2015 International Nuclear Atlantic Conference - INAC 2015
São Paulo, SP, Brazil, October 4-9, 2015
ASSOCIAÇÃO BRASILEIRA DE ENERGIA NUCLEAR - ABEN
ISBN: **978-85-99141-06-9**

COMPUTATIONAL SIMULATION OF FUEL BURNUP ESTIMATION FOR RESEARCH REACTORS PLATE TYPE

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ABSTRACT

The aim of this study is to estimate the spatial fuel burnup, through computational simulation, in two research reactors plate type, loaded with dispersion fuel: the benchmark Material Test Research – International Atomic Energy Agency (MTR–IAEA) and a typical multipurpose reactor (MR). The first composed of plates with uranium oxide dispersed in aluminum (UAlx–Al) and a second composed with uranium silicide (U_3Si_2) dispersed in aluminum. To develop this work we used the deterministic code, WIMSD-5B, which performs the cell calculation solving the neutron transport equation, and the DF3DQ code, written in FORTRAN, which solves the three-dimensional neutron diffusion equation using the finite difference method. The methodology used was adequate to estimate the spatial fuel burnup , as the results was in accordance with chosen benchmark, given satisfactorily to the proposal presented in this work, even showing the possibility to be applied to other research reactors. For future work are suggested simulations with other WIMS libraries, other settings core and fuel types. Comparisons the WIMSD-5B results with programs often employed in fuel burnup calculations and also others commercial programs, are suggested too. Another proposal is to estimate the fuel burnup, taking into account the thermohydraulics parameters and the Xenon production.

1. INTRODUCTION

Among the various parameters observed in nuclear analysis, is the fuel burnup that runs the physical phenomena associated with the interaction of neutrons. As the combustible material is fissioned, nuclear properties suffer significant changes which must be controlled. In order to compensate and track changes of the core composition, due to the consumption of fuel, studies are needed to explore its behavior during operation. For this purpose, numerous computer codes are used in the simulation of reactor core performance and research facilities and test materials contribute to this task.

The purpose of this work is to estimate the spatial fuel burnup, through computer simulation, for two nuclear research reactors: the Material Test Reactor (MTR) of the International Atomic Energy Agency (IAEA) [1] and a generic reactor we call Multipurpose Reactor (MR). The computational tools were used WIMSD-5B code and a code written in the FORTRAN language.

2. BURNUP

The importance of determining the fuel burn is related to the question of their performance as well as to the arrangement and rearrangement of the fuel loading and unloading in order to achieve a functioning that is the most economical within the design constraints, respecting the rules of safety [2]. In this regard we should note that there is fuel burning difference intended to power reactors for supplying the research reactors.
This difference is primarily associated with the type of fuel, enrichment, the core geometry, the power provided, the set cycle and the purpose of the reactor. Another distinction with respect to the unit used in accordance with [3] in the practices involving research and development is common firing be expressed in terms of percentage of fissioned heavy atoms as in the industrial area by the ratio of the thermal energy produced per day per metric ton heavy atoms.

2.1 Dispersed Fuel

According to [4], among the materials analyzed, from the international program Reduced Enrichment for Research and Test Reactors (RERTR), who were more favorable to conversion to low-enriched were UAlx-Al, the U_3O_8 and UO_2. However, according to [5] The U_3Si_2 (silicide), was the best compound identified for the development of LEU fuel (Uranium Enrichment Low).

The two research reactors presented in this paper are loaded with fuel dispersion. The MTR-IAEA with UAlx-Al (aluminum alloy and uranium dispersed in an aluminum matrix), and the typical multipurpose reactor with U_3Si_2 -. Al (silicide dispersed in aluminum matrix). These fuels are consisting of an alloy of at least two materials with different characteristics and functions in the reactor.

3. WIMSD-5B CODE

The WIMS (Winfrith Improve Multigroup Scheme) is a deterministic code, position in the cell, realizing calculation for different geometries, providing physical parameters required for the development projects of nuclear reactors of various types. Since the 60's has successfully achieved its results, and in addition is widely accepted internationally, one of the most used in the management core of nuclear reactors. Its standard library has cross sections of data to multi-group of the materials most used in nuclear reactors [6]. The code was chosen for this work because it was the latest available at Institute Engineering Institute (IEN).

The cells WIMS develops calculation in four different geometries: homogeneous cells, plates or round bars, rods or plates arrangements (cluster geometry) and multicell. In this work the calculation was based on data from a one-dimensional cell. The IAEA library was chosen which consists of 69 energy groups, being recommended by the team responsible for updating the code [6]. The WIMS Library Up-date IAEA project has a cross sections used for WIMSD-5B, that are provided by Nuclear Energy Agency (NEA) library [7].

In the code WIMSD depletion equation is written as

$$\frac{dN_i\,(t)}{dt} = -(\lambda_i + A_i).N_i\,(t) + \sum_k q'_{i,k}\,(t).N_k(t) + \sum_k q_{i,k}\,(t).N_k(t) \qquad (1)$$

N_i = nuclide concentration i,
N_k = nuclide concentration k,
λ_i = decay constant of nuclide i,
Ai = absorption rate of reaction of the nuclide i,
$q_{i',k}$ e $q_{i',k}$ = probability of k nuclide nuclide to transmute i.

For the solution of depletion equations for each material m and isotope i is used WIMSD-5B code, which integrates the method of trapezoids. According to [8] Equation (1) is solved for $\lambda i < \lambda 0$, where $\lambda 0$ assumes a specific value for which the nuclide is considered in balance. If $\lambda i > \lambda 0$, it is assumed that dN_i / dt = 0 and Equation (1) comes down- à:

$$(t + \delta t) = N_i(t) + \sum_k \frac{q_{i,k}(t).N_k(t)}{\lambda_i + A_i} \qquad (2)$$

Using the WIMSD-5B were obtained depending on the parameters nuclear burnup, information necessary to calculate the space burnup performed by the code written in FORTRAN. In Fig.1, the calculation for the cell-WIMSD 5B is represented by a diagram. Note that this code is executed only once and the data generated, it is the interpolation of the nuclear parameters necessary for the overall calculation of the core.

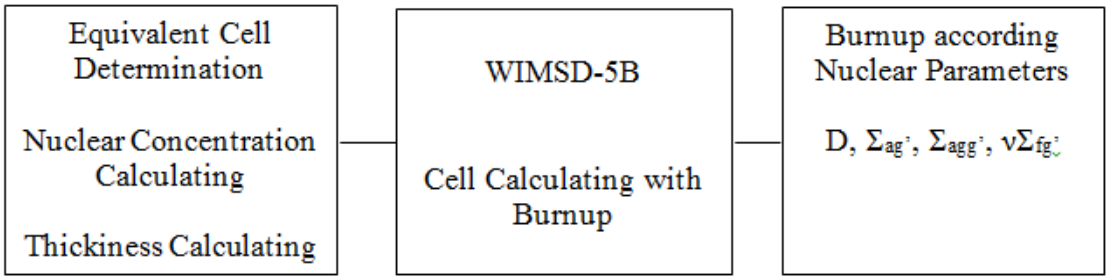

Figure 1: Nuclear homogenates parameters with WIMSD-5B.

4. FORTRAN - DF3DQ CODE

To estimate the spatial fuel burnup, it used the code in Fortran DF3DQ, developed in the IEN, based on neutron diffusion theory. The input data provided by WIMSD-5B. To solve the diffusion equations we used the Finite Difference Method (FDM), classified as deterministic and widely used in Reactor Physics a stationary model for two energy groups in three-dimensional cartesian geometry was established.
In this study, were not considered sources of external neutrons and occurrence of up-scattering, in other words, there is no scattering of lower energy group, thermal unit, for

higher energy group, fast group. Therefore, for two energy groups, which is the case this work, there is only the rapid scattering group, 1 to the thermal group, 2.
For the numerical solution of the diffusion equation was used Finite Difference Method (FDM), with the outer and inner iteration scheme using Gauss-Seidel method, with the multiplication factor being determined by the power method. The DF3DQ calculates the spatial burnup and then a subroutine nuclear interpolates the generated parameters in this step with those provided by WIMSD5 B. The new nuclear parameters resulting from the interpolation feed back to the neutron diffusion equation, and calculations are repeated according to the steps of pre-determined burnup, until program termination.

5. SIMULATIONS AND RESULTS

The first stage of the construction work was equivalent cell and calculating the thicknesses and atomic concentrations of representative cell of the fuel element (FE), the control rods safety (CRS), and other core parts of both reactors. The calculation results are used as input data for the WIMSD-5B, allowing this homogenized nuclear provide parameters associated with each day stipulated firing. With these parameters the nuclear DF3DQ code provided spatial burnup.

The WIMSD-5B and DF3DQ codes were employed in spatial fuel burnup simulations for two cases:

Case 1: Material Test Reactor MTR – IAEA
Case 2: Multipurpose Reactor – MR

5.1 Case 1: Material Test Reactor MTR – IAEA

In the first case benchmark problems we were simulated [1] for a typical reactor research and materials testing, the MTR - IAEA. Said reactor has an active core (high) of 60 cm, each fuel element. It has lateral dimensions 7.7cm x 8.1 cm. It is a reactor type pool, its fuel is composed of dispersed uranium oxide Aluminum (UAlx - Al) and power of 10 MW. The fuel element (FE) consists of 23 plates and the control rods / safety (CRS) 21 plates 17 of them being identical to those of the FE and the other made of pure Al. Fig. 2 shows the radial geometry of the reactor core. Fig. 3 depicts a cross section of the fuel element (FE). The equivalent cell of the fuel element is shown in Fig. 4.

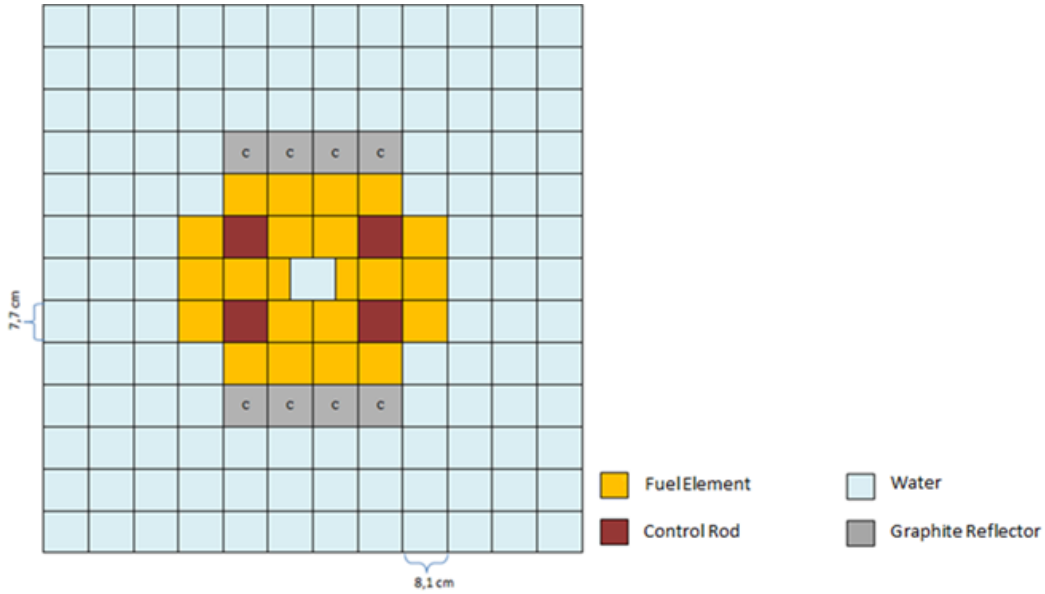

Figure 2: Reactor core– MTR-IAEA

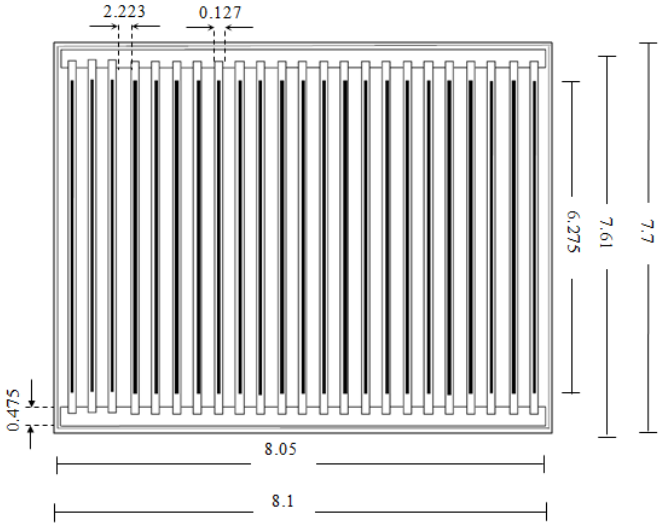

Figure 3: Fuel element representation – MTR-IAEA (dimension in cm, 20°C)

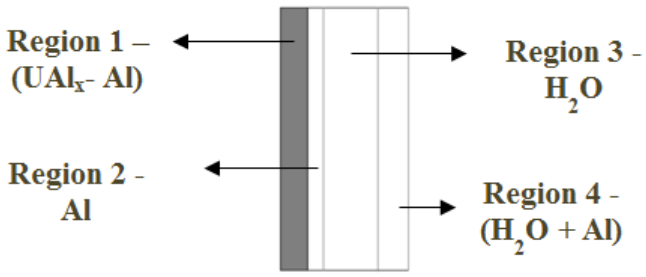

Figure 4- Equivalent cell of MTR-IAEA

The first results arose from the fuel element of the calculation cell , the control rods and safety (CRS), the control rods and safety with water replacing the four aluminum plates (CRS-water replacing aluminum plates) reflector graphite and reflector / moderator water. To avoid a very lengthy report, they are presented only the tables with the results for the FE and the CRS.

The Tables 1, 2 and 3 report the number of regions of the equivalent cells (EC), the CRS and CRS-water replacing aluminum plates. The tables also have and its corresponding isotope elements, the thicknesses and atomic concentrations of each region.

Table 1 : EC-MTR

Region	Elements and isotops	Concentration (atoms/barn.cm)		Thicknesses (cm)	
		Benchmark(*)	Calculated	Benchmark (*)	Calculated
Region 1: "meat" UAl_xAl	^{235}U	$2,2536x10^{-3}$	$2,26271 \times 10^{-3}$	$2,55 \times 10^{-4}$	$2,55 \times 10^{-4}$
	^{238}U	$8,9005x10^{-3}$	$8,93652 \times 10^{-3}$		
	Al	$3,8171x10^{-2}$	$3,83265 \times 10^{-2}$		
Region 2:cladding	Al	$6,0260x10^{-2}$	$6,02439 \times 10^{-2}$	$3,8 \times 10^{-4}$	$3,8 \times 10^{-4}$
Region 3:1/2 water channel	H	$6,6956x10^{-2}$	$6,66739 \times 10^{-2}$	$1,115 \times 10^{-3}$	$1,115 \times 10^{-3}$
	O	$3,3428x10^{-2}$	$3,33695 \times 10^{-2}$		
Region 4: Al inerts edges and excess water	Al	Not found values for comparison	$4,60492 \times 10^{-2}$	$4,02 \times 10^{-4}$	$3,97 \times 10^{-4}$
	H		$1,57441 \times 10^{-2}$		
	O		$7,87207 \times 10^{-3}$		
	O		$7,87207 \times 10^{-3}$		

(*) Source: IAEA-TECDOC, 1980

In the first three regions of this cell values calculated thicknesses are in accordance with the data provided by the [1] as well as the values of concentrations. You can assign the small difference observed due to the number of decimal places used in the calculations and Avogadro's number, which can be represented by a rounded value or with a different number of significant digits. There were no elements that would allow study of the comparison of isotopic concentrations in the region 4.

Table 2: CRS-MTR

Region	Elements and isotops	Concentration (atoms/barn.cm)	Thicknesses (cm)
		Calculated Value	Calculated Value
Region 1: "meat" UAl_xAl	^{235}U	$2,26271 \times 10^{-3}$	$2,55 \times 10^{-4}$
	^{238}U	$8,93652 \times 10^{-3}$	

	Al	3,83272 x10^{-2}	
Region 2:cladding	Al	6,02439 x 10^{-2}	3,8 x10^{-4}
Region 3:1/2 water channel	H	6,66739 x 10^{-2}	1,115 x10^{-3}
	O	3,33695 x 10^{-2}	
Region 4: Al inerts edges,water excess, pure Al plates	Al	2,99200 x 10^{-2}	1,0796 x10^{-3} (*)
	H	3,36016 x 10^{-2}	
	O	1,68008 x 10^{-2}	

(*)The thickness of this region of the cell differs from the previous case because the active area of the ECS cell is smaller and the extra area is larger.

In the region 4 of Table 2, there is a decrease in aluminum concentration, desired effect due to withdrawal of fuel plates 6 and the insert 4 of pure aluminum plates.

The following results of Table 3, for the regions 1,2 and 3, are the same as the previous cell because there was no change in the active area of the cell. In the region 4 there was a reduction in the concentration of Al, because this scheme the pure Al plates were removed and, as might be expected, the concentrations of H and O increased.

Table 3: CRS-MTR – Pure Al plates replaced by water

Region	Elements and isotops	Concentration (atoms/barn.cm)	Thicknesses (cm)
		Calculated Value	Calculated Value
Region 1: "meat"-UAl_x-Al	^{235}U	2,26271 x 10^{-3}	2,55 x10^{-4}
	^{238}U	8,93652 x10^{-3}	
	Al	3,83272 x10^{-2}	
Region 2: cladding	Al	6,02439 x 10^{-2}	3,8 x10^{-4}
Region 3: 1/2water channel	H	6,66739 x 10^{-2}	1,115 x10^{-3}
	O	3,33695 x 10^{-2}	
Regio 4: inerts edges Al + water	Al	2,15922 x 10^{-2}	1,0796 x10^{-3}

The graphs, Fig.5, show the k_∞ results obtained with the WIMSD-5B and EPRI-CELL codes and the range of concentration of some uranium isotopes as a function of burnup fuel to case 1, using the WIMSD-5B code [1].

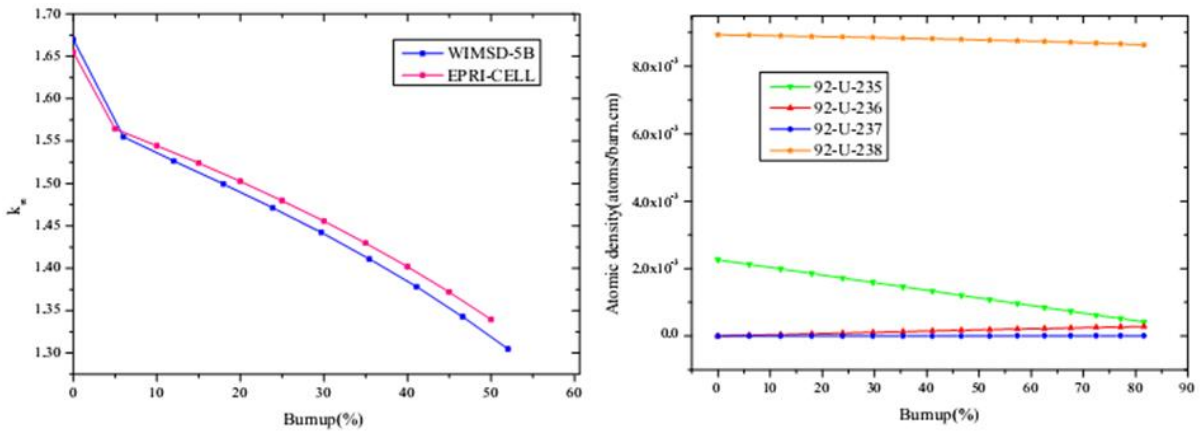

Figure 5: k_∞ from WIMSD-5B and EPRI-CELL and atomic density versus burnup – MTR-IAEA

Fig. 6 and Fig. 7 represent the thermal and fast neutron flux groups respectively at the beginning and end of the operation. Fig. 8 shows the simulation result of the accumulated burnup the 1st and 31st day. The space burnup fuel was simulated for 31 days and the unit used for burnup was the MWd / t .

From the results it can be observed that the neutron flux at the center of the reactor in Fig. 6, is smaller. This is due to the water channel positioned at the center of the core. The Fig.7 shows that, although no water fission in the peak value of the channel flow is justified for the group of thermal neutrons, which in this case is the source scattering.

Comparing the 1st and day 31, Fig. 8, it is possible to notice a significant increase in the values of burnup accumulated mainly in the central core region. As the neutron flux is larger in this region, the greater will also be burnup.

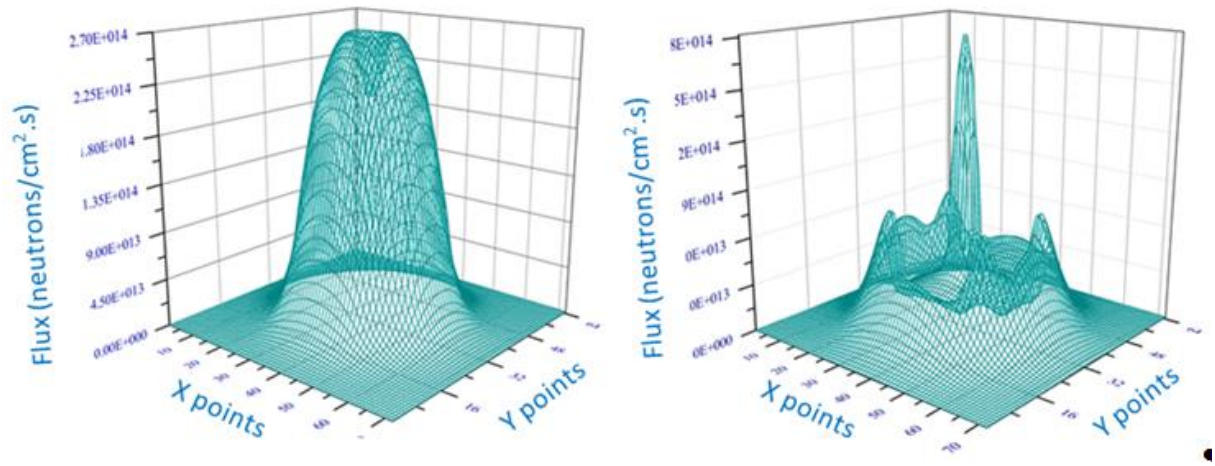

Figure 6: Thermal and fast neutron flux – Start

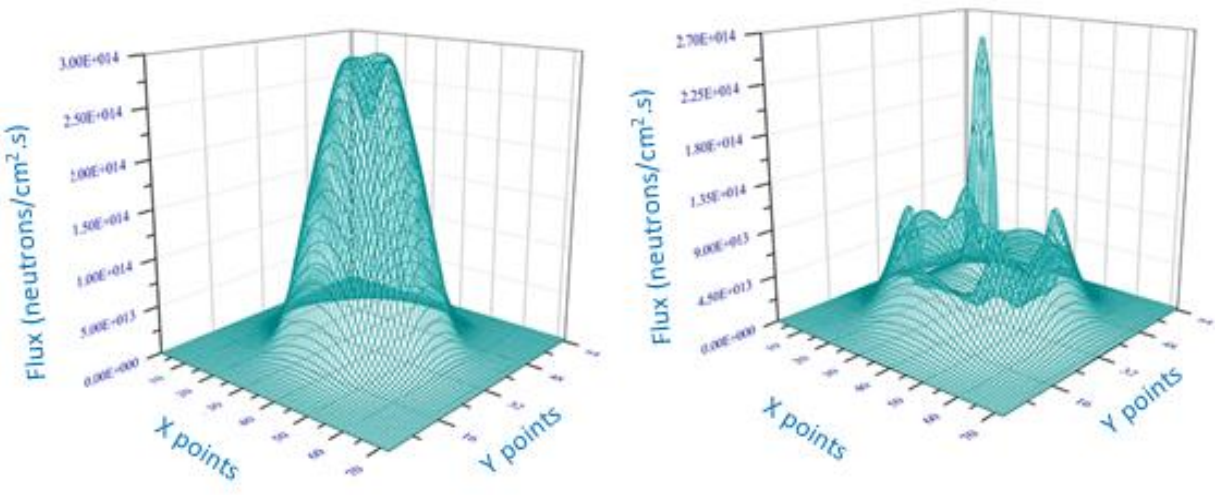

Figure 7: Thermal and fast neutron flux – End

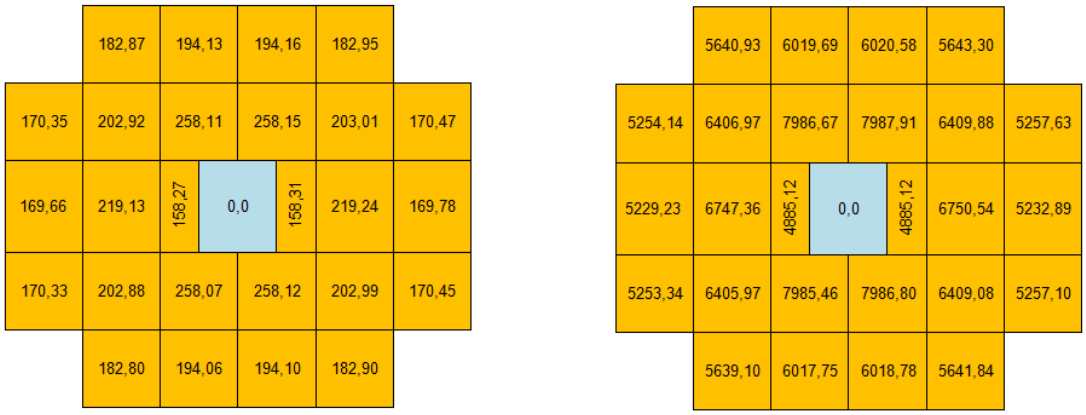

Figure 8: Accumulated burnup (MWd/t) per EC – 1º and 31º day.

5.2 Case 2- Typical multipurpose reactor (MR)

For this case, cell calculations were made for the following regions of the reactor: fuel element, control element and safety control, element guide and safety, chimney, radiating active part, radiating non-fuel region. For the same reason given in case 1 shows the tables only the FE and CRS. The multipurpose reactor (MR) typifies a reactor designed to achieve a power of 30 MW, has plate-type FE 28, with 21 plates each formed of silicide (U_3Si_2) dispersed in aluminum as well as two channels for irradiation. Regarding the first case, the differences lie in the size and fuel type, UAlx - Al.

Fig. 9 shows a cross-section (xy plane) of the multipurpose reactor and Fig. 10 to the fuel cell element.

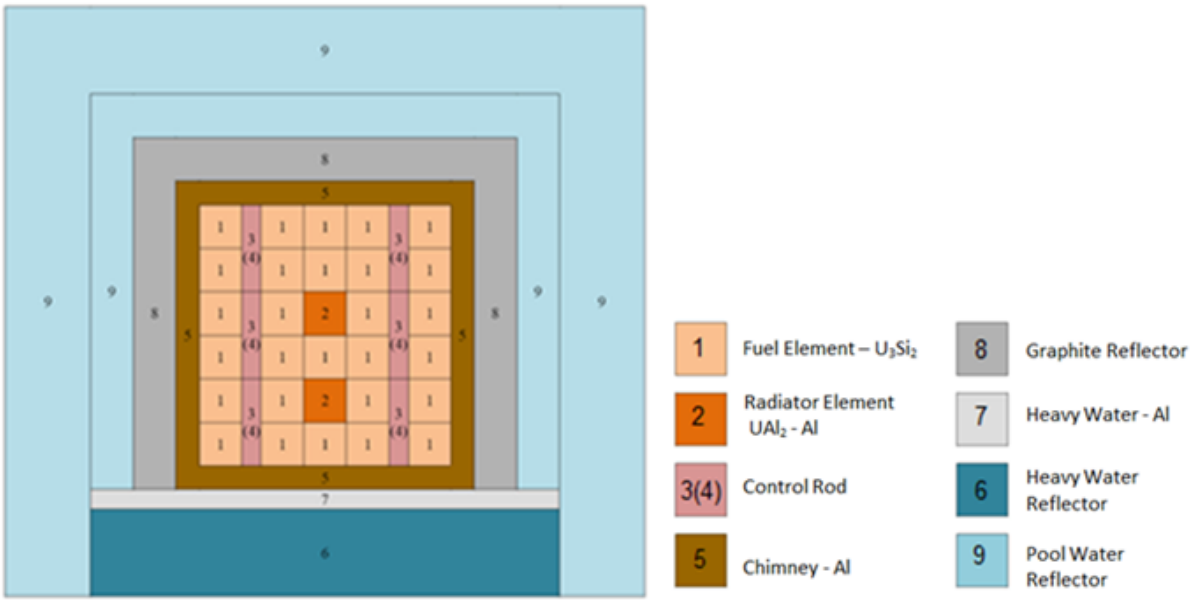

Figure 9: Cross Section (xy plane) Multipropose Reactor

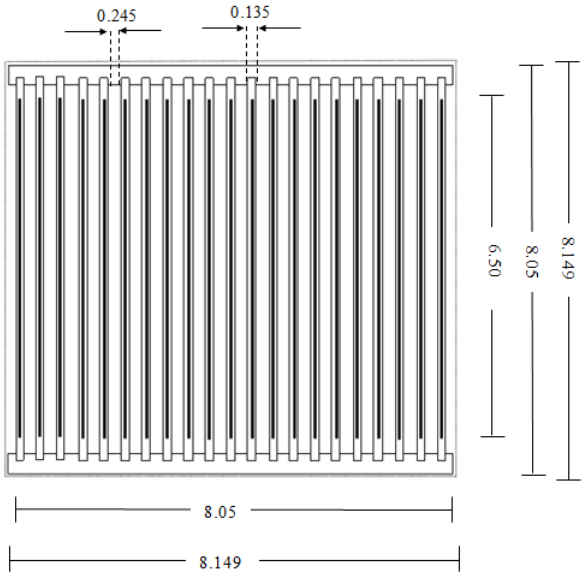

Figure 10: FE Representation – RM (dimensions cm, 20°C)

The Tables 4 and 5 report the number of regions of the equivalent cells of FE and CRS. The tables also have their corresponding elements and isotopes, the thickness and atomic concentrations of each region. The discrepancy between the values of the concentrations of ^{234}U is based on the fact that there are different ways to calculate the concentration of this isotope in the mixture. The equation used was removed from the article [9] can be written as:

$$\%U^{234} = 0{,}0015 + 0{,}0058E + 0{,}000054E^2 \qquad (3)$$

where $E = \%U^{235}$ in the mass.

Tabela 4: EC-RM

Region	Elements and isotops	Concentration (atoms/barn.cm)		Thicknesses (cm)	
		Benchmark	Calculated	Benchmark	Calculated
Region 1: "meat" U_3Si_2-Al	^{234}U	2,28116 x 10^{-5}	6,083726 x10^{-6}	0,0305'	0,0305
	^{235}U	2,28888 x 10^{-3}	2,28950 x 10^{-3}		
	^{238}U	9,16049 x 10^{-3}	9,17754 x10^{-3}		
	Si	7,63292 x 10^{-3}	7,64874 x10^{-3}		
	Al	3,61574 x 10^{-2}	3,61610 x 10^{-2}		
Region 2:cladding	Al	6,02442 x 10^{-2}	6,02439 x 10^{-2}	0,037	0,037
Region3:1/2 water channel	H	6,67462 x 10^{-2}	6,66000 x10^{-2}	0,1225	0,1225
	O	3,33731 x 10^{-2}	3,33500 x10^{-2}		
Region 4: Al inerts edges and excess water	Al	3,98094 x 10^{-2}	3,98234 x10^{-2}	0,0532	0,0532
	H	2,26389 x 10^{-2}	2,26386 x10^{-2}		
	O	1,13195 x 10^{-2}	1,13193 x10^{-2}		

In this work the chemical elements shown in Table 5 Region 2 as absorber cladding parts are available in [10] where the chemical composition is the result of the arithmetic mean of the values provided by the manufacturer (PROSIT) and measured twice by IPEN. Despite the MR not contain P and S in the absorbing cladding these elements have been incorporated into the table and in the calculation of concentrations because they represent a very small percentage compared to the other elements. Stainless steel SS-304 has different compositions depending on the manufacturer and the purpose it is intended. In SS-304 composition of the research, the components mentioned by [10] were the ones who approached the MR reality.

Table 5: CRS-MR

Region	Elements and isotops	Concentration (atoms/barn.cm)		Thicknesses (cm)	
		Benchmark	Calculated	Benchmark	Calculated
Region 1: Ag-In-Cd	^{107}Ag	2,25711 x 10^{-2}	2,25579 x 10^{-2}	0,225	0,225
	^{109}Ag	2,09773 x 10^{-2}	2,09771 x 10^{-2}		
	(*) ^{113}In + ^{115}In	7,67108 x 10^{-3}	7,67126 x 10^{-3}		
	Cd	2,61208x 10^{-3}	2,61207 x 10^{-3}		

Region 2: SS-304	Mn	$1{,}37620 \times 10^{-3}$	$1{,}46455 \times 10^{-3}$	0,1	0,1
	Si	$6{,}38380 \times 10^{-4}$	$6{,}26600 \times 10^{-4}$		
	Ni	$7{,}67040 \times 10^{-3}$	$8{,}16223 \times 10^{-3}$		
	Cr	$1{,}58100 \times 10^{-2}$	$1{,}68255 \times 10^{-2}$		
	Fe	$5{,}54450 \times 10^{-2}$	$5{,}9007 \times 10^{-2}$		
	C	$1{,}05610 \times 10^{-4}$	$1{,}11161 \times 10^{-4}$		
	Mo	$7{,}94240 \times 10^{-5}$	$8{,}45082 \times 10^{-5}$		
	Co	$1{,}63530 \times 10^{-4}$	$1{,}74028 \times 10^{-4}$		
	P	(*)	$4{,}00424 \times 10^{-5}$		
	S	(*)	$1{,}56206 \times 10^{-4}$		
Region 3: H_2O	H	$6{,}67462 \times 10^{-2}$	$6{,}66700 \times 10^{-2}$	0,375	0,375
	O	$3{,}33731 \times 10^{-2}$	$3{,}33350 \times 10^{-2}$		
Region 4: Al	Al	$6{,}02442 \times 10^{-2}$	$6{,}02439 \times 10^{-2}$	0,30	0,30
Region 5: 1/2 water channel	H	$6{,}67462 \times 10^{-2}$	$6{,}66700 \times 10^{-2}$	0,1225	0,1225
	O	$3{,}33731 \times 10^{-2}$	$3{,}33350 \times 10^{-2}$		
Region 6: fuel plate cladding	Al	$6{,}02442 \times 10^{-2}$	$6{,}02439 \times 10^{-2}$	0,037	0,037
Region 7: U_3Si_2-Al	^{234}U	$1{,}42572 \times 10^{-5}$	$9{,}97368 \times 10^{-6}$	0,061	0,061
	^{235}U	$1{,}43055 \times 10^{-3}$	$1{,}43064 \times 10^{-3}$		
	^{238}U	$5{,}72531 \times 10^{-3}$	$5{,}72299 \times 10^{-3}$		
	Si	$4{,}77057 \times 10^{-3}$	$4{,}78034 \times 10^{-3}$		
	Al	$4{,}51967 \times 10^{-2}$	$4{,}51967 \times 10^{-2}$		
Region 8: fuel plate cladding	Al	$6{,}02442 \times 10^{-2}$	$6{,}02662 \times 10^{-2}$	0,037	0,037
Region 9:1/2 water channel	H	$6{,}67462 \times 10^{-2}$	$6{,}66700 \times 10^{-2}$	0,1225	0,1225
	O	$3{,}33731 \times 10^{-2}$	$3{,}33350 \times 10^{-2}$		

(*)Due to the small abundance of ^{113}In, their concentration was added to the ^{115}In.
(**) The elements P and S are the SS-304 steel components, information was obtained from the document used as a reference for calculating the concentrations of this region.

For case 2, the behavior k_∞ comparison, as in a case 1 was not possible due to the EPRI-CELL unavailability.

The spatial burnup was simulated for a period of 21 days. The effect of CRS, Fig. 11 and Fig. 12 is very clear in regions where the flow profile appears a depression. In the region corresponding positions of the radiators channels there are two peaks of which the flow of neutrons is slightly higher for one of them, thus indicating the proximity of the influence of this channel with reflector of heavy water.

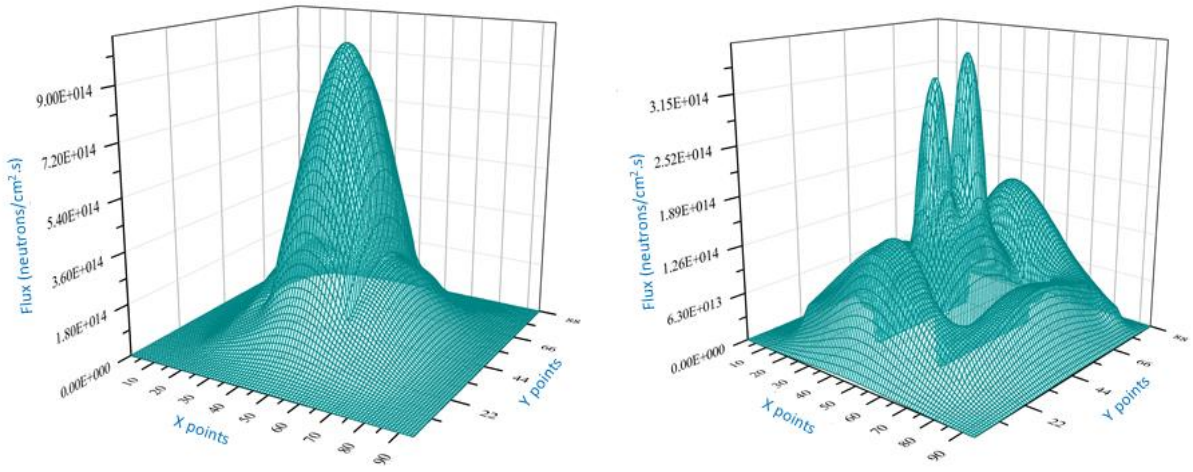

Figure 11: Thermal and fast neutron flux – Start.

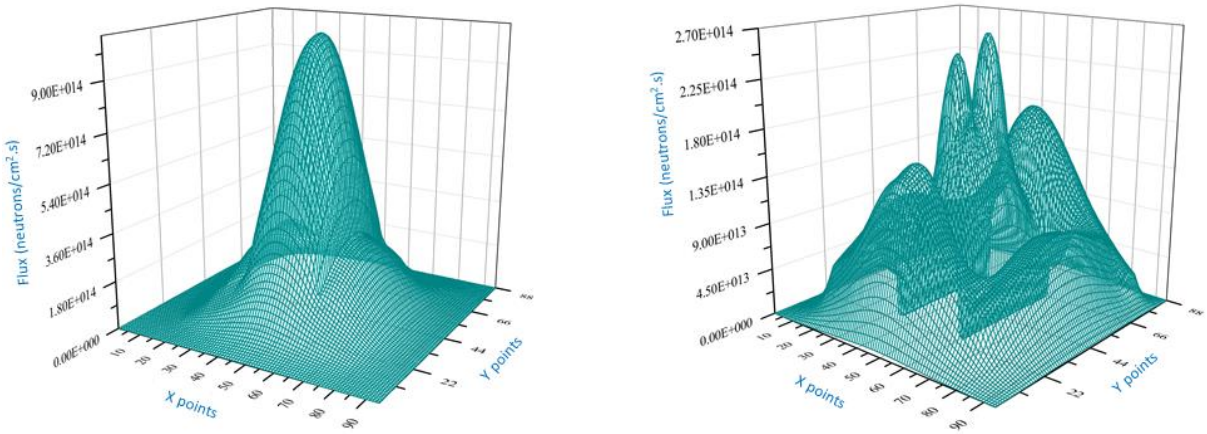

Figure 12: Thermal and fast neutron flux – End

In the case of burnup accumulated, Fig. 13, already there from the 1st day burnup is higher for FE in the central region, as these are subject to higher radiation due to the neighboring elements. In both cases, 1 and 2, there is shown that the burnup does not occur evenly over the core, Fig. 8 and Fig.13, showing a dependency of positioning of each fuel element.

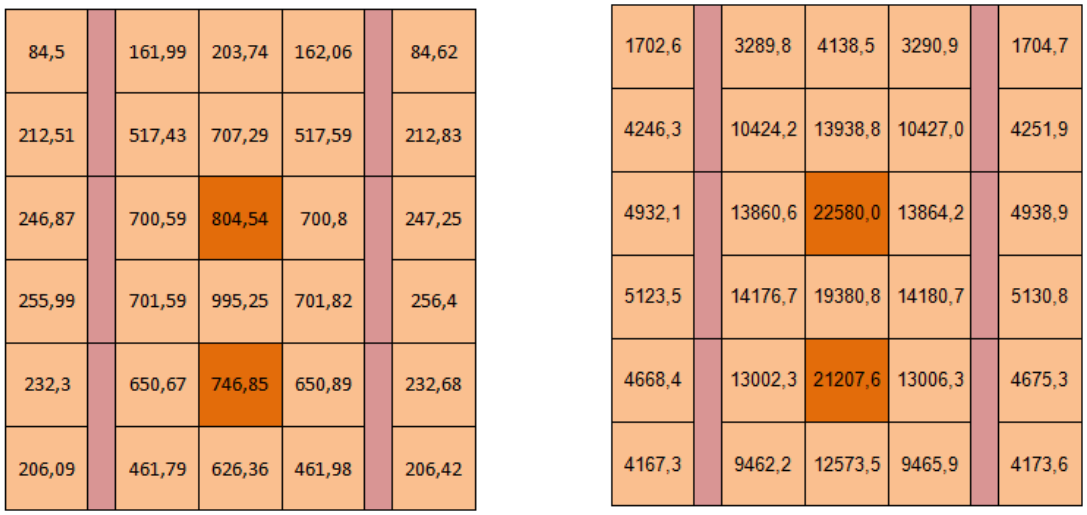

Figure 13: Burnup accumulated (MWd/t) per FE – 1º and 21º day.

6. CONCLUSIONS

The fuel burnup calculations are essential in nuclear reactor projects. At the core of managing numerous reactors computer codes already implemented and others under construction are employees seeking greater efficiency in these burnup calculations. The present study, the determination of the equivalent cell and thereby obtaining the thicknesses and nuclear concentration, and the cell calculation, the generation of nuclear parameters using WIMSD-5B code, when compared with the reference values, were well successful. To simulate the spatial burnup using DF3DQ code, it could not perform the comparison because it was not found benchmarks. However, the methodology is shown which can be applied to other research reactors.

For future work are suggested simulations use WIMS other libraries, including extensions to 172 energy groups, other configurations of the core, including different positions of control roads security (CRS) and irradiation channels. They are also suggested comparisons of WIMSD-5B results with often employed programs in spatial burnup calculations and also commercial programs. Another proposal is to estimate the fuel burnup, taking into account the thermohydraulics parameters and the appearance of xenon.

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