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Neutronic evaluation of a GFR of 100 MWt with reprocessed fuel and thorium using SCALE 6.0 and MCNPX

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Abstract. A GFR core model with 100 MWt was evaluated using three different fuel compositions: conventional (U, Pu)C and two reprocessed fuels with transuranic (TRU) (Pu, Am, Np, Cm). One reprocessed by UREX+ technique and spiked with depleted uranium, (U,TRU)C, and the other reprocessed by the same technique but spiked with thorium, (Th,TRU)C. The reprocessed fuel came from a PWR standard fuel (33,000 MWd/T burned) with 3.1% of initial enrichment and left in the pool by 5 years. Some important nuclides were followed for burns and neutron absorption and k_{inf} was evaluated 1400 days of burnup. Tests were also made for B4C absorber insertion and the temperature coefficient. The simulations were made comparing results of MCNPX and SCALE 6.0 programs. The goal is to validate the simulated model and evaluate the possibility to use TRU spiked with Th in a GFR conception.

1. Introduction

Based on the proposals of the GEN-IV International Forum [1], some researchers proposed GFR models with different objectives, considering neutronic parameters, thermos-hydraulics, and tests with new materials. In an article published in 2010 [2], researchers from *Universidad Autónoma del México* also used such information to propose an assembly for a GFR conception. In the following year, 2011, the core was designed based on its assembly model, always meeting the recommendations of the GEN-IV for the geometry and fuel composition, in this case (U, PU) C [3]. Following the recommendations, these researchers were able to propose in 2013, a simplified GFR core of 100 MWt, including the concentration of the entire composition of this [4]. The "simplified core" was thus named because it has the following characteristics:

- 1. To be considered homogeneous;
- 2. Have the seven absorber assemblies filled with helium;
- 3. Outside the reflective edge is considered a vacuum;
- 4. All components of the core are considered at the temperature of 1200 K.

Based on the GFR core proposed in [3, 4], the work described in [5.6], the conventional fuel (U,Pu)C was substituted by (U,TRU)C and (Th,TRU)C. The focus was to validate a heterogeneous model of a GFR using SCALE 6.0 code [7] based on a study that presents detailed geometry and compositions for a homogeneous assembly using (U,Pu)C as fuel [6]

and then, to evaluate the possibility of using TRU as fuel. Two fuels were evaluated: (Th,TRU)C and (U,TRU)C. The TRU were obtained from a PWR spent fuel, reprocessed by UREX+ technique and then spiked with Th, (Th,TRU)C, and spiked with depleted U, (U,TRU)C. Details of the spent and reprocessed fuel can be found in [5,6]. The fuel composition was chosen to obtain similar k_{inf} found by [4]. All simulations using SCALE 6.0 were performed skipping the first 30 out of 530 generations with 4000 neutrons. Now, the focus is to simulate the GFR core to compare the neutronic behavior using different fuels during the burnup. The model has been modified according to the following characteristics:

- 1. The heterogeneous model will be considered instead of the homogeneous model;
- 2. The operating temperature of 1200 K for all core components used in [3,4] have been modified to real values;
- 3. Since the interest is only to evaluate the fuel depletion, the core will be simplified in the sense of replacing the zirconium reflectors with the total reflection boundary condition;

The goal of this work is to simulate the GFR core using SCALE6.0 and MCNPX and analysis some neutronic characteristics.

2. Validation of the Proposal Model

The assembly proposed in reference [2], as well as the core proposed in references [3, 4], were homogeneously modeled with MCNPX using respectively JEFF 3.1 and 3.2 and ENDF-B-VI libraries. Both assemblies and core were properly validated in [5, 6]. Nevertheless, it is important to remark that there is a migration from the homogeneous system to a heterogeneous one, maintaining the same geometric characteristics and physical properties of the systems. In this case, the simulations with MCNPX at steady state and burnup mode were performed with the ENDF-B-VII libraries. With the SCALE system, the same library is used for calculations at steady state. For the burnup, it was used the library of 238 groups collapsed from ENDF-B-VII. FIG. 1 shows a scheme for the assembly and details of a fuel rod.



FIG. 1. Heterogeneous assembly and details of a fuel cell.

The operating conditions in both codes are identical. Both of them were burned up in 1400 days, divided into 12 equal steps, 4000 particles will be used in 500 cycles with a dismissing the first 30 cycle. The specific power for both the assembly and the core is 48 W/g.

2.1 The GFR Core

FIG. 2. shows a scheme for the simplified core.



FIG. 2. Simplified GFR core configuration.

With the SCALE 6.0, the burnup is done with the TRITON module. The library used will be the continuous data library of 238 groups, collapsed from ENDF-B-VII and with MCNPX, it uses the CINDER module with its respective library. The operating temperatures highlighted in Table 1 below were based on the work of *WFG van Rooijen* [7], *Anthony M. Judd* [8] and *Peter Yarsky* [9] replacing the reference system [2, 3, 4] which uses the same temperature of 1200 K for all core components.

Components	Temperature (Kelvin)
Fuel	1000
Fuel cladding	800
Cladding to the fuel rods	600
Gap coolant"gap"	1000
control rods coolant	600
fuel assembly coolant	600

TABLE 1. TEMPERATURES FOR THE CORE COMPONENTS.

TABLE 2 shows the percentages of fissile material in each evaluated fuel.

	Program / Fuel						
	MCNPX and SCALE 6.0						
	(U, Pu)C	(U, TRU)C	(Th, TRU)C				
Fissile material (%)	11.33%	13.06%	15.78%				

TABLE 2. PERCENTAGE OF PHYSICAL MATERIAL IN EACH FUEL.

2.2 Burnup Calculation and $k_{\text{inf}}\,Evolution$

TABLE 3 shows the values of k_0 which corresponds to the beginning of cycle (BOC) and k_{12} representing the end of cycle (EOC).

TABLE 3. INITIAL AND FINAL k_{inf} FOR THREE FUELS IN 1400 DAYS OF BURNUP

	FUEL / k _{inf}					
$\mathbf{k}_{\mathrm{inf}}$	MCNPX			SCALE 6.0		
	(U, PU)C	(U, TRU)C	(Th, TRU)C	(U, PU)C	(U, TRU)C	(Th, TRU)C
k ₀	1.30270	1.30039	1.29860	1.30713	1.30499	1.30353
k ₁₂	1.17824	1.18847	1.23279	1.17080	1.18142	1.22089

FIG. 3 shows the evolution of k_{inf} at each burnup step. After a little more than 300 days of burnup, the fuel spiked with thorium undergoes a proportional decrease, evidencing the effects of the ²³³U build-up.



FIG. 3. k_{inf} comparison to the three fuels in 1400 days of burnup.

The small differences between the codes can be attributed to the different libraries of nuclear cross sections of the codes used. In order to gain a better understanding of these differences, FIG. 4 represents the absolute difference between the k_{inf} values obtained between the two codes, MCNPX and SCALE, for each fuel.



FIG. 4. The difference between the values of k_{inf} in the respective fuels and codes.

Only three of the 12 points studied present a difference greater than 10^{-3} . They are in the 1st and last burnup steps, respectively.

2.3 Nuclides Evolution

FIG. 5 shows the Pu, isotopes such as ²³⁸Pu, ²³⁹Pu, ²⁴⁰Pu, ²⁴¹Pu. FIG. 6 shows actinides ²⁴⁴Cm, ²⁴¹Am e ²³⁷Np. In the sequence, FIG. 7 shows the ²³³Th and ²³³Pa, giving rise to ²³³U.



FIG. 5. Plutonium isotopes evolution during the burnup.



FIG. 6. Evolution of fissile actinides during the burnup.



FIG. 7. Evolution of ²³³U and their predecessors, ²³³Th and ²³³Pa.

The (Th, TRU) C was the fuel that most created fissile material, due to the build-up of ²³³U that occurs simultaneously to the build-up of ²³³Pa from ²³³Th. The concentration of ²³³U reaches almost its maximum value exactly when the fuel has its highest reactivity by increasing its concentration, in about 150 days burnup. Therefore, the Protactinium, which is a high absorber, does not change during burnup, which shows that the same amount of ²³³Pa is transmuted from ²³³Th creating the ²³³U. This fact causes a decrease in the burnup rate of the fuel spiked with thorium. With more fissile material being created, k_{inf} decreases at a much lower rate when compared to the other two fuels.

2.4 Temperature Coefficient

To evaluate the Doppler coefficient, a temperature gradient of 100 Kelvin for the fuel has been simulated. FIG 8 shows that this coefficient remains negative for all fuels during the burnup for the both codes.



2.5 Criticality Evaluation with B₄C Absorber

In this simulation, the seven absorbers initially filled with helium will give rise to the boron carbide absorber (B₄C), in the following proportion: 90% ¹⁰B and 10% ¹¹B. The goal is to verify the criticality of the core every 10 cm of insertion of the rods, at steady-state. FIG. 9 shows the results for every 10 cm of insertion of B₄C rods.

Initially, it was found that only for fuel (U, Pu) C, the system reached subcriticality, remaining supercritical for the other two fuels with TRU. In this condition, the absorber mass was just over 272 kg. The solution given was to increase the diameter of the rod, in order to increase the amount of absorber. After some tests, it was found that this increase should be 1.0 mm in the radius of the rod. This allowed the addition of 143 kg of boron carbide, totaling a mass of 415 kg of this absorber.



FIG. 9. k_{inf} behavior for the three fuels with the height variation of the absorber.

The absolver insertion shows that for the fuel (U, Pu) C, the core becomes subcritical with about 90% of the rods inserted. For fuel (U, TRU) C, subcriticality would only be achieved with the rods inserted almost entirely. For fuel (Th, TRU) C, however, there is a slight divergence in the results. Although the MCNPX program showed a minimal difference of 10^{-5} , being the k_{inf} value with 100% of the uncertain bars equal to 1.00006 the nucleus was not subcritical by the same difference, whereas, according to SCALE, it would already be subcritical in the same condition.

2.6 CONCLUSIONS

The k_{inf} calculation results using the MCNPX and SCALE 6.0 with their respective libraries shows similarity between their values, which encourage to continue the studies with the different fuels. The rates at which concentrations evolve are practically identical when compared to the data provided by MCNPX and SCALE. The simulations showed that the parameters temperature coefficient and the insertion of an absorber are consistent with each other and obtain good agreement with the one obtained for a fast reactor. This work also shows that for the parameters evaluated, the use of different codes and libraries produce expected and coherent results between them. The substitution of traditional fuel (U, Pu) C by other TRU-based fuels also proved to be compatible. The fuel spiked with thorium presents basically the same expected differences in the evolution of the burnup. Finally, the build-up of nuclides pointed out by the two codes also showed high compatibility. In this way, the model proposed here and the proposed reprocessed fuels present expected behaviors and consistent with each other. DEN-UFMG is continuing its research with the aim of soon proposing its own GFR model based on the latest publications of the GEN-IV International Forum.

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