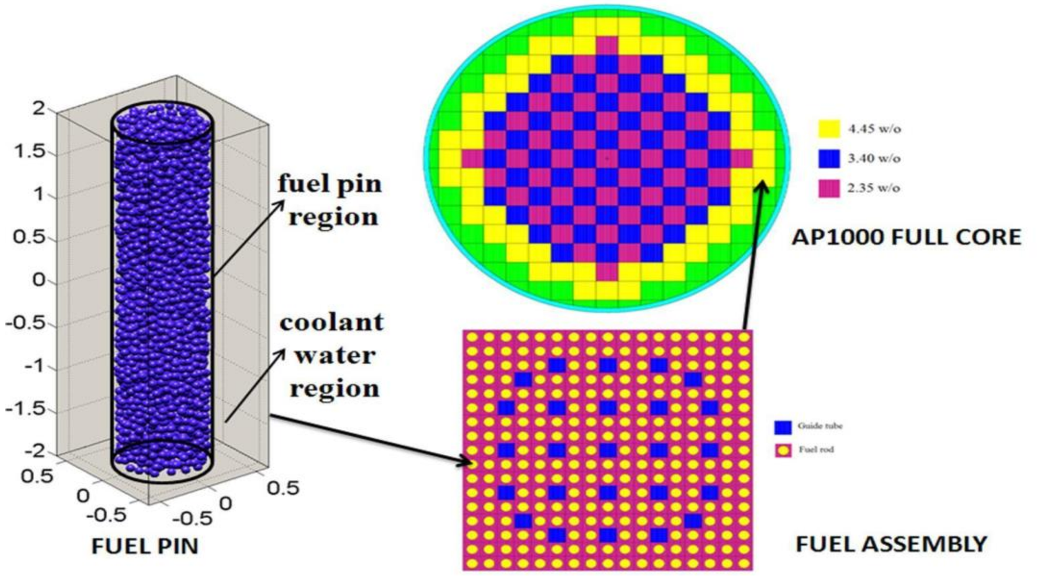

Figure 2: Schematic for the AP1000 reactor core, fuel assembly and fuel pin [5].

The middle position of the fuel assembly iskept free for the eventual insertion of instrumentation. Other 24 remaining positions are guide tubes where the control elements travel. There are also positions where fuel rods are replaced by burnable poison to provide better reactivity control as the fuel is burned up.

3. UTILIZED METHODS

This section describes the computer codes utilized to calculate reactor physics parameters, the composition of the materials used in the simulations, reactor configuration and methods used to obtain specific parameters. The cross-section library used for all simulations was the ENDF/B-VII.0 [9]. The MCNP 6 and SERPENT codes were chosen due to their capability of conducting fuel depletion calculations, versatility and the reliability.

3.1. Computer codes

The MCNP (Monte Carlo N-Particle) is a code used in multiple purposes such as radiation protection, dosimetry, radiography, medical physics, nuclear criticality safety, design and detector analysis, accelerator design, project design, fusion and fission reactor design, decontamination and decommissioning of reactors. The MCNP can be used for neutrons, photons, electrons or coupled neutron/photon/electron transport [7]. The code treats an arbitrary three-dimensional configuration of materials in geometric cells bounded by first- and second-degree surfaces and fourth-degree elliptical tori.

The MCNP code provides numerous flexible tallies: surface current & flux, volume flux (track length), point or ring detectors, particle heating, fission heating, pulse height tally for energy or charge deposition, mesh tallies, and radiography tallies.

The SERPENT code is also a Monte Carlo codes, uses a universe-based combinatorial solid geometry [8], which allows the description of practically any two- or three-dimensional fuel or reactor configuration. The geometry consists of material cells, defined by elementary quadratic and derived macrobody surface types as spheres and cylinders.

ACE format cross section libraries based on JEF-2.2, JEFF-3.1, JEFF-3.1.1, ENDF/B-VI.8 and ENDF/B-VII. Interaction data is available for 432 nuclides at six temperatures between 300 and 1800K.

The burnup capability in SERPENT is entirely based on built-in calculation routines, without any external coupling. The number of depletion zones is not restricted, although memory usage becomes a limiting factor for SERPENT when the number of burnable materials is large.

Fission products and actinide nuclides are selected for the calculation without additional user effort. Burnable materials can be subdivided into depletion zones automatically. The irradiation history is defined in units of time or burnup. Reaction rates are normalized to total power, specific power density, flux or fission rate and the normalization can be changed by dividing the irradiation cycle into a number of separate depletion intervals.

3.2. Material composition and temperatures

The modeling of all nuclear systems whether reactors, radiation shielding and others depend essentially on how the nuclear radiation interacts with matter. This section will show the composition of each material used to model the reactor in mass fraction, such as its density and temperature. Tables 1 and 2 show the composition of materials used in the modeling.

Table 1: composition of the fuel, water and GAP.

Material	Isotope	Composition (mass fraction)	Material	Isotope	Composition (mass fraction)
Water clean	O-16	0.8900000	UO_2 (3.4 w/o) 10.47635 g/cm³	U-235	0.0299707
	H-1	0.1100000		U-238	0.8607902
Water zero soluble boron[1]	O-16	0.8892640		O-16	0.1184944
	H-1	0.1099090	UO_2 (4.45 w/o) 10.47635 g/cm³	U-235	0.0392257
	B-10	0.0001650		U-238	0.8422518
	B-11	0.0006620		O-16	0.1185225
UO_2 (2.35 w/o) 10.47635 g/cm³	U-235	0.0207072	GAP	He-4	1.0000000
	U-238	0.8607902			
	O-16	0.1185026			

[1] 827 ppm of soluble Boron in BOL.

Table 2: Fuel coating composition [10].

Material	Isotope	Composition (mass fraction)	Material	Isotope	Composition (mass fraction)
Zirlo 6.5 g/cm³	Nb-93	0.01200	Zirlo 6.5 g/cm³	Sn-122	0.00037
	Fe-54	0.00008		Sn-124	0.00046
	Fe-56	0.00119		O-16	0.00160
	Fe-57	0.00003		Zr-90	0.50272
	Sn-112	0.00008		Zr-91	0.10963
	Sn-114	0.00005		Zr-92	0.16757
	Sn-115	0.00003		Zr-94	0.16982
	Sn-116	0.00116		Zr-96	0.02874
	Sn-117	0.00061		Nb-91	0.02736
	Sn-118	0.00194			
	Sn-119	0.00069			
	Sn-120	0.00261			

The density of water varies with temperature. It was treated here that thermal power is when the reactor operates with a moderator at 600K and a density of 0.700 g/cm³. As for the reactor at zero power, the moderator temperature is 300K and thus its density is equal to 0.998 g/cm³. The fuel temperature for the hot reactor is considered 900 K, and cold reactor 600 K.

3.2. STRUCTURAL DESCRIPTION OF THE CORE COMPONENTS:

The internals of the reactor were not modeled, only it is considered the moderator, the fuel elements and the barrel. Table 3 provides data on the structural modeling and Figure 3 schematically shows a fuel element rod.

Table 3: Structural Data.

	Fuel Assemblies		**Fuel Rods**
Number	157	Number	41448
Rod Array	17x17	Outside diameter	0.94996 cm
Fuel Rods per assembly	264	Diameter gap	0.01651 cm
Rod Pitch	1.26 cm	Clad thickness	0.05715 cm
Overall transverse dimensions	21.40 cm x 21.40 cm	Clad material	Zirlo
Fuel weight, as UO2	95974 kg		
			Fuel Pallets
Material	UO2	Lenght	0.98298 cm
Density	95.5 % of theoretical	Mass os UO2 per m	6.53602 Kg/m
Diameter	0.81915 cm		

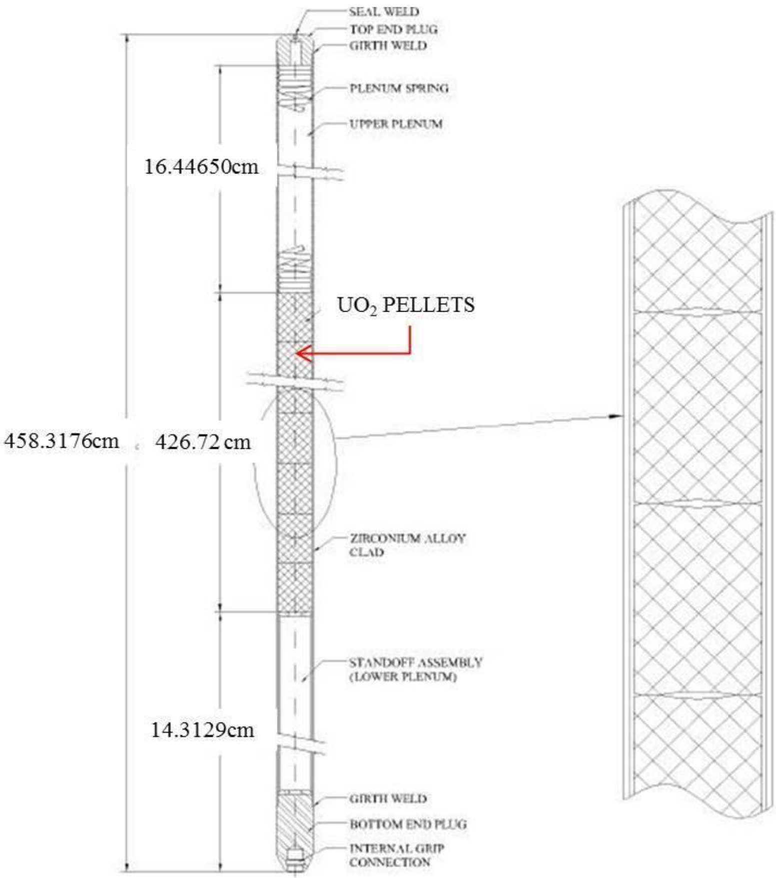

Figure 3 – Fuel rod [2].

3.3. NORMALIZATION OF F4 TALLIES IN A CRITICALITY CALCULATION

The MCNP provides the flux of neutrons through the tally F4, result is normalized to a source of neutrons and must be sized properly for absolute values. The result of F4 can be normalized to the desired power using the equation 3.4.1 [19] providing the corresponding flux Φ.

$$\Phi\left[\frac{n}{cm^2 s}\right] = \frac{P[W]\bar{\upsilon}\left[\frac{neutron}{fission}\right]}{\left[1.6022.10^{-13} J/_{MeV}\right] w_f \left[{}^{MeV}/_{fission}\right]} \frac{1}{k_{eff}} \Phi_{F4} \left[\frac{1}{cm^2}\right] \qquad (3.3.1)$$

Where P is power, $\bar{\upsilon}$ average number of neutrons released by fission, $w_f$the energy released by fission of 198 MeV order and Φ_{F4} the result given by the tally F4.

3.4. Thermal Analysis

Thermal analysis of a nuclear reactor becomes critical because enable anchoring in practice the greatest power released in view of the reactor material properties. Since the maximum power generated in a reactor should be transferred from the nuclear fuel into the coolant in the form of heat[10]. Thus, the thermal analysis are tools for validating the neutronic analysis and establish safety parameters for nuclear reactors.

The maximum power to be produced by the core of a reactor is determined by the heat removal capacity in the hottest channel reactor or the fuel temperature limits in the position of the hottest point of the core. In the case of water-cooled reactors, the prevention of occurrence of critical heat flux (CHF), which is a sudden drop of the heat transfer coefficient of a surface which is evaporating or boiling, is the main concern of the designer, from the term-hydraulic point of view.[11]

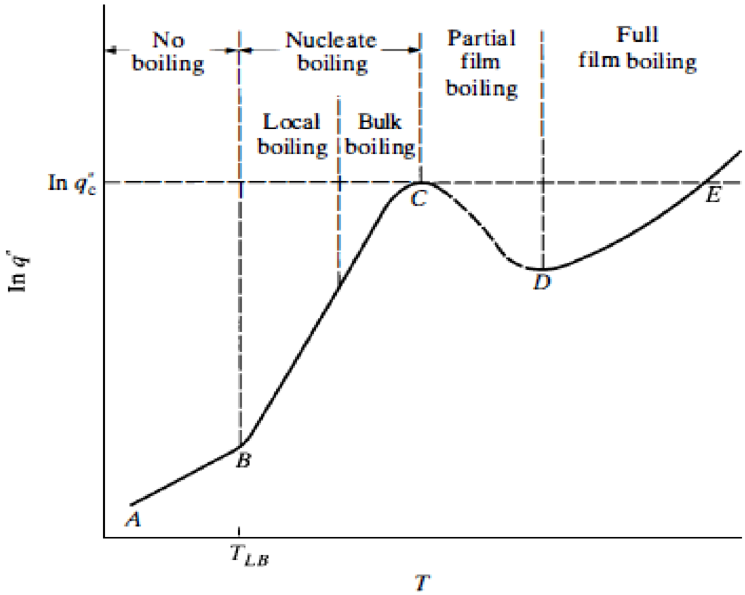

Figure 4 - Boiling regimes. [12]

In a nuclear reactor design should keep the temperature less than the temperature where the heat flux becomes critical (point C in Figure 4), as once reached, this temperature may undergo an abrupt change due to the accumulation of heavy bubbles in the boundary layer and nucleate boiling pass scheme for full boiling film, and thus, inevitably, the temperature reach the melting point of fuel, causing very serious damage to the reactor. This effect is known DNB (Departure from Nuclear boiling)[13].

In a nuclear reactor design should keep the heat flux less than the critical heat flux (CHF) [13]. The thermal limit is the DNBR and DNB (Departure from Nuclear boiling Ratio) which is a measure that determines the DNB performance. It is defined as:

$$DNBR = \frac{q''_{CHF}}{q''_{actual}} \tag{3.4.1}$$

Where q”CHF is the critical heat flux and q” actual is the local heat flux. The criticalheat flux is obtained from empirical correlations. In this paper we adopted the W-3 correlation [14]. For design purposes, the minimum value of the DNBR for PWR reactors is 1.3 [13,15]. this value that exactly matches the hottest channel of the rod, the point where the flow of heat and enthalpy is maximum, as shown in the figure below.

The q”$_{CHF}$ is calculatedby empirical correlations. In this paper is used the W-3 Correlation which was the result of work done at the Westinghouse Atomic Power Division the following correlation was developed from available uniform heat flux with water [14]. It is given by:

$$q''_{CHF} = \left[(2.022 - 0.00623952p) + (0.1722 - 0.00142717p)e^{(18.177 - 0.0598861p)x}\right] \quad (3.4.2)$$
$$\bullet \left[(0.1484 - 1.596x + 0.1729|x|.x)((G/1356.23) + 1{,}037)\right] \bullet \left[1.157 - 0.869x\right]$$
$$\bullet \left[0.2664 + 0.8357e^{-124.055D_e}\right] \bullet \left[2605.06 + 1.076846(h_{sat} - h_{in})\right]$$

Where G is a mass velocity, p - pressure, D - Hydraulic diameter , x - Steam void content, h $_{in}$ – Inlet enthalpy, L – length and q” $_{CHF}$ is a critical heat flux in SI units.

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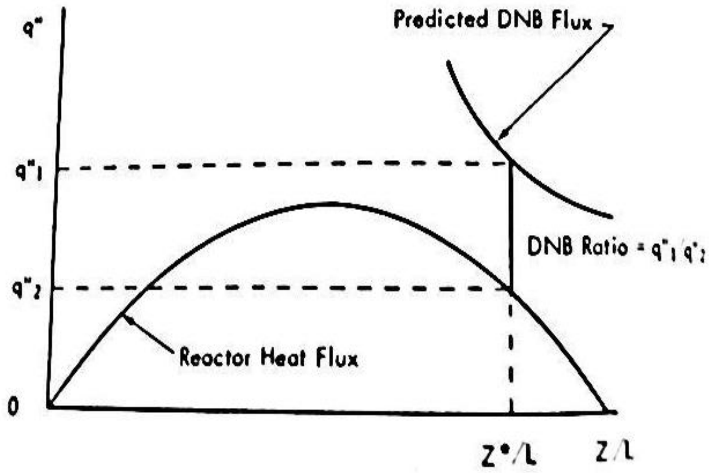


Figure 5 – Development of DNBR as a function of the ratio of the height by the length of the core rod (Z/L) [14]

Below, in Table 4 are given the input values for calculating the DNBR.

Table 4: Input values for DNBR calculation [16]

Fuel Rods	
Number	41448
outside diameter(cm)	0.94996
Diametral gap (cm)	0.01651
clad thickness (cm)	0.05715
Rod pitch(cm)	1.25984
Fuel Pellets	
Diameter (cm)	0,81915
lenght (cm)	0,98298
Coolant Flow	
Total vessel thermal design flow rate (kg/s)	14300.76
Effective flow rate for heat transfer (kg/s)	13456.57
Effective flow area for heat tranfer (m^2)	3.855476
Average velocity along fuel rods (m/s)	4.84632
Average mass velocity ($Kg/s.m^2$)	0.003269
Coolant Temperature	
Nominal inlet (°C)	279.4444
Average in core (°C)	303.3889
Average in vessel (°C)	300.8889

With such input values, it was possible to calculate the titles, enthalpy, q''_{CHF} e q''_{actual} so as to then be calculated DNBR, whose value was 1.42.

4. RESULTS

The calculations conducted with the SERPENT and MCNP6 codes were validated against results from Ref. 2.

4.1. Excess reactivity in Begin of Life and Doppler Temperature coefficient

The excess reactivity is the the parameter that will provide us the life of the reactor to the need for a new cartridge and the amount of absorbent material which should be inserted to provide safety and power control. The maximum core excess reactivity of the reactivity of the reactor (Keff). It was calculated for the arrangement depicted in figure 2 at zero power, cold and 827 ppm boron dissolved in moderator.

The maximum fuel assembly excess of reactivity (k_{inf}) used the same parameters used in the k_{eff} for the Reactor, where the enrichment of this fuel element was 4.45 w/o, and with reflected boundary condition. The excess reactivity is the parameter that will provide the life of the reactor to the need for a new cartridge and the amount of absorbent material which should be inserted to provide safety and power control. The maximum core excess reactivity of the reactor (K_{eff}) was calculated for the arrangement shown in Figure 2 at zero power, cold and 827 ppm boron dissolved in the moderator.

The Doppler Temperature coefficient (α_{iso}) is an important parameter for the safety of the reactor, because when negative, it prevents the positive reactivity feedback. The Doppler Temperature coefficient was calculated for the case described above and in figure 2 the fuel temperature to 600 K, 900 K and 1200K, being measured in each interval is 300 K. The values found are shown in Table 5 below and show up all well consistent with the reference value.

Table 5 – Multiplication Factor and Doppler Temperature coefficient.

	Ref. 2	MCNP6	SERPENT
Maximum core K_{eff}	1.205	1.20450 ± 0.00009	1.20421±0.00051
Maximum Fuel Assembly K_{inf}	1.328	1.32797 ± 0.00022	1.32758±0.00062
α_{iso}(pcm/°F)	-3.5 to -1.0	-1.3 ± 0.3 to -0.9 ± 0.2	-1.1± 0.2 to -1.0 ± 0.1
Cold, zero power, zero soluble boron, beginning of cycle and zero soluble boron (827 ppm)			

4.2. Neutron Flux

The flux form however does not change the power; however, the magnitude of the neutron flux is determined by the power, which the reactor operates. Thus the neutron flux is very important for practical consequences, in Figure 6 it is possible to see the distribution of the neutron flux in the reactor.

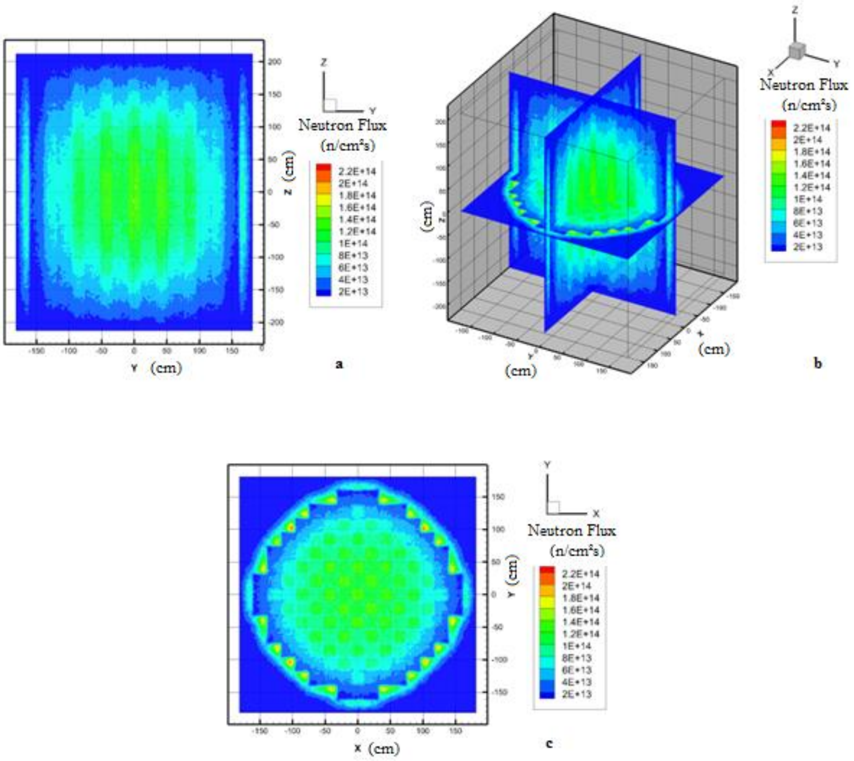


Figure 6 – Thermal Neutron flux distribution in reactor core (a) Axial (b) 3D (c) Radial

The values obtained were compared to the level of typical flux of Westinghouse [2], the comparison between the results can be seen in Table 6 and demonstrate the compatibility of the modeling performed.

Table 6. Typical Neutron Flux at full Power

	Reference[2]	MCNP
Energy (MeV)	0.625 eV > E	
Core Center (n/cm^2s)	5.47E+13	7.16E+13 ± 6.26+E12
Core outer radius at midheight (n/cm^2s)	1.83E+13	1.92E+13 ± 4.39E+12
Core top, on axis	2.17E+13	1.99E+13 ± 3.22E+12
Core bottom, on axis	2.40E+13	1.99E+13 ± 2.42E+12

4.3. Uranium Depletion and TRU production

Knowledge of the isotopic inventory of a reactor and its evolution over time is a fact of utmost importance to recharge planning and disposal of material. The validity and reliability of this data is what makes possible the objective behind this work which is to use a reference reactor for studies of breeder reactors with thorium MOX.

All calculations performed by the references was made with the use of MCNP and the SERPENT. To show the validity of a comparison between the firing results MCNP and the SERPENT is modeled full core to the default configuration (given in figure 2), operating full power for 450 days and with no moderator dissolved boron (clean water). Figure 7 gives us the evolution of the multiplication factor over time for both codes, it can seeing that the MCNP and the SERPENT have very consistent results. There were used 200,000 stories on this modeling, which ensures uncertainty for the multiplying factor about $10^{-05.}$

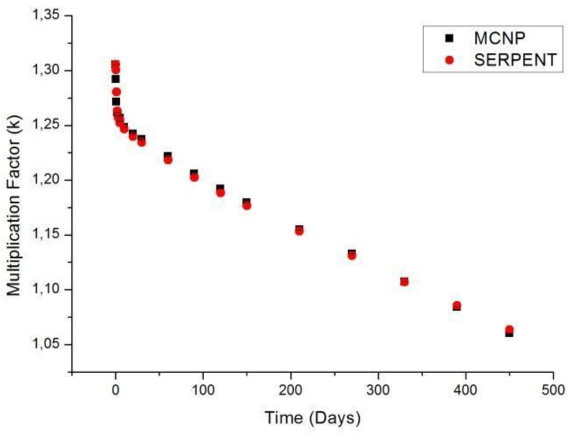
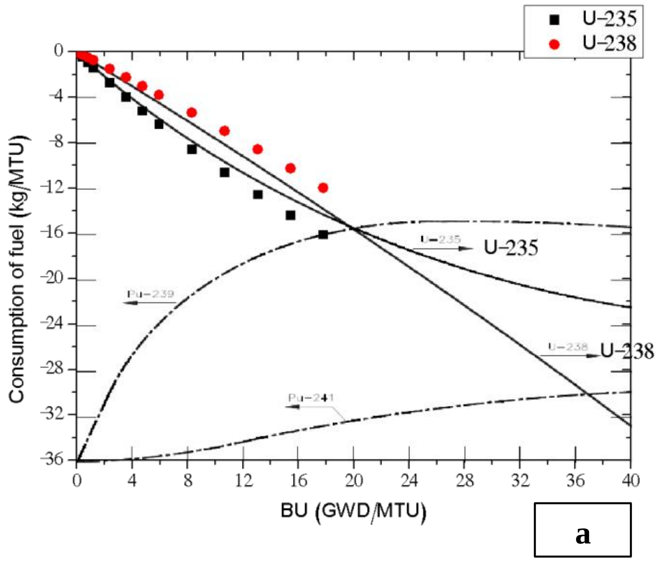


Figure 7 – Multiplication Factor versus Time in full core reactor, Full Power and unborated water.

Figure 7 is also an indication that the reactor can operate for a year and a half without recharging, which is confirmed in the AP1000 reference data [2].

A fuel assembly enrichment equal to 4.45 w/o is burned in a total of 40 GWd / MTU, Figure 8 shows the data of Westinghouse (black lines) and the calculations made in this study (black squares and red circles). In this study the simulations were done differently of the Westinghouse's, was calculated fuel consumption and production of TRU for 450 days of operation, this way you can compare the scale and note that they are very close. Figure 8 (a) is the production of transuranic elements and Figure 8 (b) fuel consumption over time. The results can be seen in Figure 8 below and are consistent with the results of Westinghouse.



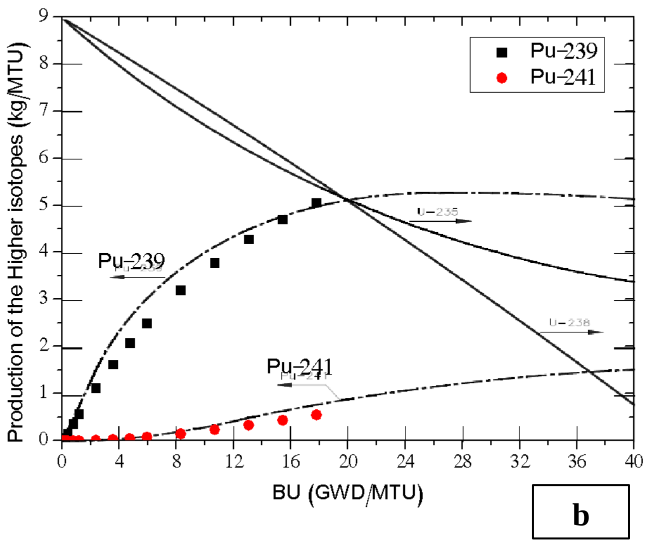


Figure 8 – TRU production and fuel burnup calculations with SERPENT code compared with Westinghouse[2].

4.4. Thermal- Hydraulic Calculations

The reactors should be designed such that the fission products remain confined up with fuel during the entire time and during adverse conditions: be the normal operation, shutdown and during accident conditions, when the refrigerant can not normally cool the fuel down. Below, in Table 7 are given the input values for calculating the DNBR. With such input values, it was possible to calculate the titles, enthalpy, q''_{CHF} e q''_{actual} so as to then be calculated DNBR, whose value was 1.42.

5. CONCLUSIONS

The results obtained were well consistent with what was expected. For 450 days, a little less than one and a half (540 days), we obtained a keff EOL of 1.06026 ± 0.00008 (MCNP) and 1.06372 ± 0.00003 (SERPENT) where the reactor was depleted with no burnable poison or control rods. In other words, approximately 18 MWD / TU per cycle, so in three cycles that would be about 54 MWD / TU which is a value close to the expected by the Westinghouse for the fuel duration that would be 62 MWD / TU

The excess reactivity at the beginning of life for the parameters given in [2] show compatibility with the 1.205 value used as a reference diluted to 827 ppm boron, was obtained the values of 1.20450 ± 0.00009 (MCNP6) and 1.20421 ± 0.00051 (Serpent). The Doppler Temperature coefficient and neutrons fluxes have also demonstrated values close to expected, as can be seen in Tables 5 and 6, in the data analysis section.

The production of TRU and fuel consumption also shown in order of magnitude as the relatory given in [2].

The Thermal-hydraulic point of view, calculate the DNBR, despite having higher values than those mentioned in [21], it is still within the acceptable limit. The ratio between the value of the DNBR shown in last reference and calculated in this problem is 0.88.

The difference may be likely in the choice of correlation for calculating q''_{CHF}, since the correlation used in [21] is WRB - 2M [22]. But, within that context, the evaluation is positive.

As a suggestion for future work, the use of correlations with gifts correction factors, such as W-3 R- Grid[23], can yield more interesting results.

This study met expectations, demonstrating a good compatibility of the computational modeling with the expected results for the PWR AP1000. The results also demonstrated compatibility between the codes MCNP-6 and SERPENT, to be used for a future study involving fuel of ThO_2-UO_2, using as reference the AP1000 reactor.

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