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Characterization of the GBC-32 Fuel Assembly Source Terms

Mario Matijević, Matej Pekeč

Summary — **This paper presents burnup/depletion calculations of the typical Westinghouse 17x17 fuel assembly to be used as a radioactive waste package in a Generic Burnup Credit cask benchmark problem with 32 elements (GBC-32). This first phase is addressing spent fuel source terms calculation while evaluation of the shielding performance of the GBC-32 cask is planned for the second phase. The TRITON-NEWT methodology of the SCALE6.1.3 program package was used in a tandem with ORIGEN-S code for deterministic 2D calculation of the GBC-32 fuel assembly neutron multiplication factor, providing spatial-temporal fluxes and isotopic concentration change. The burnup simulation was done up to 60 GWd/tU with sensitivity analysis of relevant physical parameters influenced by the working cross-section library. This approach also allowed generation of the specific user-defined collapsed cross-section libraries as a function of fuel enrichment and burnup level. Calculation of isotopic concentrations, decay heat, neutron-gamma spectra and major actinides activity for different fuel assembly cooling periods was performed using ORIGEN-ARP module.**

Keywords — **SCALE, NEWT, TRITON, burnup, depletion**

I. Introduction

The Generic Burnup Credit cask (GBC-32) benchmark problem represents a real-life burnup credit style cask, preserving all important features through approximations, hence eliminating nonessential details and proprietary information [1]. The purpose of the GBC-32 benchmark is to provide a reference configuration for estimation of spent fuel (SF) reactivity margin available for fission products and minor actinides as a function of initial enrichment, burnup, and cooling time. Estimates of the additional reactivity margin for this reference configuration may be compared to a similar burnup-credit cask to provide an indication of the validity of specific design characteristics. A conservative approach to criticality safety analyses of commercial PWR fuel assembly (FA) storage and transport casks assumes the SF to be fresh or unirradiated, with isotopic concentrations defined by allowable enrichment [2]. This provides upper bounding value for reactivity, ignoring fuel operational history and simplifying analysis. However, this approach is lacking the decrease in reactivity of SF as a result of irradiation, giving conservative safety margin which limits cask capacity. A more realistic approach is including reduction in reactivity due to fuel burnup which is known as burnup credit. This will explicitly model reduction of fissile nuclides and the production of actinides and fission-product neutron absorbers. To provide a reference results for a burnup credit cask, resembling to a typical real-life configuration, a generic GBC-32 cask with 32 spent FAs was developed [1]. The reference results can be used to estimate additional reactivity margin coming from actinide nuclides and fission products. The essential part of criticality safety analyses is thus a detailed knowledge of FA geometry, initial material composition, operational history, and neutron-gamma source terms after cooling period.

This paper is presenting application of SCALE6.1.3 [3] transport theory codes for detailed isotopic analyses of an optimized Westinghouse 17x17 fuel assembly (OFA) in the framework of the GBC-32 benchmark. The performed TRITON [4] calculations quantified neutronic and isotopic characteristics of OFA by means of 2D deterministic transport theory code NEWT [3][5]. The depletion calculations of OFA were done in tandem with ORIGEN-S code up to a burnup of 60 GWd/tU using nominal power of 40 W/gU. Calculated k-eff values are provided as a function of burnup and cooling time for initial enrichments of 2 w/o, 3 w/o, 4 w/o, and 5 w/o of ^{235}U. The values are provided for burnup up to 60 GWd/tU with 20 time steps (75 days per step), and for cooling period up to 40 years (9 time steps). These TRITON-NEWT calculations coupled with ORIGEN-S also allowed generation of the specific user-defined collapsed cross-section libraries with 49 groups as a function of fuel enrichment and burnup level. Calculation of isotopic concentrations, decay heat, neutron-gamma spectra and major actinides activity for different fuel assembly cooling periods was performed using ORIGEN-ARP module [6]. These OFA results will be used as a starting point for the development of Monte Carlo (MC) GBC-32 cask model, which will be further analyzed with MAVRIC/Monaco shielding sequence of SCALE6.1.3 code package.

This paper is organized as follows. Chapter 2 gives basic description of an optimized 17x17 Westinghouse fuel assembly, which is used in the GBC-32 benchmark. The SCALE6.1.3 computational methods for deterministic 2D burnup/depletion of FA are presented in Chapter 3. The OFA TRITON model is given in Chapter 4. Chapter 5 gives TRITON-NEWT standalone results for OFA presenting method of generating weighted (collapsed) cross-section library with user defined 49 groups. The TRITON depletion calculations of OFA are presented in Chapter 6, together with ORIGEN-ARP results for neutron-gamma source terms. Discussion and conclusions are given in Chapter 7, while reference list is given at the end of the paper.

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II. Optimized Fuel Assembly in GBC-32 Cask

The burnup credit can increase storage and transport cask capacities by 1/3, so for a standard rail-type cask this means increase from 24 to 32 FAs for large PWR assemblies or 40 FAs for smaller fuel matrix [1]. The design of GBC-32 cask was directed by OECD/NEA concept, with the following criteria:

1. dimensions and geometry should be representative of typical U.S. rail type-casks;
2. the canister must accommodate at least 30 FAs;
3. the FA cell size must accommodate all common PWR designs;
4. design should be general without unique or proprietary information.

The GBC-32 design is based on merging OECD/NEA concepts with several U.S. cask vendors. Additional details on dimensions and materials of the cask can be found in report [1]. The reference fuel assembly design used in GBC-32 cask is the Westinghouse 17x17 Optimized Fuel Assembly (OFA) because it was shown to be the most reactive FA in most fresh-fuel cask designs. This fact streams from a zero burnup (fresh fuel) and high moderator-to-fuel ratio, which will at the same time produce less reactive fuel at typical discharge burnups. The OFA physical specification can be found in Table 1, while fresh fuel material specification for different fuel enrichments (2 w/o, 3 w/o, 4 w/o, and 5 w/o) can be found in report [1]. Figure 1 is showing NEWT 2D model of the OFA (green - fuel pins), which is placed inside GBC-32 cask cell.

Table I

The OFA physical parameters

OFA parameter	inches	cm
Fuel outside diameter	0.3088	0.7844
Cladding inside diameter	0.3150	0.8001
Cladding outside diameter	0.3600	0.9144
Cladding radial thickness	0.0225	0.0572
Rod pitch	0.4960	1.2598
Guide tube inside diameter	0.4420	1.1227
Guide tube outside diameter	0.4740	1.2040
Guide tube radial thickness	0.0160	0.0406
Instrument tube inside diameter	0.4420	1.1227
Instrument tube outside diameter	0.4740	1.2040
Instrument tube radial thickness	0.0160	0.0406
Active fuel length	144	365.76
Array size	17x17	
Number of fuel rods	264	
Number of guide tubes	24	
Number of instrument tubes	1	

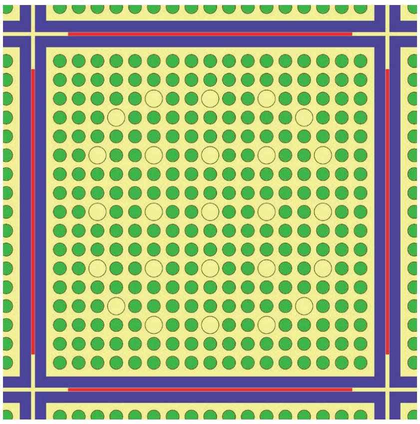

Fig. 1. Cross sectional view of OFA cell inside GBC-32 cask

III. SCALE Computational Tools

The SCALE6.1.3 code system was developed for the U.S.NRC to satisfy a need for a standardized method of analysis for the evaluation of nuclear facilities and package designs. In its present form, the system has the capability to perform criticality, shielding, radiation source term, spent fuel depletion/decay, reactor physics, and sensitivity analyses using well established functional modules tailored to the SCALE6.1.3 system [3]. The TRITON sequence of the SCALE6.1.3 code system performs problem-dependent cross-section processing followed by calculation of neutron multiplication factor k-eff for a 2D FA configuration using NEWT. The NEWT module is a multigroup discrete-ordinates (SN) radiation transport code with flexible meshing capabilities that allows two-dimensional (2D) neutron transport calculations using complex geometric models. The differencing scheme employed by the NEWT, the Extended Step Characteristic approach (ESC), allows a computational mesh based on arbitrary polygons. This functionality can be iterated in tandem with ORIGEN-S depletion calculations to predict isotopic concentrations, source terms, and decay heat as a result of time-dependent fluxes calculated in a 2D deterministic fashion (NEWT) or in a 3D stochastic approach (KENO V.a or KENO-VI). Because spatial fluxes are burnup dependent, changing with nuclide inventories, and because mixture cross-sections will also change with burnup, the depletion sequence uses a predictor-corrector approach to update both fluxes and cross-sections as a function of burnup [4]. The rigorous SN treatment in NEWT coupled with ORIGEN-S depletion capabilities and CENTRM resonance self-shielding processing within TRITON sequence provides a high-fidelity approach for various FA designs. The cross-section processing can be CENTRM-based rigorous SN solution by default ("parm=centrm") or a more relaxed two-region approximation in CENTRM (similar in nature to NITAWL) but retaining continuous-energy processing ("parm=2region").

The main codes for this study thus simulate burnup/depletion (ORIGEN-S) and 2D neutron transport with eigenvalue search (NEWT) under TRITON. The ORIGEN-ARP code is used lastly to quantify isotopic source terms for different FA cooling periods. The use of this sequence requires availability of the cross-section libraries for a specific FA design. These may be obtained from pre-generated libraries distributed within SCALE6.1.3 or can be generated by the user for a specific FA design using true flux (not generic PWR) for cross-sections weighting.

A. TRITON-NEWT broad group library

The TRITON-NEWT parameter "weight" will trigger MALOCS module to generate a weighted broad group cross-section library in AMPX master format (newxnlib file). The calculated NEWT problem-averaged flux spectrum is then used as the weighting function for the spectral collapse, while user provides energy group structure in the "collapse" input block. For this analysis, the v7-238 group master library (148 fast + 90 thermal groups) based on ENDF/B-VII.0 [7] is collapsed to a user-defined 49-group library (v7-49g), with grouping structure tailored to important PWR flux peaks and windows. The distributed v5-44g library (based on ENDF/B-V) was developed to capture significant aspects of LWR spectrum, while newer 49-group structure introduced in SCALE6.0 includes additional energy groups in the upper thermal energy range.

B. ORIGEN-S cross section libraries

During TRITON depletion calculations, the module COUPLE is creating and updating a cross-section database (ft33f001 file) for each depleted material, thus providing cross-sections as a function

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of burnup in specific ORIGEN-S file format. The TRITON produces one additional library with flux-weighted averaged cross-sections (ft33f001.cmbined file), which can be read by the ORIGEN-ARP module for rapid calculation of source terms. This procedure was adopted in this research for creating OFA libraries with different enrichment and burnup steps.

IV. Triton OFA Model

Based on the GBC-32 benchmark specification provided in Section 2, a computational model of the OFA was developed for TRITON-NEWT and TRITON depletion sequence. A cross sectional view of the NEWT 2D computational model is shown in Figure 2 for a symmetric 1/4 of the FA geometry. The calculations were performed using reasonably conservative cycle-average operational parameters for fuel temperature (1000 K), gap and clad temperature (620 K), moderator temperature (600 K), soluble boron concentration (650 ppm), and OFA specific power (40 MW/tU).

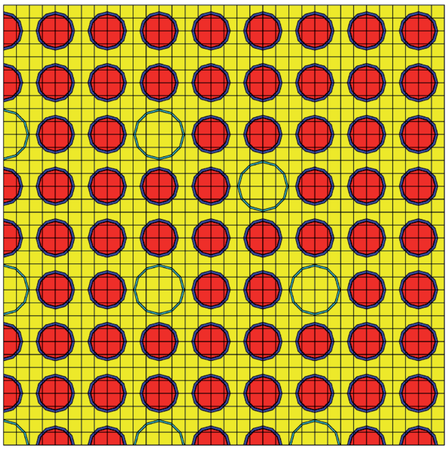

Fig. 2. NEWT model of the OFA with SN mesh (1/4 geometry)

The OFA fuel matrix is square 17x17 type (22.0 cm pitch) with 264 fuel rods and 24+1 control guide tubes. The fuel enrichment varies from 2 w/o to 5 w/o in ^{235}U using nominal thermal power of 40 MW/tU. The unit cell (1.2598 cm pitch) is comprised of fuel rod (1000 K), gap (620 K), clad (620 K) and moderator region (600 K) with 650 ppm of soluble boron. The cladding is Zirconium and the moderator is ordinary water. The NEWT model used S6 angular segmentation with P3 Legendre polynomial expansion for moderator (P1 for other materials), where unit cell had subdivision of 4x4 (recommended value). The forward transport solution was k-eff search with active collapse block (49 groups). The original coarse mesh finite difference (CMFD) acceleration was used for rectangular-domain configuration with enabled second-level two-group accelerator. All spatial and eigenvalue convergence criteria were set to value of $1 \cdot 10^{-4}$. The boundary conditions were all reflective type.

The TRITON depletion sequence was run using total of 20 time steps with duration of 75 days/step, giving total discharge burnup of 60 GWd/tU. The depletion with constant power was defined only for one material (UO_2 mixture, same for all pins) and three different libraries were used for k-eff comparison: v5-44g (broad built-in), v7-49g (user collapsed) and v7-238 (master built-in). The trace quantities of certain nuclides important for proper characterization of depleted fuel material were selected with "addnux=3" option, which adds 230 nuclides in depletion calculations.

The "parm=weight" option is very useful since TRITON depletion calculations require a significant amount of computer resources. This option allows generation of problem-dependent 49-group cross-section library at the start of depletion: steady-state NEWT calculation using v7-238 library is done only once at the beginning to determine neutron spectrum for spectral collapse. The 49-group library is then used for all subsequent depletion steps. This makes transport calculations run faster with minimal bias in total solution (typically less than 200 pcm for LWRs) [4]. Accurate depletion of heterogeneous FA designs in TRITON generally requires a different fuel mixture for every individual fuel pin inside a lattice, because spatial flux distribution varies significantly throughout a lattice model. Additionally, the flux distribution changes as a function of depletion. This results in space-time varying flux so fuel pin mixtures must be depleted individually in order to accurately track isotopic concentrations change [4]. Furthermore, depletion with a constant power is justified for fuel materials, but not for targets, structural materials and burnable poisons (i.e. IFBA rods). These materials are affected by neighboring fluxes and they do not contribute to power production, so depletion with a constant flux is a better option. Allowing mixed mode depletion with TRITON also improves the time-dependent flux distribution across fuel assembly.

V. Triton-NEWT OFA Results

The steady-state TRITON-NEWT results of k-eff are shown in Table 2 for different fuel enrichments using v7-238 master library (CPU time 11.5 min) and 49-group collapsed library (CPU time 2.1 min). One can notice small k-eff differences for v7-49g (40 pcm to 60 pcm) compared to v7-238 groups while CPU time reduction using broad library has almost linear scaling with the number of energy groups, i.e. v7-238 has over four times more groups than v7-49g. Figure 3 shows qualitatively neutron flux distribution over the 2D OFA model with e=2 w/o for the first and the last energy group. One can notice change in relative position of the local neutron sources from fuel rods (fast group) to water filled guide tubes (thermal group). The eigenvalue delta, or the change in k-eff with outer iterations is shown in Figure 4 using logarithmic scale to point out how final convergence will not be achieved until all groupwise inner iterations per outer iteration have converged.

Table II

NEWT steady-state k-eff solution

enrichment (w/o)	2.0	3.0	4.0	5.0
k-eff (v7-238)	1.11577	1.23911	1.31240	1.36101
k-eff (v7-49g)	1.11646	1.23977	1.31302	1.36158
k-eff rel.err. for v7-49g (pcm)	62.2737	53.7871	47.5313	41.9365

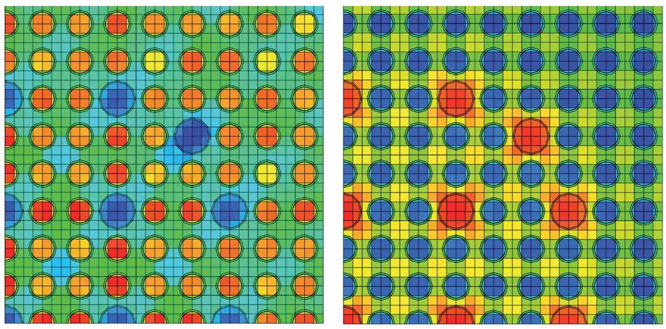

Fig. 3. NEWT flux distribution over OFA model (left-first group, right-last group)

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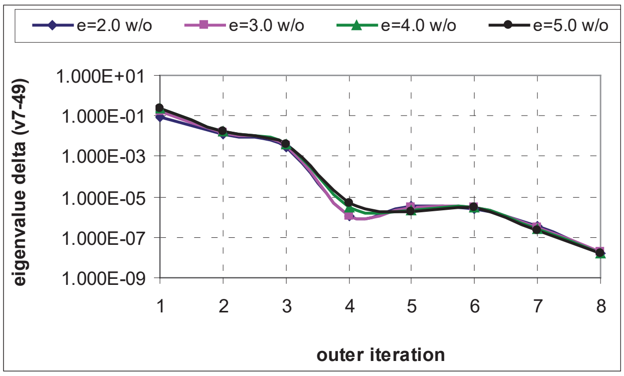

Fig.4. NEWT k-eff delta for v7-49g library

VI. Triton OFA depletion results

This section summarizes the depletion results for different enrichments of OFA model. Different cross-section libraries were used to investigate spectral effects on reactor physics parameters. The ENDF/B-VII.0 library v7-238 is generally recommended, but significantly prolongs CPU time per depletion step. Using a broad group library will automatically speed up the calculation, but the built-in v5-44g library (based on ENDF/B-V) was collapsed with LWR spectrum that is different than the specific OFA spectrum. This library is good for scoping and test calculations, but it is not recommended for production stage calculations. A good tradeoff between speed and accuracy can be obtained using the "parm=weight" option, which uses the problem-dependent neutron spectrum to collapse the master library v7-238 to a 49-group structure, which becomes working library for TRITON depletion sequence. The k-eff results for OFA (e=2.0 w/o) are shown in Figure 5, while v5-44g and v7-49g comparison to a master library v7-238 is shown in Figure 6. These trends are similar for other fuel enrichments and demonstrate justification of using collapsed v7-49g library for depletion calculations, reducing CPU run time by factor 4. One should also notice how delta k-eff for v7-49g library is bounded by an error interval of ± 100 pcm, which is a much smaller value compared to a built-in library v5-44g.

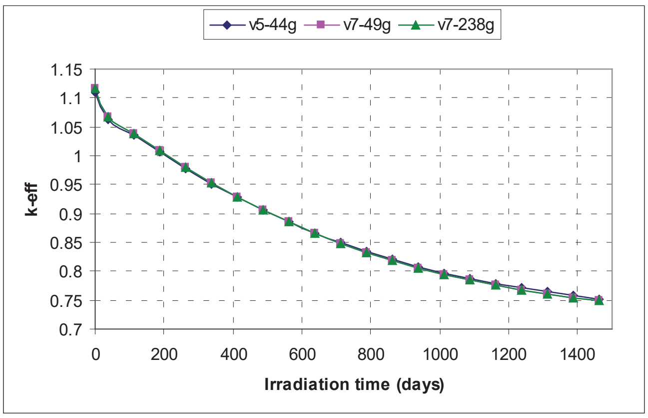

Fig. 5. TRITON k-eff depletion results (e=2.0 w/o)

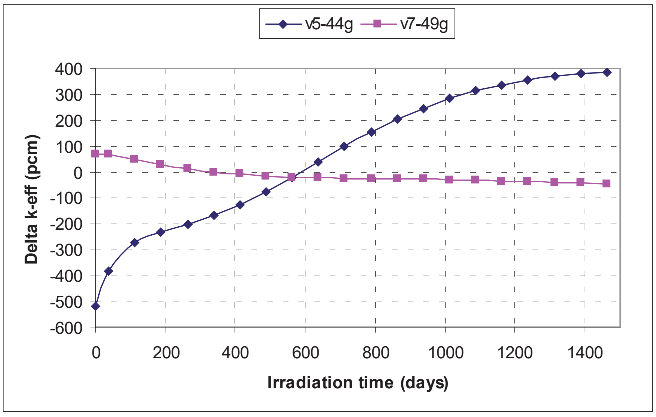

Fig. 6. Delta k-eff (pcm) for v5-44g and v7-49g libraries (e=2.0 w/o)

It is interesting to notice how delta k-eff curve of v5-44g library is being shifted to lower values for higher OFA enrichment levels, so Figure 7 is presenting this trend for e=5.0 w/o.

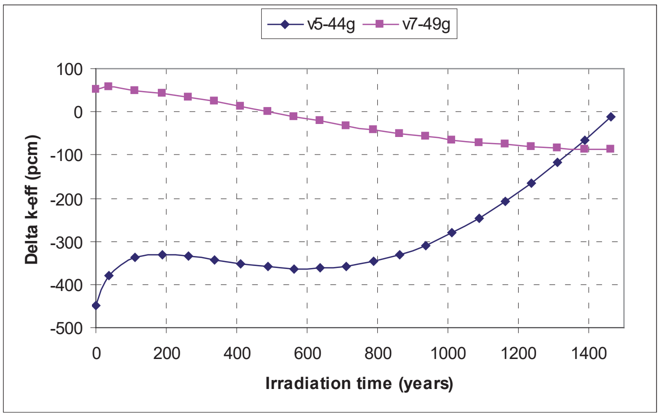

Fig. 7. Delta k-eff (pcm) for v5-44g and v7-49g libraries (e=5.0 w/o)

Relative pin power distribution of the OFA model is shown in Figure 8 for the fresh fuel (left) and at the end of irradiation (right). The peak pin power of 1.0655 was in the fuel rod (5, 6) for the fresh fuel and 1.0646 in the same position for burnt fuel, respectively.

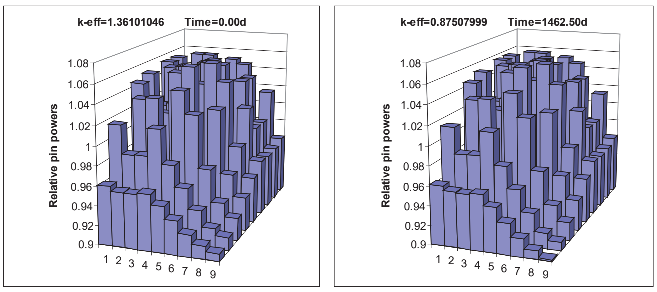

Fig. 8. Relative pin power distribution in the OFA (e=5.0 w/o)

Another useful result obtained with TRITON depletion is generation of ORIGEN-S cross-section libraries for depleted material. These burnup-dependent libraries were appended to SCALE6.1.3 data directory so ORIGEN-ARP module could be used for a rapid calculation of OFA source terms. The ORIGEN-ARP results are presented next using PlotOPUS program [3] for v7-27n19g shielding library, burnup of 60 GWd/tU, specific power of 40 MW/tU, 3 burnup cycles, and cooling periods of 0, 1, 3, 10, 30, and 40 years. The multigroup gamma and neutron spectra are shown in Figure 9 and Figure 10, while Figure 11 shows primary contributors (light elements, actinides and fission products) for decay heat production in order of their importance, but total value is for all nuclides in the problem. The multigroup neutron and gamma sources (particles/s/tU) are depicted in Figure 12 and Figure 13 for e=2.0 w/o, while total n-g sources as a function of cooling time are depicted in Figures 14 and 15, showing characteristic falling-off trend.

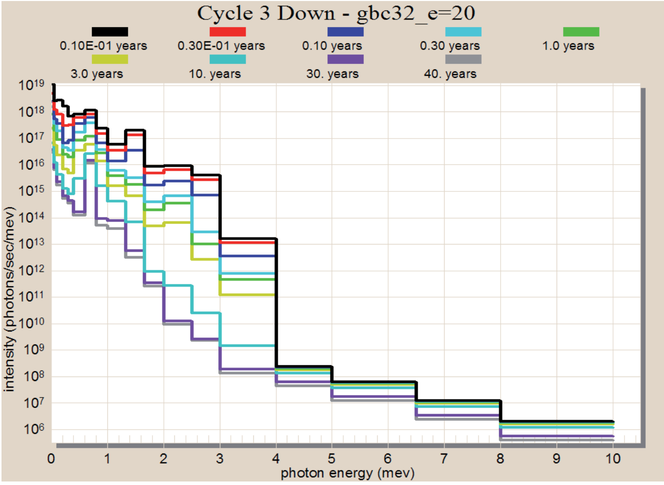

Fig. 9. Gamma spectra in photons/s/MeV (e=2.0 w/o)

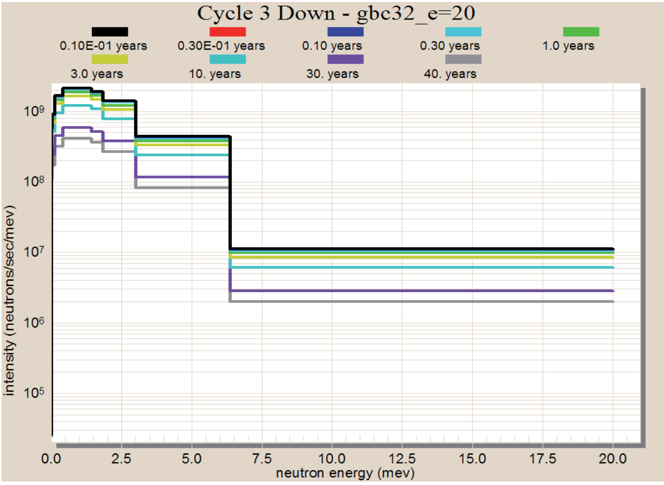

Fig. 10. Total neutron spectra in neutrons/s/MeV (e=2.0 w/o)

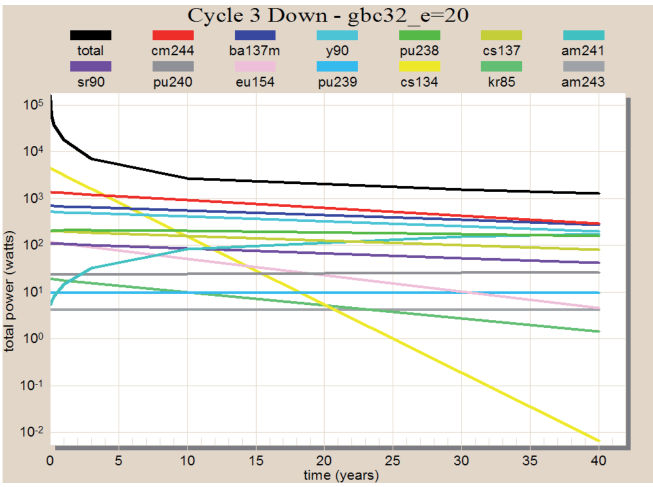

Fig. 11. Decay heat primary contributors (e=2.0 w/o)

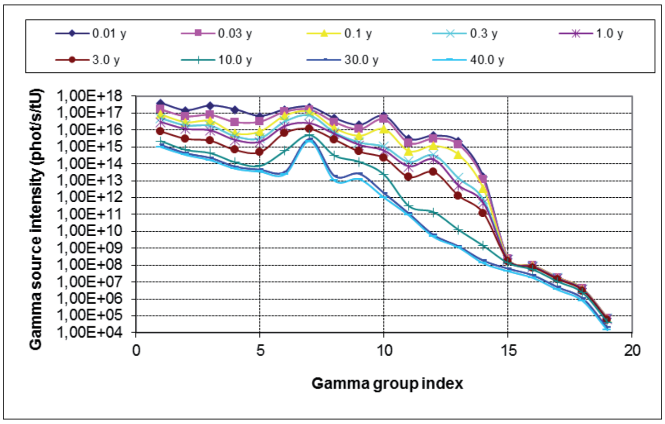

Fig. 12. Gamma source intensity (phot/s/tU) for different groups (e=2.0 w/o)

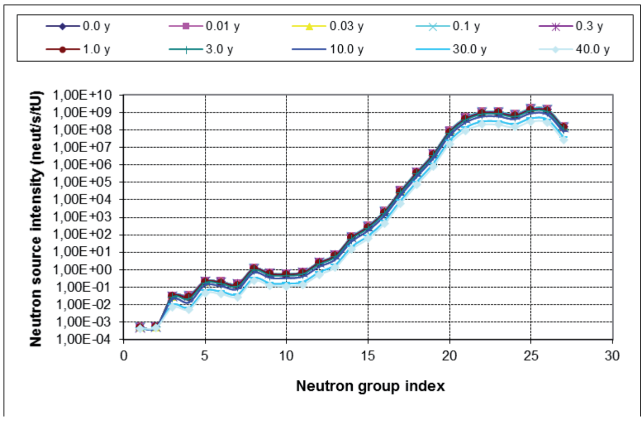

Fig. 13. Neutron source intensity (neut/s/tU) for different groups (e=2.0 w/o)

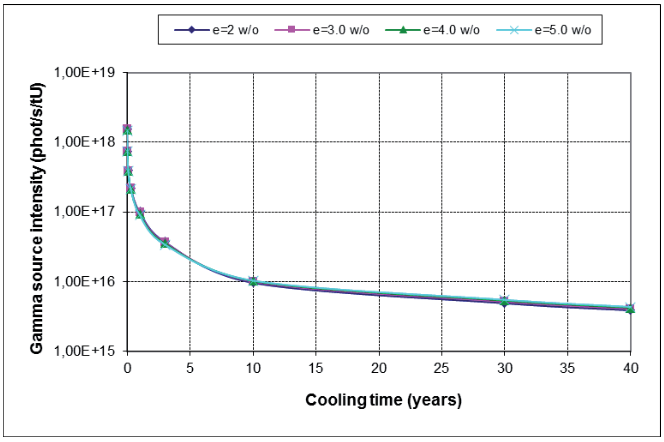

Fig. 14. Gamma source intensity (phot/s/tU) as a function of cooling time

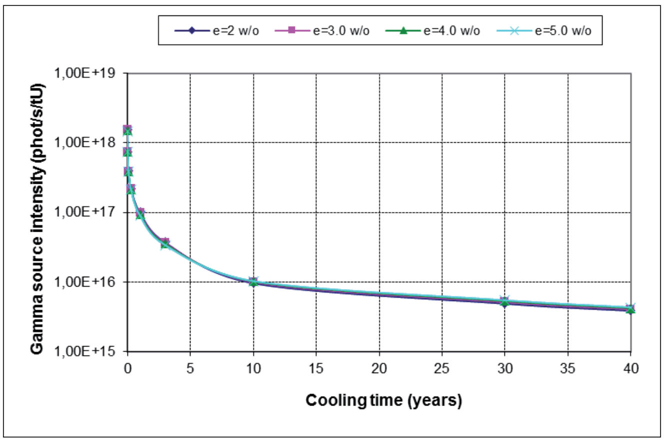

Fig. 15. Neutron source intensity (neut/s/tU) as a function of cooling time

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VII. Discussion and Conclusions

This paper presents selected results of TRITON-NEWT and TRITON depletion simulations of the OFA model in the framework of GBC-32 cask benchmark. This first phase is addressing accurate source terms characterization, since OFA model contains small modifications compared to the standard Westinghouse 17x17 FA model. Besides quantification of neutron-gamma source terms, during burnup and cooling time periods, this methodology provides ability to generate cross-section database (ft33f001 file) for each depleted material as a function of burnup in ORIGEN-S format. Such approach will use the initial v7-238 NEWT flux solution of the OFA model as a weighting function in production of the v7-49g collapsed cross-section library, which will accelerate remaining TRITON depletion calculations with a minimal bias in a solution. The obtained time-dependent databases can be directly used with ORIGEN-ARP interpolator to produce comprehensive source term characterization. The obtained results will be used in preparation of specific neutron-gamma source terms for the future MAVRIC/Monaco shielding calculations of GBC-32 cask.

The presented calculations utilize symmetry of the OFA model, so only 1/4 of FA was modeled with reflective boundary conditions. On top of that, each fuel pin had the same UO_2 matrix as the only depleted material, which is a gross approximation for modern FA designs. In practice, considerable CPU time goes on cross-section processing (CENTRM module) prior to NEWT calculations if one chooses to deplete a large number of fuel mixtures [8]. Moreover, this CPU time becomes prohibitively large with multiple unit cells, which are necessary for capturing spatial effects of fuel depletion. This problem is a well-known issue in depletion of modern, heterogeneous FA designs, that even with symmetry inclusion one typically gets dozens of fuel pin locations which need to be independently depleted. To simplify cross-section processing paradigm, it has been recognized that the macroscopic response of spent fuel is much more sensitive to the number densities of constituent nuclides than the nuclide cross-sections [3][4].

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