

# NEUTRONIC COMPARISON OF TRADITIONAL FUEL ASSEMBLIES USING UO2 (URANIUM DIOXIDE) AND UN (URANIUM MONONITRIDE) FUEL IN THE SCALE 6.0 (NEWT) CODE.

Raphael H. M. Silva<sup>1</sup>, Clarysson A. M. da Silva<sup>1</sup>, Cláubia Pereira<sup>1</sup>

 <sup>1</sup> Departamento de Engenharia Nuclear Universidade Federal de Minas Gerais
Av. Antônio Carlos, 6627, Campus UFMG PAC 1 – Anexo Engenharia, Pampulha, 31270-90 Belo Horizonte, MG, Brazil <u>Raphael.HMS@outlook.com</u>

## 1. Introduction

The UN (uranium mononitride) fuel had some important characteristic related to fissile material, as the larger theorical density and greatest transfer of heat to the cooling than the uranium dioxide. It also presents as other feature, the high thermal conductivity and melting point, irradiation resistance and great behavior with structural materials. The UN has lower coefficient of linear expansion and "swelling" rates compared to  $UO_2$ , as well as a higher density of heavy metal, in which it has the values of 10.96 and 14.32 kg/m<sup>3</sup>, respectively of  $UO_2$  and UN. In this context, the present work involves simulation of two nuclear fuel assemblies 16x16, with the main objective to compare the criticality (burnup) and the final isotopic composition the both typical PWR assembly. The neutronic code used to estimate the parameters were the SCALE 6.0/Newt (Standardized Computer Analyses do for Licensing Evaluation). This process was carried out to identify the main advantages of the UN compared with the traditional fuel assembly  $UO_2$  fuel have been used in the PWR reactor [1].

## 2. Methodology

The simulations of nuclear fuel assemblies carried out into this paper had the main objective to estimate the  $k_{inf}$  under the conditions of "Hot Full Power", burnup and composition, which were obtained in (SCALE 6.0/Newt) code. The libraries used by code was the ENDF/B-VII. The work was performed out in two stages, the first, the critically (burnup) was associated with the two nuclear fuel assemblies (16x16) using the UO<sub>2</sub> and UN fuels and the second step, isotopic composition associated the burnup of both fuels were compared.

Neither nucler fuel assemblies were simulated with negative reactivity insertion, that is without diluted boron concentration, control rods or gadolinium oxide rods, the fuel assemblies (16x16) simulated are according to the nomenclature described below. The Fig.1 shows the disposition of the fuel rods and the guides tubes of the annular and traditional fuel assemblies used in the research.

✓ TFA 16 - Traditional Fuel Assembly 16x16.



Figure 1: Traditional fuel assemblies (a)  $UO_2$  - (b) UN.

The nuclear fuel assemblies (TFA 16) used the enrichment of 5.0% (Tab.1). The operation's temperature carried out in the first step of the work are 900 K, 618 K and 587 K to fuel/gap, cladding and moderator respectively [2].

In relation to the other compositions, was used Zircaloy-4 to the cladding, helium in the gap and light water as moderator. In relation to the geometry, all parameter of modeling the TFA 16 as fuel rod, pitch and guide tube are demonstrated in the Tab.1 above.

| Parameter       |          | TFA 16 |  |
|-----------------|----------|--------|--|
|                 | Fuel     | 0.4583 |  |
| Radium (cm)     | Gap      | 0.4659 |  |
|                 | Cladding | 0.5385 |  |
| Radium          | Inner    | 0.6200 |  |
| Guide tube (cm) | Outer    | 0.6900 |  |
| N° Fuel Rods    |          | 236    |  |
| N° Guide Tube   |          | 20     |  |
| Pitch Distance  |          | 1.43   |  |

Table 1: Parameter of geometry in TFA 16.

In order to compare the values of the infinite multiplication factor, the reactor physics needs an equation, in which parameters related to the neutron population need to be considered. Neutron production, disappearance rates and other important variables should be written in order to establish a general balance of the system. Such main parameters of analysis are associated with Reproduction ( $\eta$ ), Thermal utilization (f), Resonance escape probability ( $\rho$ ) and Fast fission ( $\xi$ ). The burnup was established in 33 GWd/tU and specific density of power 38 W/g. To set up a great comparison between the burnup in each fuel, the burnups were carried out in the program Origin S into the SCALE 6.0–Newt.

## 3. Results and Discussion

In the Fig.2, is demonstrated an important factor related to the difference of neutron multiplication factor (Tab.2), that is, associated with macroscopic cross-section, more precisely the radioactive capture. Comparing these behaviors, was observed that the element N (nitrogen-UN), has a higher absorption of neutrons in the

thermal and epithermal region compared with O (oxygen-UO<sub>2</sub>), consequently. For this reason, the values of  $k_{inf}$  have been shown are highest in the fuel UO<sub>2</sub> than UN [3]

This provides the transmutation of element <sup>14</sup>N to <sup>14</sup>C, which is highly reactive with steam or water. The transmutation increased the caution, related to cladding problems in order to avoid explosions in the reactor. This whole context contributes to a considerable reduction in the values of the neutron multiplication factor of the analysis [4] [5]

| Fuel   | TFA 16   |  |  |
|--------|----------|--|--|
| $UO_2$ | 1.433170 |  |  |
| UN     | 1.297543 |  |  |



Table 2: Parameter related to k<sub>inf</sub> in the fuel assemblies.

Figure 2: Relation between cross sections (radiative captures) of <sup>14</sup>N and <sup>16</sup>O.

In relation to Reproduction factor ( $\eta$ ), Fast fission ( $\xi$ ), and Resonance escape probability ( $\rho$ ) (Tab.3), demonstrated the most relevant differences, related to the higher theoretical density of UN, which the isotope <sup>238</sup>U has direct influence on effects such as self-shielding and neutron loss (resonance and radiative captures) in the System. The Thermal utilization factor remained practically identical in both fuels.

| Factors                                 | UN       | $UO_2$   |
|---|----------|----------|
| Reproduction $(\eta)$                   | 1.808065 | 1.913134 |
| Thermal utilization (f)                 | 0.961007 | 0.945700 |
| Resonance escape probability ( $\rho$ ) | 0.500111 | 0.605930 |
| Fast fission (ξ)                        | 1.492313 | 1.306590 |
| k <sub>inf</sub>                        | 1.296783 | 1.432388 |

| Table 3: Neutronic parameter of simulated fuel assembli |
|---|
|---|

The Fig.3 (a) shows the spectrum analysis performed in the two fuels simulated, in which the energy variation is from the thermal to the fast range. In the energy range of main interest (thermal/epithermal), the absorption of thermal neutrons in the fuel is lowest in the UN than UO<sub>2</sub>, confirming the lowest neutron multiplication factor value of uranium mononitride. In Fig.3 (b), it shows the transmutation, mainly, the <sup>238</sup>U to <sup>239</sup>Pu. Such information demonstrates in the process of burnup, largest concentration of the <sup>239</sup>Pu in UN than the UO<sub>2</sub>, a factor of concern regarding the proliferation of weapons.



Figure 3: Spectrum neutron in the fuels (a) and <sup>239</sup>Pu production in the burnup (b).

In the Tab.4 presents the initial and final values of burnup, it showed the  $UO_2$  had greatest value of  $k_{inf}$  compared than the UN, in neutronics parameters, the  $UO_2$  fuel has a greater possibility of burnup extension.

|         | LIO .           | TINI            |
|---------|-----------------|-----------------|
| GWd/tU  | $UO_2$          | UN              |
| BOC/EOC | 1.43317-1.08224 | 1.29754-0.99760 |

| Table 4: | Burnup | of the | fuel | assemblies. |
|----------|--------|--------|------|-------------|
|----------|--------|--------|------|-------------|

### 4. Conclusions

Based on the neutronic results at the work, which have been presenting disadvantages ( $k_{inf}$ /burnup/<sup>239</sup>Pu) of UN fuel related to the UO<sub>2</sub>. Thermohydraulic parameters are required to evaluate heat transmission (rod/coolant) and determine the efficiencies the both fissile materials. Since, the greatest advantage of UN fuel, is associated with the high thermal conductivity compared to the UO<sub>2</sub>.

### Acknowledgements

The authors express their gratitude to CAPES, FAPEMIG, CNPq, CNEN and the all researchers and students of Departamento de Engenharia Nuclear – Escola de Engenharia–Universidade Federal de Minas Gerais (UFMG).

### References

[1] Hassan, Ibrahim A. et al, *Viability of uranium nitride (UN) as annular fuel for AP-1000*, Progress in Nuclear Energy, vol. 110, pp. 170-177 (2019).

[2] Rio de Janeiro (Estado) Eletrobrás Termonuclear, S. Final Safety Analysis Report-FSAR Angra 2. Electronuclear, Rio de Janeiro (1999).

[3] Long, Yun. *Modeling the performance of high burnup thoria and urania pwr fuel*. Tese de Doutorado, Massachusetts Institute of Technology, (2002).

[4] Brown, Nicholas R. et al. *Neutronic performance of uranium nitride composite fuels in a PWR*. Nuclear Engineering and Design, vol. 275, pp. 393-407 (2014).

[5] Zakova, J., Wallenius, J. *Fuel residence time in BWRs with nitride fuels*, Ann.Nucl. Energy vol. 47, pp. 182–191 (2012).