

## BOUNDARY CONDITION MODELING EFFECT ON THE SPENT FUEL CHARACTERIZATION AND FINAL DECAY HEAT PREDICTION FROM A PWR ASSEMBLY

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### ABSTRACT

In this paper, two main exercises have been carried out to describe the effect that varying an albedo boundary condition has in the computation of observables such as decay heat, neutron emission rate and nuclide inventory from a PWR fuel assembly (or a configuration of assemblies) during a depletion scenario. The SERPENT2 code was then employed to emphasize the importance of modeling a proper boundary condition for such purposes. Moreover, the effect of taking into account more than a single fuel-pin region for depletion studies while varying the type of boundary condition, was also accounted for. The first exercise has the main objective of comparing in a single fuel assembly the albedo variations ranging from 1.1 up to full vacuum conditions. By comparing to the reference assembly (considered to be the case of full reflective conditions), relative differences up to +17% were observed in decay heat and up to almost -30% in neutron emissions. Also, a clear dependence on the albedo was detected if more than one depletable zone was considered while computing the integral value of observables of interest. Regarding the second exercise, where a  $3 \times 3$  configuration of fuel assemblies is being now considered with a reflector section in the middle, a negligible effect on the observables was observed for the single fuel pin zone case; instead, an effect in the  $^{244}\text{Cm}$  computation when analyzing two fuel pin-zones produced a change in the neutron emission rate during cooling time up to 2.5% (while comparing it to the reference single assembly case).

**KEYWORDS:** albedo sensitivity, neutron emission rate, isotopic inventory, decay heat, PWR assembly depletion

## 1. INTRODUCTION

Nowadays, computer codes are widely used for the determination of spent fuel nuclide inventory, decay heat, fuel loading analysis of nuclear reactors, among other studies [1-3]. For example, depletion calculations of Light Water Reactors (LWR's) that have been used for the aforementioned purposes with large scale models (e.g. full core or core symmetric-quarter) had been mostly based on the so-called "two-step" approach, where a set of few-group homogenized cross-sections (usually at the assembly level) are set to form a core model in order to feed a simulator that would solve the diffusion-Bateman equations [4-5]. Meanwhile, modern simulation efforts for depletion analyses are being based on high-fidelity multi-physics and multi-scale approaches by solving the transport equation relying on state-of-the-art numerical methods [6]. Nevertheless, it is nowadays still customary to carry out such type of studies at lower scales than the core level (e.g. at the assembly level or a group of assemblies sharing similar characteristics such as fuel batches), in order to find a good compromise between the computational costs in time and power that an accurate computation of the observables of interest would require. When this holds true, the use of appropriate boundary conditions becomes necessary in the modeling strategy, with the intention to properly emulate the environmental effects that the neutron flux would otherwise encounter in a large scale system.

The constraint in defining a certain type of boundary condition might have an impact in the assessment of observables of interest as a function of burnup. For instance, the use of reflective boundary conditions along all directions assumes a physical modeling corresponding "to an infinite system", which might be correct if the surrounding media is composed by the same geometrical and material characteristics for several neutron mean free paths from the domain boundaries. On the other hand, albedo ( $\beta$ ) boundary conditions are commonly applied when a change of environment is expected to take place, producing a high net neutron current with the eventual shift of the energy-spectra (i.e. around reflectors or strong absorbers like control rods). It is actually common to find this strategy along in-core fuel management depletion calculations of commercial reactors in well established codes like CASMO-SIMULATE [7] and PHOENIX-POLCA [8], where instead of defining a macroscopic cross-section region of non-fissile materials such as axial and radial reflectors, a two-group albedo boundary condition is used instead for the solution of the nodal two-group diffusion equation [7-8].

In this paper, the study of the impact that changing the surroundings of either a single fuel assembly (by means of changing the albedo) or, on the other hand, the impact that changing the surroundings of a fuel assembly batch group (by imposing a reflector in the middle of the configuration) has on the prediction of the decay heat, nuclide inventory, and neutron emission rates, was performed along a hypothetical scenario consisting of 4 cycles with a final 5 year cooling period of time. This parametric study was carried out solely with the SERPENT2 code [9], and one of the main objectives is to assess the relative variation that exist between such depleted observables with respect to other ones that have been previously computed from an assembly modeled with full-reflective boundary conditions (i.e. albedo equal to unity), and that was ran for the same cycle scenario [3]. Moreover, another important objective of this work is to verify if by considering all possible materials that contain the same type of fuel as a single "burnable" region, the computation of the addition of the aforementioned observables of interest differ too much (due to the change of albedo or type of boundary), from the case where separate "burnable" regions containing fuel pins of the same type where instead consider for the integral computation of the results.

## 2. DESCRIPTION OF THE MODELING EXERCISES

A reference 2D model from a previous benchmark study conducted by the authors [3] is being referenced for this work. It conveys a typical  $17 \times 17$  PWR assembly with reflective boundary conditions, assuming a Zircaloy-4 cladding and a 4 w/o UOX fuel that is irradiated along 4 cycles of 300 days each, with interim cooling periods of 30 days. At the end of the 51000 MWd/tHM burnout, a final 1-1000 year period cooling of time is taken into account. Table I below summarizes all important characteristics of the model. The only

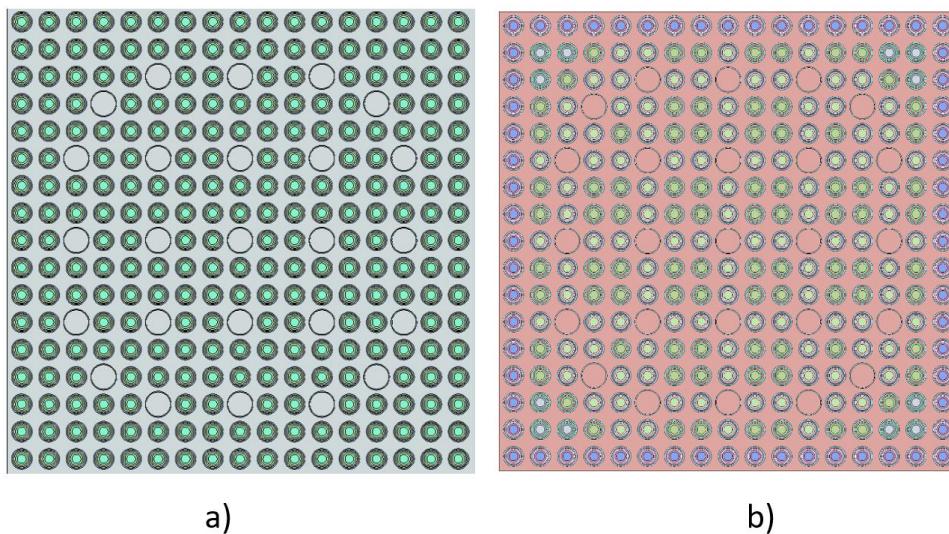
notable difference from the reference model in Ref. [3] is a change of moderator/coolant temperature from 600 K to 580 K and the corresponding change of water density to provide more realistic irradiation conditions of a typical PWR assembly.

**Table I. Model characteristics in SERPENT2**

Power [each cycle]	Constant levels of 50, 50, 40 and 30 MW/tHM	
Density [g/cm <sup>3</sup> ]	Fuel	10.4
	Moderator/Coolant (with constant boron level of 800 ppm)	0.655
Temperature [K]	Fuel	900
	Cladding	600
	Moderator/Coolant	580
Geometrical dimensions [mm]	Fuel pellet radius	4.095
	Cladding (inner/outer) radii	4.18/4.75
	Pin pitch	12.6
Cycle time steps [days]	1, 10, 14, 3 × 25 and 4 × 50	
Nuclear data library	ENDF/B-VII.1 [10]	
Radial zones per pin during depletion	4	

## 2.1. Model for the albedo sensitivity studies

To fulfill the exercise 1 of this work, a single fuel assembly is enough. The aim is to vary the albedo boundary conditions ranging from an over-reflective case ( $\beta = 1.1$ ), passing by the reference full-reflective case ( $\beta = 1$ ) and ending up at full-vacuum boundary ( $\beta = 0$ ) in order to compare the behaviour of the observables, both of these are computed assuming only one fuel material region to be depleted (see Figure 1a) as well as with four different regions (as highlighted in Figure 1b). The first zone in blue at the periphery; the second region at the corners; the third region around the control/instrumentation tubes; and the fourth region elsewhere). It has to be remarked that in both cases, each pin is radially meshed four times. In the end, the effect of having a separate pin treatment in a fuel assembly for catching albedo dependencies in the assessment of observables as a function of time is the objective of the exercise.

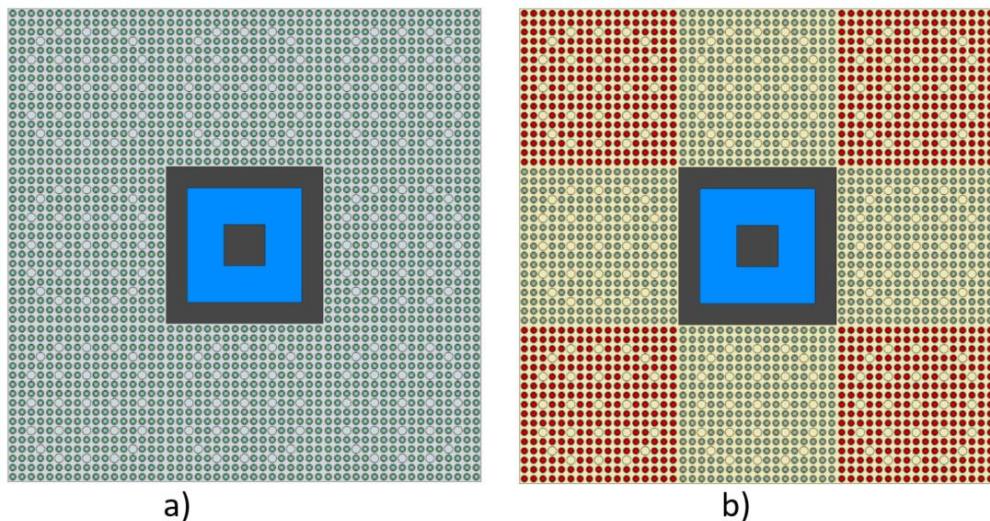


**Figure 1. a) Assembly with one depletion zone; b) Assembly with four depletion zones (albedo study).**

## 2.2. Model for the reflector analysis

A more realistic way of modeling a true albedo would be to actually include a reflector zone in the domain of study. In this exercise, a  $3 \times 3$  fuel assembly configuration is used, with the exception that the central assembly is replaced with a reflector zone formed by a heterogeneous configuration of steel and water. Fuel assemblies have the same characteristics as in exercise 1. This type of modeling was divided in two parts: one corresponding to fuel assemblies with one “burnable” region, and a second one where the corner assemblies are considered a separate “burnable” region from the rest of the assemblies. This can be appreciated in Figure 2a and 2b, respectively. In Figure 2 the black zone corresponds to the type of stainless steel (SS-304), while the blue part is being filled with regular coolant.

The objective of this exercise 2 is two-fold. Firstly, to study the impact of a reflector zone on decay heat, nuclide vector and neutron emission rate compared to the reference case of full-reflective conditions from exercise 1. And secondly to study the effect of modeling more than one “burnable” region on previous comparison.



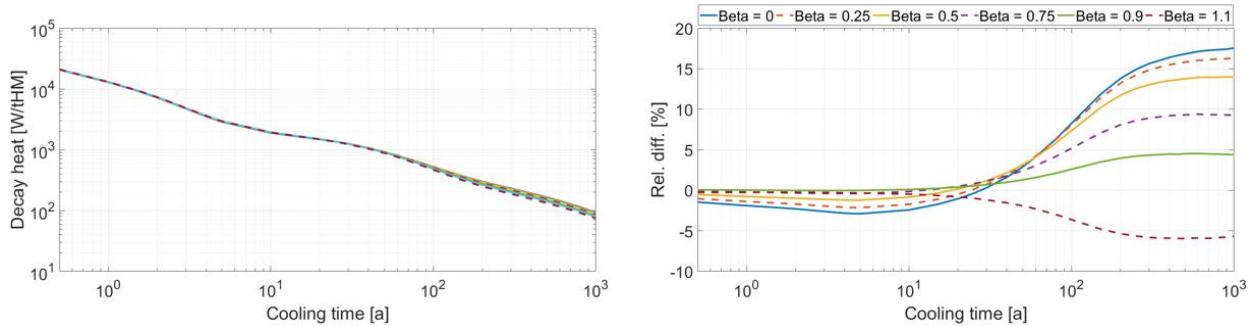
**Figure 2. a)**  $3 \times 3$  configuration with one depletion zone; **b)**  $3 \times 3$  configuration with two depletion zones (reflector study).

## 3. RESULTS

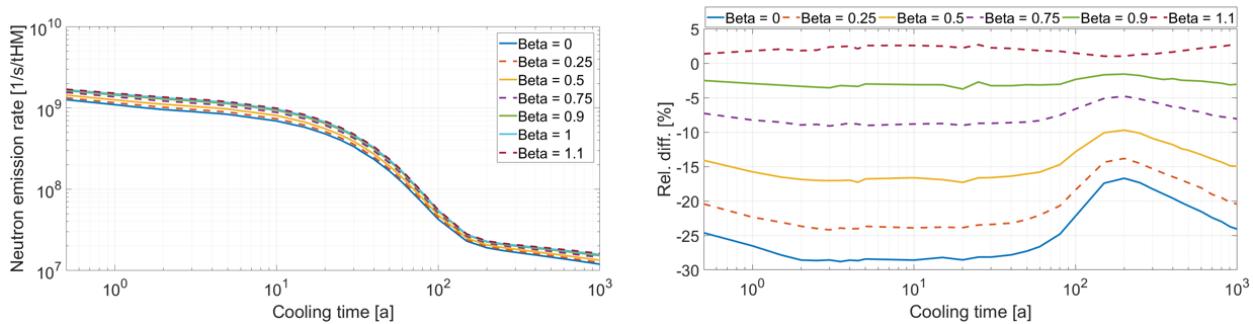
### 3.1 Albedo sensitivity studies

The computation of decay heat and neutron emission rates are based on the methodology from Ref. [3]. The results for exercise 1 are subdivided into two different set of figures. On one hand, depletion observables as a function of time for different albedos (which range from 0 to 1.1) when only one fuel-pin zone is considered are shown in Figures 3 to 6. Decay heat and neutron emission rates are only depicted during cooling times, while for the behavior of some nuclides such as  $^{241}\text{Am}$  and  $^{244}\text{Cm}$ , the full irradiation plus cooling time is being accounted for. This analysis also describes the relative difference that such parameters display for different albedos with respect to the reference case of albedo equaling to unity.

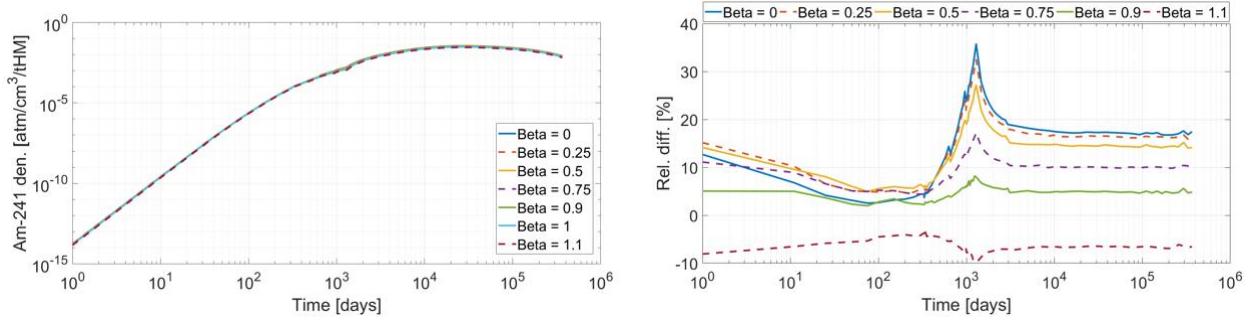
On the other hand, the second set of Figures (comprised between Figure 7 and 10) shows 3D plots, displaying the relative differences between the assemblies with one fuel pin zone with respect to the assembly with four fuel pin zones at different albedos. To outline the impact of employing either one or four “burnable” regions on the computation of observables of interest at a certain time, it was decided to show the decay heat and neutron emission rates trends as a function of albedo after exactly 5 years of cooling for both cases. Meanwhile, the same type of study was performed for prediction of  $^{241}\text{Am}$  and  $^{244}\text{Cm}$  masses at the end of irradiation.



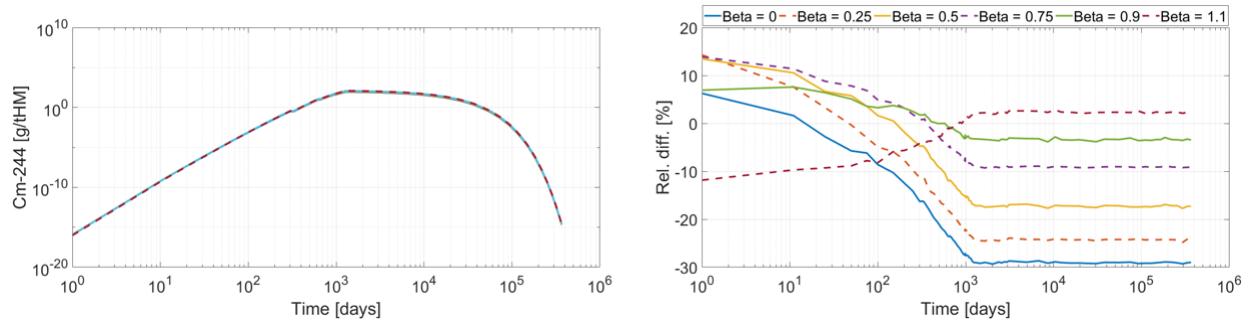
**Figure 3.** Decay heat rate as a function of cooling time for different albedo boundary conditions.



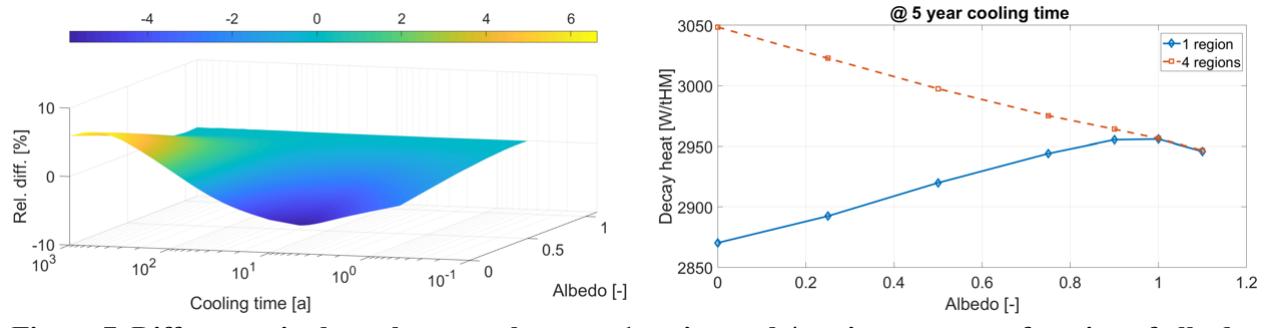
**Figure 4.** Neutron emission rate as a function of cooling time for different albedo boundary conditions.



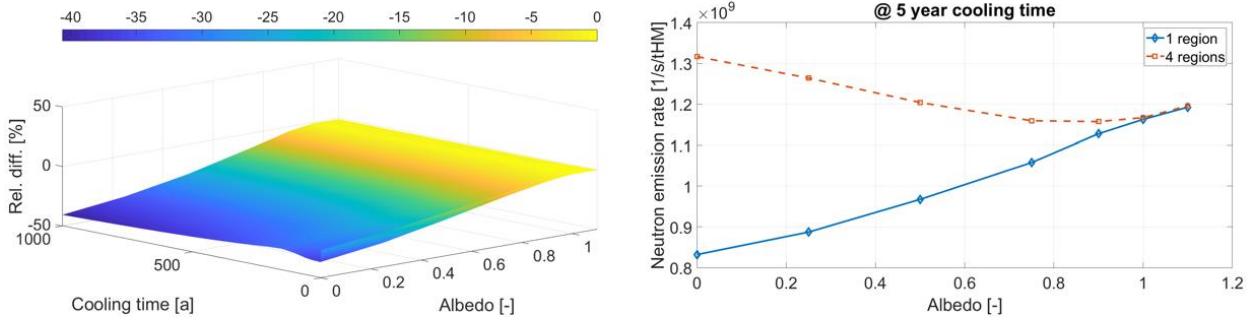
**Figure 5.**  $^{241}\text{Am}$  mass as a function of irradiation + subsequent cooling time for different albedo boundary conditions.



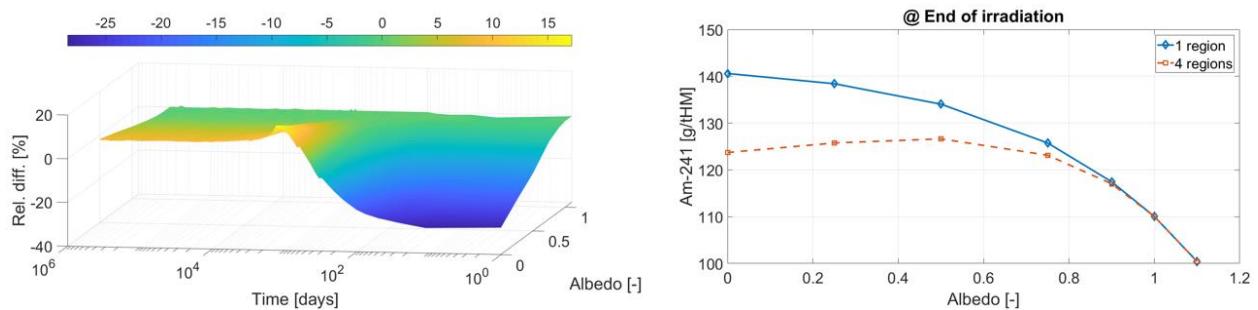
**Figure 6.**  $^{244}\text{Cm}$  mass as a function of irradiation + subsequent cooling time for different albedo boundary conditions.



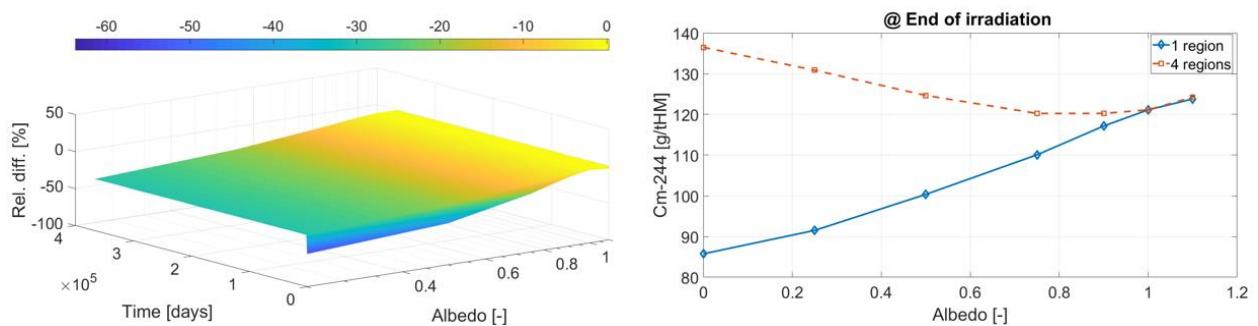
**Figure 7.** Differences in decay heat rate between 1 region and 4 region cases as a function of albedo and cooling time.



**Figure 8.** Differences in neutron emission rate between 1 region and 4 region cases as a function of albedo and cooling time.



**Figure 9. Differences in  $^{241}\text{Am}$  concentration between 1 region and 4 region cases as a function of albedo and irradiation + subsequent cooling time.**



**Figure 10. Differences in  $^{244}\text{Cm}$  concentration between 1 region and 4 region cases as a function of albedo and irradiation + subsequent cooling time.**

For the albedo sensitivity studies in a single assembly, the following can be concluded for each computed parameter:

- Decay heat is sensitive to albedo changes consistently from the reflective reference, specifically after 50 years of cooling time. For albedos lower than unity and after 100 years of cooling, decay heat relative differences increase and stabilize accordingly to the albedo reduction with a greatest value of +17%. For albedos greater than unity, the opposite effect is observed; decay heat decreases and stabilizes at a maximum relative difference of about -6%.
- The opposite effect is observed while studying the neutron emission per unit time. Consistently, the lower the albedo, the greater minimum difference is observed with respect to the reference case (e.g. up to almost -30% for the vacuum boundary condition case). On the other hand, computations for emission rates corresponding to albedos of 90% or 110% are within -5% and +5%, respectively, from the reference case.
- At the beginning of irradiation, the prediction of  $^{241}\text{Am}$  concentration relative to the reference case varies between -10% and +15%. At the end of irradiation, such relative difference tends to stabilize as  $^{241}\text{Am}$  is being build up in the fuel. A sudden peak (up to +35% difference) and stabilization takes place during cooling time until the end of the study. Accordingly, the lower the albedo, the greater the relative difference in its final prediction is being observed.

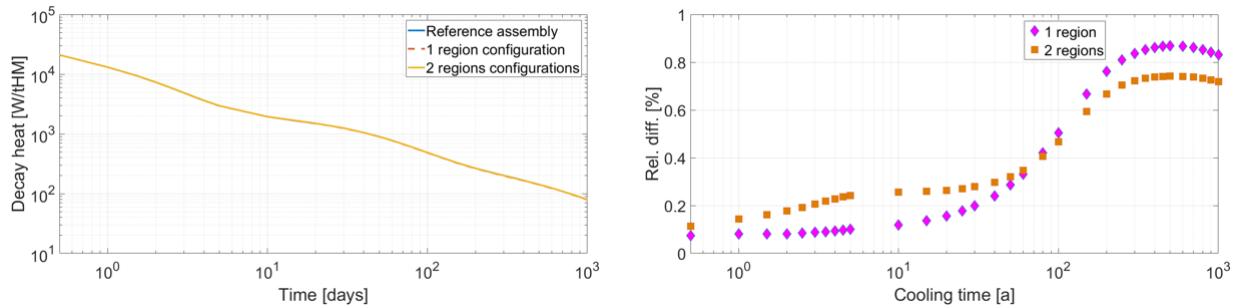
- The  $^{244}\text{Cm}$  case ranges from almost +15% to just below -10% at the beginning of irradiation, following a steady-increase until stabilization at the end of irradiation and beginning of cooling time. Accordingly, and inversely proportional to the decrease of albedo, the maximum final relative difference is about -30% for the black (vacuum) boundary case.

Regarding the study between a single and four depletable regions, it is clear that the lower the albedo is from the reflective case, the more divergent the computation of the observables becomes. Thus, a high impact is observed, with an under-estimation for low albedos if a single zone is used compared to four regions (except for the case of  $^{241}\text{Am}$ , where an over-estimation was observed instead).

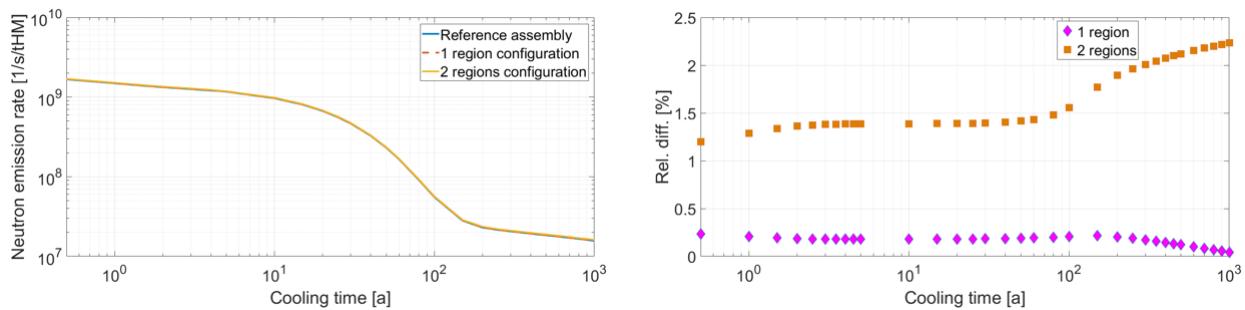
### 3.2 Reflector configuration results

In this section, results of observables per tHM for different reflector configurations (one or two fuel-pin regions) are being compared to calculations from the reference fuel assembly (i.e.  $\beta = 1$  and one fuel-pin zone). By following the same trend of describing results from the previous exercise, Figures 11 to 14 depict the difference (both in absolute and relative terms) between decay heat and neutron emission rate during cooling time, as well as for normalized  $^{241}\text{Am}$  and  $^{244}\text{Cm}$  masses along the complete time of the scenario.

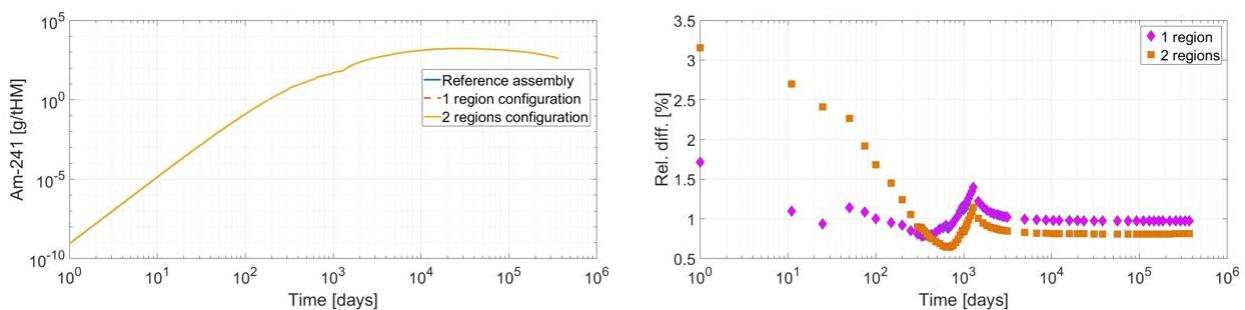
In general, it can be said that no significant impact is observed when a single or two regions are considered in a configuration with a central reflector area for decay heat computations. However a significant impact is observed in the computation of the neutron emission rate (it goes up to 2.5 times higher compared to the nominal case). This is caused mainly by curium concentrations around the different zone averages (in Figure 14, the  $^{244}\text{Cm}$  calculation at the beginning of irradiation is up to 10% different than the nominal model). Thus, it can be said that neutron source is more dependent on the reflector boundary compared to decay heat, due to influence of neutron spectra on the production of higher actinides.



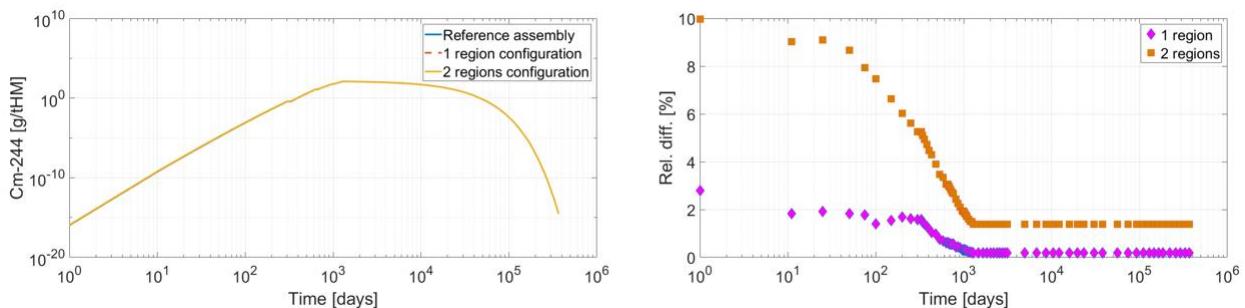
**Figure 11. Decay heat rate as a function of cooling time for different assembly configurations with respect to the reflector.**



**Figure 12.** Neutron emission rate as a function of cooling time for different assembly configurations with respect to the reflector.



**Figure 13.**  $^{241}\text{Am}$  mass as a function of irradiation + subsequent cooling time for different assembly configurations with respect to the reflector.



**Figure 14.**  $^{244}\text{Cm}$  masses as a function of irradiation + subsequent cooling time for different assembly configurations with respect to the reflector.

#### 4. CONCLUSIONS

This paper described in two different exercises, the effect that the quantitative albedo has in depletion calculations from different PWR-type assembly configurations. It shows that the neutron emission rate is more sensitive to albedo changes in a single fuel assembly than decay heat (i.e. -30% vs. +17% in relative difference, respectively). Likewise,  $^{244}\text{Cm}$  production is more sensitive than  $^{241}\text{Am}$  within this framework at the cooling time of 100 years (+17% vs. -30%, respectively), except at the end of irradiation where  $^{241}\text{Am}$  exhibits a peak up to +38% relative difference from the nominal scenario. Moreover, it is clear that at low

albedos, for an accurate computation of integral depletion observables several fuel-pin depletion regions need to be considered (four in this work).

Regarding the assessment of having a reflector inside a  $3 \times 3$  fuel assembly configuration, the relative change in output observables normalized to tHM and compared to the reference assembly is negligible. On the other hand, an effect was in fact noted when different depletable zones were being considered in the study; then, the accumulation of actinides like  $^{244}\text{Cm}$  makes the neutron source more dependent on the type of boundary condition (a relative difference at some point during cooling time of up to 2.5% was observed for this particular case).

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