Comparison Among Monte Carlo Based Burnup Codes Applied to the GFR Demonstrator ALLEGRO

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Abstract: This paper aims to compare three Monte Carlo (MC) burnup based codes, i.e. MCNP6, Monteburns and Serpent on a future prototype reactor, named ALLEGRO, based on Gas cooled Fast Reactor (GFR) technology. GFR reactors are one of the proposed Generation-IV fast reactors; ALLEGRO facility is scheduled to be built in Europe as a GFR demonstrator, so its deepened simulation can help in its future development. The present study follows other researches already performed and aims to exhibit the different approaches in burnup calculations applied to a gas cooled fast reactors, i.e. this paper would like to show and to compare some results concerning nuclear parameters as k_{eff} and flux spectra, as well as the mass inventories versus burnup for some nuclides evaluated with different Monte Carlo codes. From obtained results, it seems to exist some differences in evaluation of nuclear parameters, mainly in effective multiplication factor and in mass inventories. The remaining differences are mainly related to calculation time: indeed between the fastest, that is SERPENT, and the slowest, that are MCNP6 and MONTEBURNS, the differences are about one order of magnitude. As far as precision is concerned, it was considered the standard only for effective multiplication factor and it seems that all codes are in good agreement.

Keywords: MCNP, Serpent, Monteburns, ALLEGRO, GFR, Generation-IV, Fast Reactors, Neutronics.

1. INTRODUCTION

As known, Monte Carlo (MC) codes are a useful tool to simulate nuclear reactors. Nowadays nuclear activities work toward new generations of reactors: innovative nuclear facilities are the best way to reach the nuclear fuel cycle closure and to further increase safety features. Therefore, more complex geometries, materials, and an improved neutronic economy are needed in order to achieve these purposes. In particular, the numerical simulations have an important role in new nuclear facilities: they can help researchers and designers to better define nuclear and technological features before their building. This paper is a part of a wider research activity about MC codes applied to innovative facilities with the main purpose of analyze the nuclear fuel cycle closure (see, as examples [1-10].

Here, the idea is to compare three MC based burnup codes, namely MCNP6, MONTEBURNS and SERPENT2. These codes can work in criticality and burnup modes. The first two codes use the "classical" MCNP for static calculations coupling it with different codes (in case of MCNP6 incorporated as an inner subroutine) for burnup/depletion calculations; instead SERPENT2 is self-operating, having an inner ad-hoc

subroutine to perform burnup calculations. Additionally the three codes work in different ways as far as the evaluation of nuclear parameters is concerned; moreover they present different run times and precisions (statistical error) *vs*. computational resources. Then, this paper aims to show the different approaches and results when these MC codes are applied for a GFR-like benchmark simulation.

The present comparison has been carried out on the research reactor named ALLEGRO: it is a Gas cooled Fast Reactor (GFR) prototype proposed in order to evaluate the GFR full power ("commercial") reactor proposed by Generation-IV International Forum [7]. An important feature of GFR should be the contribute to nuclear fuel cycle closure [11]: as a consequence, the verification of codes suitable for transmutation analyses can be very useful. Thus, the purpose of this paper is to show some comparison results using different MC burnup codes, and to study some nuclear parameters about ALLEGRO reactor. From obtained results, we can see a quite good agreement between codes as far as mass inventories and 69-group flux spectra, while some differences exist relating to the trends of effective multiplication factors versus burnup.

2. CALCULATION CODES

The MC burnup codes chosen for this comparison are widely known in nuclear simulations. MCNP6 is available for researchers after an agreement with Los

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Alamos National Laboratories. MONTEBURNS is available for public use through NEA-OECD Organization, after signing an user agreement. SERPENT2 is a beta version that is provided by VTT Technical Research Centre of Finland LTD to the nuclear community already using SERPENT1 supplied by NEA-OECD.

MONTEBURNS uses a coupled routine with MCNP code to run in burnup mode, while MCNP6 and SERPENT2 have an inner burnup subroutine.

All these codes need of cross sections to run: to have more comparable results, it was chosen to use the same cross section dataset, i.e. the JEFF dataset. Particularly we used the JEFF-3.1 version because this one is internationally well known and already tested in many nuclear simulations. In following sub-paragraphs these codes will be analyzed in detail.

2.1. MCNP6

The MCNP6 [12] is the merging result of MCNP5 [13] and MCNPX Monte Carlo codes. From this effort, a code with the features of both (besides new features that have been implemented) is born. MCNP6 is a general-purpose code; more than its capability of track many particle types over broad ranges of energies, its main characteristics are the continuous-energy, the generalized-geometry, the time-dependent and the radiation-transport. As far as new features is concerned, they are underlined: the capabilities to handle a multitude of particles and to include model physics options for energies above the cross-section table range, the burnup mode calculations and the production of delayed particles. Moreover, some features were improved about: tally, source, variance-reduction options and plotting capability.

Here, only the new burnup feature is described. Indeed, this calculation mode can be employed through a BURN card that must be defined in the input file: the depletion/burnup feature can be used only in KCODE problems. For performing the burnup calculations, MCNP6 uses a link process with CINDER90 code 1.a.i.[14]. The procedure that involves the codes work in this way: the steady-state calculation is done by MCNP6 to determine the system eigenvalue, the 63-group flux spectrum, the energy-integrated reaction rates, the fission multiplicity and the recoverable energy per fission. These values are used by CINDER90 to do depletion step and then to calculate new materials densities for following step. These last

values of densities are provided to MCNP6 to run a new time step. MCNP6 carries out burnup calculations only on those isotopes listed in material card and obtained from a fission product tier or a generator algorithm. Unlike other codes under analysis, in MCNP6 it is not possible to define a list of nuclides to follow in burnup process, but the chain of isotopes of interest must be inserted in material card. If these isotopes are not present at begin of cycle (e.g. products and scraps of fission processes) they must have low atomic or weight fraction values.

2.2. Monteburns

The Monteburns [15] is a burnup code coupling MCNP [13] with Origen2 [16]. Monteburns works through a Perl script file (*Monteburns.pl*) that executes MCNP, Origen2 and the *monteb.f* code written in FORTRAN77 language. This interaction between *Monteburns.pl* and *monteb.f* acts on input and output from MCNP and Origen2 to generate the burnup tool. Through this way MCNP supplies the one-group microscopic cross-sections and fluxes to Origen2 for burnup calculation; after Origen2 and MCNP have run, results are written onto output files. After these steps, from new data of Origen2 burnup calculation, a new MCNP input file is created with new isotopic compositions and new densities for each material under analysis. Origen2 is a deterministic depletion code based on the matrix exponential method. Some initial data are required by codes as: initial compositions and volumes of materials to burn, one-group cross sections for each isotope, thermal power and burnup time. For burnup calculation Origen2 requires the initial cross section libraries: 30 different cross sections types, useful for different systems, are provided: in this calculation the Fast Flux Test Facility Cross sections (FFTFC) were used. Monteburns uses a "predictor midpoint step routine" to increase the burnup calculation accuracy. In burnup calculation Origen2 runs halfway through designated burn step so that, at the midpoint of the burn step, MCNP calculates spectrum-averaged, one-group cross-sections and fluxes. This isotopic composition is considered as a reasonable approximation of composition of entire burn step. Burn time steps should not be too much long, so that midpoint value could be representative of entire burn step.

2.3. Serpent2

The SERPENT [17, 18] is a continuous-energy Monte Carlo code developed by VTT Technical Research Centre of Finland. Serpent code is provided

by NEA: base release is Serpent 1.1.7. Serpent2 is a new and beta version of this code: it is actually provided to researchers who have a good experience with Monte Carlo simulations and, above all, with SERPENT1. Indeed, it need to be tested to solve problems related to new features before make it available to public distribution (e.g. at NEA and RSICC). The Serpent version used in the present paper is 2.1.20 dated April 2014. About 80% of Serpent2 is compatible with Serpent1: new features and capabilities are discussed through a dedicated forum, in this paragraph only some of them will be reported. In general, main features of Serpent2 are very similar to those of version 1: this code is written in standard ANSI-C language, the input file can be only one (in some problems can be used an external file to define different features of source, geometry etc.) and it is composed by some command cards, i.e. cell cards, surface cards and miscellaneous cards. For solving depletion equations Serpent uses by default the CRAM matrix exponential method [19]. Respect to Serpent1 new features were implemented, particularly relating to: tracking and geometry routine, physics and interaction data, physics and interaction data, burnup calculation, parallelization. Particularly, in Serpent2 were implemented some burnup routines that work through some advanced options for predictor-corrector calculation: they were tested higher order methods to solve the depletion solutions in burnup calculations [20]. However, in this comparison it was used a standard predictor-corrector routine based on CE/LI algorithm (CE: Constant Extrapolation for the predictor, LI: Linear Interpolation for the corrector) [21].

3. CALCULATIONS

The ALLEGRO 75 MW$_{th}$ prototype has been already studied in GoFastR Project [22, 11, 7, 3, 4] and derives from some previous nuclear concepts initially developed by CEA. Two configurations have been proposed: "MOX pin" and "CERAMIC" cores [23-30]: in this paper we used as benchmark the MOX pin core (MOX24 pin S/A) design with the addition of some Experimental Sub-Assemblies (Exp-S/A) designed for full power reactor. Active core is surrounded by reflectors and neutronic shields both in radial and in axial directions and is composed as follows:

- 6 CSD S/A – Control and Shutdown Devices

- 4 DSD S/A – Diverse and Shutdown Devices

- 81 MOX24 pin S/A – sub-assemblies fill by 169 cylindrical pins each; the fuel is oxide of U-Pu, the claddings are made of stainless steel

- 6 Exp-S/A – sub-assemblies as test of GCFR fuel Exp-S/As; the fuel is U-Pu carbide, geometry derives from GCFR fuel slab configurations [32, 33] and the materials compositions is similar to that of pin S/As

The ALLEGRO is cooled by helium at 70 bar pressure and at an average (on the whole core) temperature of 410 °C. The fuel pins and plates have average temperatures around 880 °C. Further ALLEGRO design data (e.g. materials and geometric features) are confidential, thus they cannot be shown explicitly.

All the criticality calculations were performed adopting the following neutronic parameters:

- 50000 neutrons source

- 500 active cycles

- 50 inactive cycles

These simulation parameters were chosen as good agreement for this paper (also relating to calculation power available), however a more detailed analysis on source convergence could be object of further comparisons.

Burnup calculations were performed considering 1000 total burnup days divided in 10 steps of 100 days each one corresponding to 2.927 MWd/kg$_{HM}$. All codes adopted the JEFF-3.1 cross sections dataset [31].

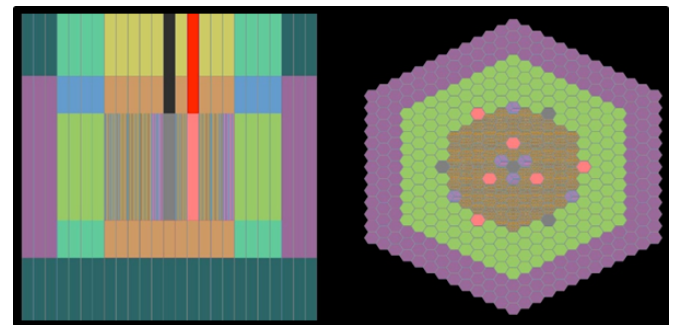In the next figure **1** the Y-Z and X-Y geometrical sections of ALLEGRO reactor are shown.

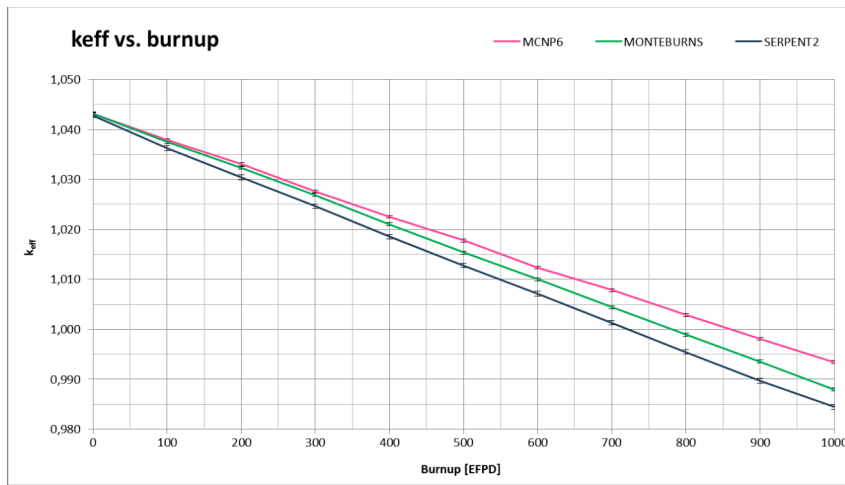**Figure 1:** ALLEGRO Y-Z (left) and X-Y (right) geometrical sections.

Figure 2: Comparison of k_{eff} trends calculated by MCNP6, MONTEBURNS and SERPENT2.
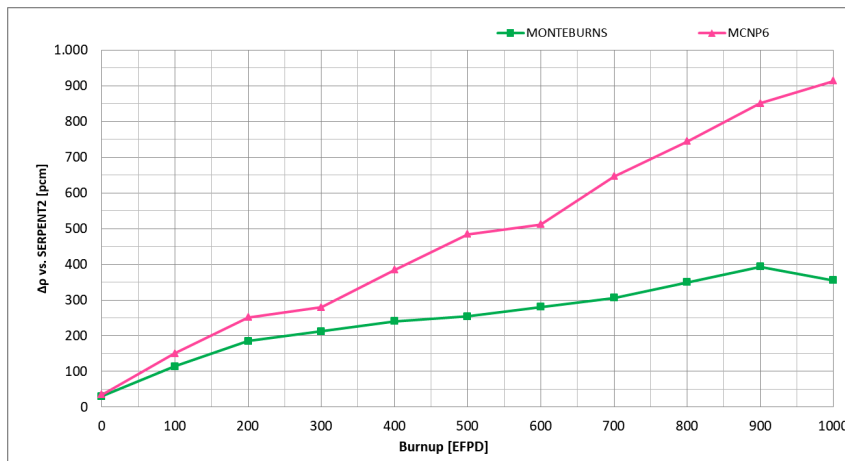

Figure 3: Relative differences in reactivity values.

4. RESULTS

In this paragraph, the results obtained by burnup calculations are shown: The begin of calculation, is indicated as BoC (Begin of Cycle), while the end of burnup process (i.e. 1000 equivalent full power days, EFPD) is indicated as EoC (End of Cycle). SERPENT2 was chosen to consider this one as the reference code, because SERPENT2 was already tested for burnup calculations on innovative gas cooled reactors. This assumption does not imply that SERPENT2 should be, a priori, more accurate in burnup calculations than other codes.

In the figure **2** the trends of k_{eff} *vs.* burnup for the three codes under evaluation are shown, (the 3σ uncertainty for each codes is also indicated).

At BoC, all the codes have the same value, but at EoC there are some differences, probably mainly due

Table 1: Relative Differences in 6-Group Spectra with Respect to SERPENT2

Relative Differences with Respect to SERPENT2 (at BoC)			
# Group	Energy	MCNP6	Monteburns
1	E-9<MeV<E-7	0.00000%	0.00000%
2	E-7<MeV<E-6	18.63293%	17.25084%
3	E-6<MeV<E-4	0.44968%	-0.34332%
4	E-4<MeV<E-1	1.04700%	0.02199%
5	E-1<MeV<E0	-0.70670%	-0.00711%
6	E0<MeV<2E1	-0.95057%	-0.04024%

to the differences in Pu^{239} quantities. Monteburns shows a bigger variation in the trend at the first step: this variation seems to exist only one time, so it could be due to a different evaluations of masses and cross sections, and therefore to the reaction rates, in the first depletion step. Those differences can be highlighted in figure **3**, which shows the reactivity relative differences in comparison with SERPENT2: non-negligible differences exist for both MCNP6 and Monteburns, although it appears to be bigger for MCNP6.

In the figure **4** and the table **1**, the 6-group spectra evaluated at BoC on whole core are shown: a good agreement exists between all codes, although MCNP6 seems to have a slight softer flux. It is important to note that the second group has almost no neutrons (more

than 3 order of magnitude less than in the third group), so the reported differences (in %) could be a bit misleading. In general, the MCNP6 shows the greatest relative differences for all the energy groups.

In figure **5** the 69-group spectra evaluated at BoC on whole core are shown: it can be noted that exists a very good agreement between all the codes under evaluation.

In the next figures the trends of some (selected) nuclides amounts *vs.* burnup (in MWd/kg$_{HM}$) are shown: these inventories are represented as the atomic concentration in the fuel pin material. As it expected, there is a constant consumption of the U^{235} and Pu^{239} and a non-linear increase of Am^{241}.
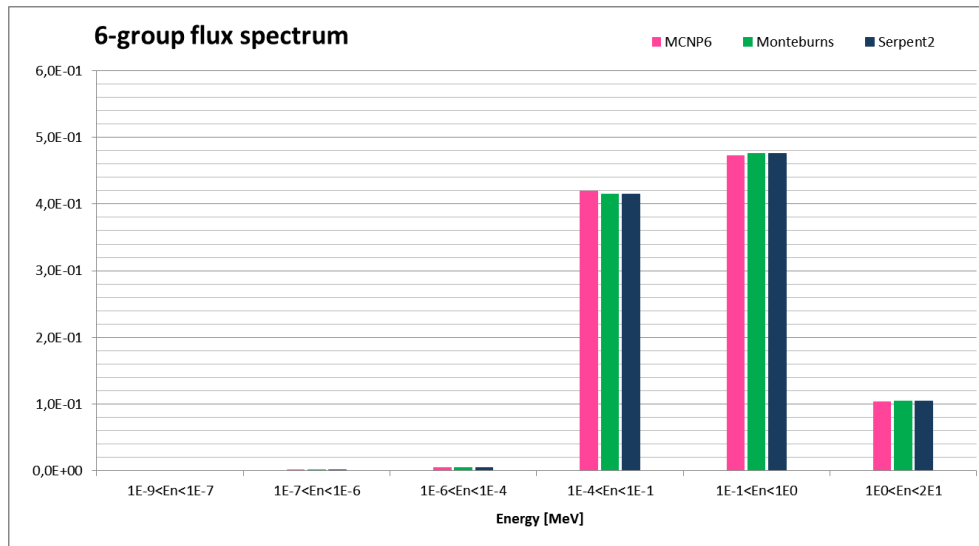

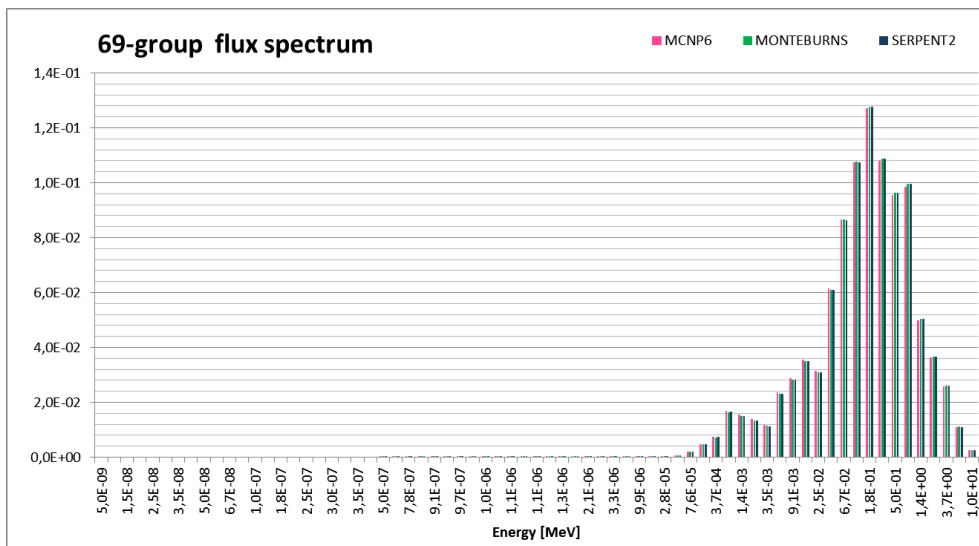**Figure 4:** Comparison of 6-group spectra of reactor core at BoC.

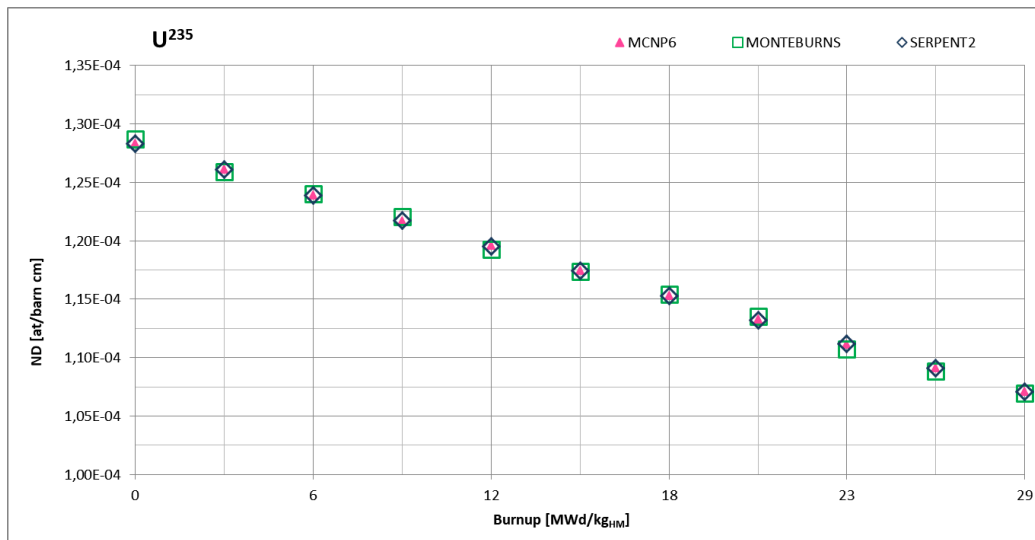**Figure 5:** Comparison of 69-group spectra of reactor core at BoC.
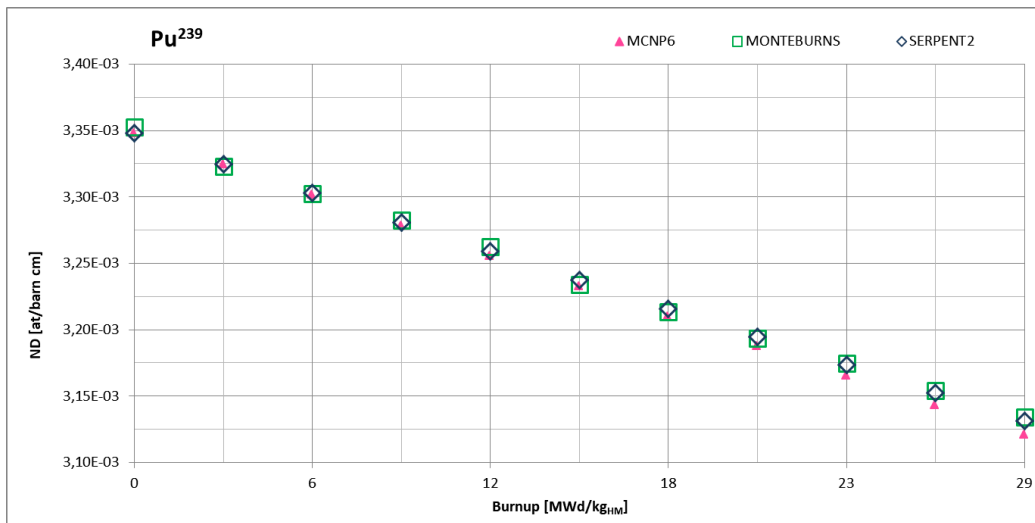
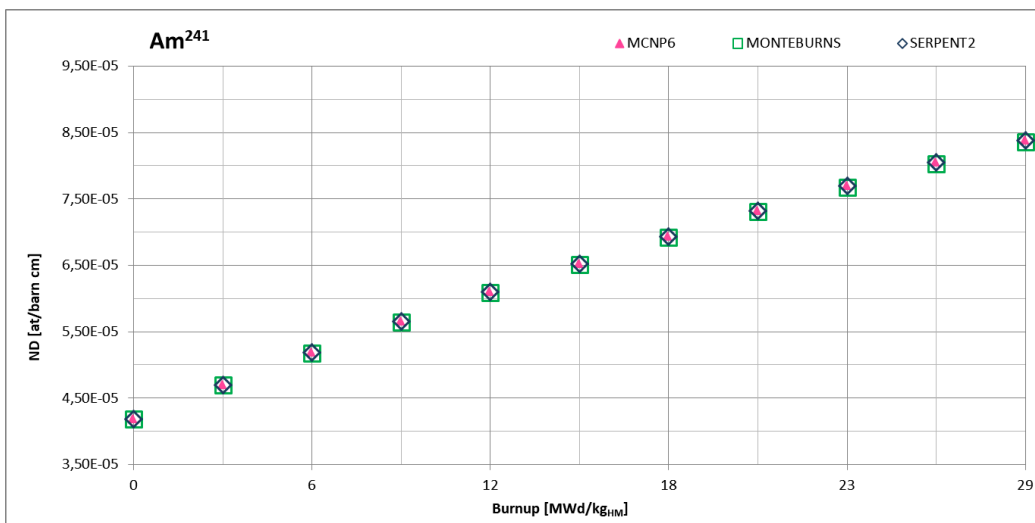**Figure 6:** Inventory of U^{235} *vs.* burnup.

Figure 7: Inventory of Pu^{239} *vs.* burnup.

Figure 8: Inventory of Am^{241} *vs.* burnup.
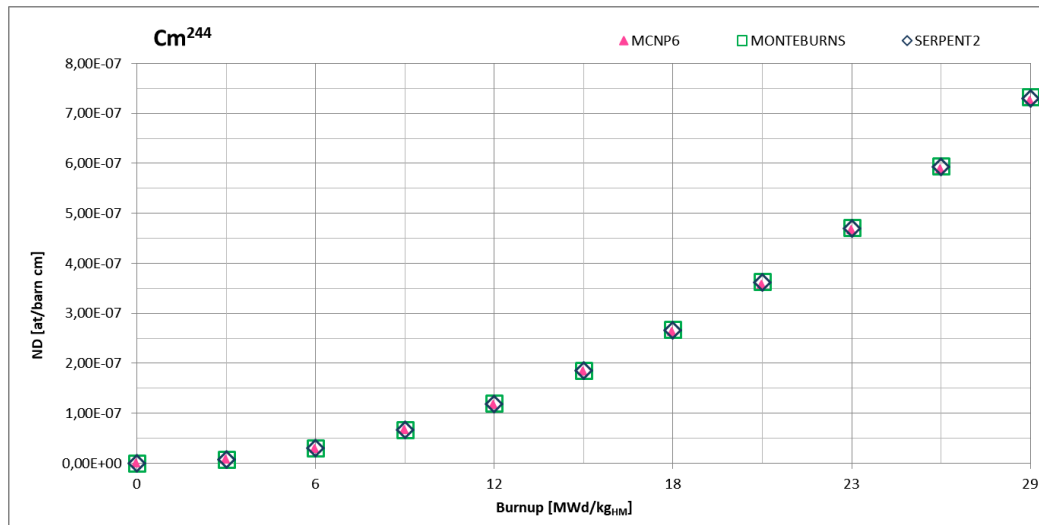
Figure 9: Inventory of Cm^{244} *vs.* burnup.

Table 2:   Differences with Respect to SERPENT2 of Nuclides Inventories

Inventory at EoS - Difference with Respect to SERPENT2		
	MCNP6	**Monteburns**
# Step	**MWd/kg$_{HM}$**	**U^{235}**
1	2.927	0.03095%	-0.13788%
2	5.854	0.01575%	0.08734%
3	8.781	-0.01749%	0.30315%
4	11.708	0.00297%	-0.23443%
5	14.635	0.00680%	-0.05363%
6	17.562	-0.00923%	0.11384%
7	20.489	0.03290%	0.27574%
8	23.416	-0.02394%	-0.37501%
9	26.343	-0.02195%	-0.25767%
10	29.270	-0.04224%	-0.15818%
# Step	**MWd/kg$_{HM}$**	**Pu^{239}**
1	2.927	-0.00918%	-0.06164%
2	5.854	-0.02878%	-0.00238%
3	8.781	-0.07895%	0.05396%
4	11.708	-0.10757%	0.10650%
5	14.635	-0.14089%	-0.11395%
6	17.562	-0.17925%	-0.07078%
7	20.489	-0.22249%	-0.03139%
8	23.416	-0.24376%	0.03105%
9	26.343	-0.29739%	0.06224%
10	29.270	-0.32862%	0.08912%
# Step	**MWd/kg$_{HM}$**	**Am^{241}**
1	2.927	-0.00792%	-0.04476%
2	5.854	-0.02786%	-0.17799%
3	8.781	-0.02280%	-0.09930%
4	11.708	-0.03715%	-0.15058%
5	14.635	-0.03591%	-0.18167%
6	17.562	-0.04365%	-0.20577%
7	20.489	-0.04322%	-0.23215%
8	23.416	-0.05428%	-0.26782%
9	26.343	-0.05039%	-0.30827%
10	29.270	-0.06054%	-0.26681%

Table 1 Continued…

Inventory at EoS - Difference with Respect to SERPENT2			
		MCNP6	Monteburns
# Step	MWd/kg$_{HM}$	Cm^{244}	
1	2.927	-1.38117%	0.47675%
2	5.854	-1.28414%	0.26233%
3	8.781	-1.19444%	0.43724%
4	11.708	-1.10680%	0.47434%
5	14.635	-1.00882%	0.46660%
6	17.562	-0.95227%	0.33198%
7	20.489	-0.88119%	0.46721%
8	23.416	-0.81366%	0.33080%
9	26.343	-0.73448%	0.28783%
10	29.270	-0.64520%	0.29089%

It is important to underline that, a reasonably agreement exists for all nuclides, although non-negligible differences (with reference to SERPENT2) can be noted for both MCNP6 and MONTEBURNS. For a clearer comparison, in the table **2**, the relative differences in comparison to SERPENT2 (applied for each nuclide at each End of Step, EoS) are shown. The greatest differences are reported for Cm^{244} and Pu^{239}, although the values remain well below 1.5 % for the whole campaign.

Finally, in table **3** the main computational parameters for the three considered codes are summarized (remembering that all the calculations have been run on the same hardware with the same available RAM).

CONCLUSIONS

As already shown also in some previous works (see, as examples, [1-10,34,35]), ALLEGRO remains a suitable benchmark test for code-to-code assessment focusing on the main neutronic data: it is mainly due to the peculiar neutronic characteristics (such as the use of He as coolant), transparent to the neutrons, and the future concrete possibility to be located in the central

Europe [36]. The comparison concerned some nuclear parameters and material data evaluated by MCNP6, Monteburns and Serpent2 Monte Carlo based burnup codes have been shown with particular attention given to Serpent2 as reference calculation.

Significant differences are shown in effective multiplication factor trends, particularly for Serpent2 if compared to MCNP6 and Monteburns. However, the maximum relative differences are lower than 1%.

Moreover, the 6-group and 69-group flux spectra were analyzed at begin of cycle (BoC): some differences were highlighted during the performing the calculation benchmark analysis, however it is evident that MCNP6 seems to supply a slightly softer spectrum.

As the final step of the research activity, the trend of mass inventories versus burnup was analyzed for some selected nuclides in order to complete the comparison. These values come from masses provided by each code calculation; however, due to the confidential nature of some data, the results are shown only as atomic densities in the fuel pin materials.

Table 3:   Comparison of Some Codes Features

Features		MCNP6	MONTEBURNS	SERPENT2
Platform (SO)		Windows/Linux	Windows	Linux
MC code used for transport calculation		MCNP6	MCNP5	SERPENT (stand alone)
Cross sections dataset		JEFF-3.1 continuous-energy	JEFF-3.1 continuous-energy	JEFF-3.1 continuous-energy
Type of Doppler broadening correction (cross sections temperature correction)		increasing / decreasing	increasing / decreasing	increasing
Depletion code/subroutine		CINDER90	ORIGEN2	SERPENT (stand alone)
Calculation time [order of magnitude in hours]	criticality	E1	E1	E1
	burnup	E3	E3	E2

It is important to remark that some important differences exist in the calculation times in burnup mode for each code: the fastest code remains SERPENT2, while MCNP6 and MONTEBURNS are slower (about one order of magnitude in time for the burnup calculations).

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