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Benchmarking of MONTEBURNS against measurements on irradiated UOX and MOX fuels

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This work shows that MONTEBURNS is able to accurately model the depletion of UOX and MOX fuels up to 71.0 GWd/T and 47.2 GWd/T respectively. As the reference scheme depends on the continuous energy libraries used and on the exact representation of the real geometry only, it is also able to model any configuration representative of the future PWR, BWR, HTR and VHTR reactors with the same accuracy.

KEYWORDS: Monteburns, UOX fuel, MOX fuel, PWR, HTR

1. Introduction

MONTEBURNS [1] simulates the depletion of any nuclear fuel through the coupling of MCNP4 [2] and ORIGEN2 [3]. It handles input/output data, manages exchanges between the two codes and edits the Keff, the neutron flux, the nuclear power and isotopic compositions of the various depleted mediums at any selected time-step.

MONTEBURNS can be used, under certain conditions, to assess a new reactor design [4] or as a numerical reference for validating deterministic codes, generally in the absence of representative experiments.

The precision of MONTEBURNS is due to the "exact" solving of transport equations by MCNP4 when the exact geometry is input and adequate continuous energy nuclear libraries are used, and to ORIGEN2's ability to represent more than 1200 isotopes, provided the single energy group cross-section tables input for solving the Bateman equation are correct. In fact, MONTEBURNS makes MCNP4 calculate the required cross-section tables at each depletion step, taking into account the actual change in the energy spectrum with depletion.

Both MCNP4 and ORIGEN2 are internationally recognized and both have been benchmarked against a wide range of experiments. However, benchmarking against experiments of the MCNP4-ORIGEN2 coupling is still in the early stages, and there are few publications describing such benchmarks [5], [6].

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2. The analyzed fuel rods

This paper presents a MONTEBURNS benchmark performed against the results of isotopic analyses of 13 UOX and MOX rods:

- 9 UOX rods to 4.48 % U235 burned from 26.9 to 71.0 GWd/T
- 2 UOX rods to 3.31 % U235/gadolinium to 4.9% burned 2.96 and 6.34 GWd/T
- 2 MOX rods to 5.64 % Pu burned 28.6 and 47.2 GWd/T

These rods cover most of the enrichments currently used in the French nuclear fleet.

C/M comparison is carried out for the 8 main heavy isotopes (HI) (U234, U235, U236, PU238, PU239, PU240, PU241 and PU242). A 9th, U238, is used to normalize the concentrations. A comparison is carried out in parallel for 3 tracer isotopes produced by burnup: Nd145, Nd148 and Cs137.

For 2 UOX rods with gadolinium, the concentrations of the odd isotopes Gd155 and Gd157 are compared.

The isotopic analysis of the irradiated rod relates to a segment of the order of one cm located at middle height of the core. At this height we have an "asymptotic" spectrum with respect to the edges of the core (leakage has no impact on the spectrum); the analysis can thus be carried out by a 2D model.

The power history relates to the analyzed rod, whereas power modelling relates to the assembly or cluster of MONTEBURNS. The irradiation of the assembly containing this rod is thus simulated in order to obtain the required rod burnup.

3. Calculation parameters and sensitivity studies

Given the calculation time necessary to perform MCNP4 calculations with sufficient accuracy, the different parameters of the MONTEBURNS calculations have to be optimized according to the desired accuracy of the results. These parameters are:

- the number of depleted mediums of the studied rod
- the modeling of the surrounding of the studied rod
- the length of each time step,
- the convergence of MCNP4 calculations,
- the importance fraction which is input by the user to select the isotopes for which the cross-sections are to be updated by MCNP4
- the fission energy used during depletion and
- the cross-section libraries.

3.1 Number of depleting mediums

By analogy with deterministic calculation schemes, we carried out most of our analysis with a rod split into 5 depletion rings, whereas the surrounding rods (for computing time reasons) were modeled with one depleting medium only. This approximation is acceptable only when the neighboring rods provide the average neutron spectrum. On the other hand, when the surrounding rods also provide indicators such as power and burnup (GEDEON experiment) they are modeled in the same way as the analyzed rod. Thus the number of depleted mediums for the cluster containing the 13 analyzed rods varies from 6 (UOX/2, 3, 4, 5 cycles) to 24 (GEDEON, UOX+Gadolinium, see figs. 1a, 1b, 2a, 2b, 3a and 3b). We consider that there is no uncertainty related to this parameter for the depletions obtained with 5 rings in the fuel rod. Since the computing time is proportional to the number of depleted mediums, one can, in certain cases, have less than 5 rings to carry out faster sensitivity analyses. Comparisons between 5 and 1 ring for the studied rod show for example that C/M results are comparable (see table 3).

Figure 1a: Quarter of UOX assembly with 9 depleting mediums

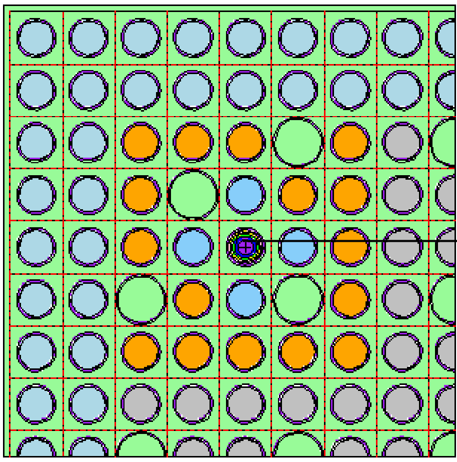


Figure 1b: Five depleting mediums for the studied UOX rod

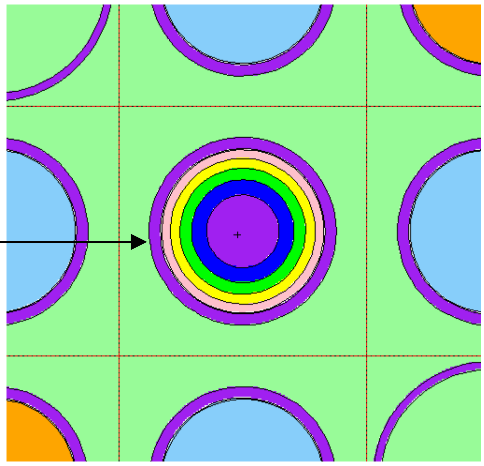


Figure 2a: Quarter of MOX assembly with 8 depleting mediums

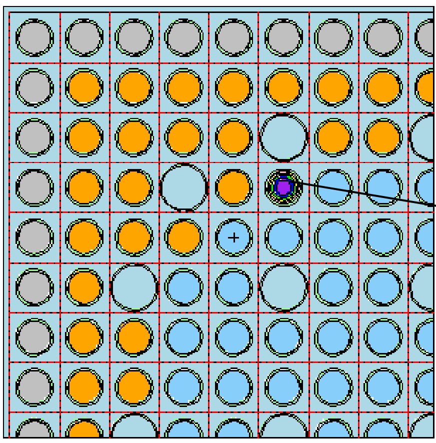


Figure 2b: Five depleting mediums for the studied MOX rod

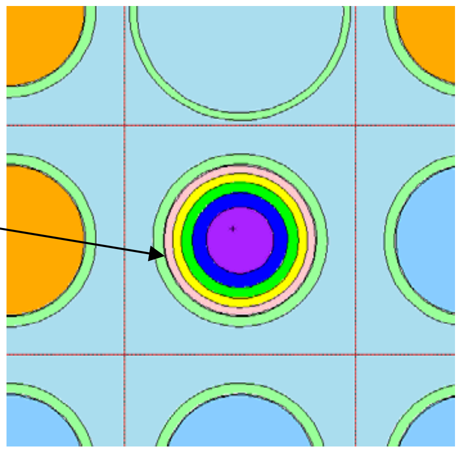
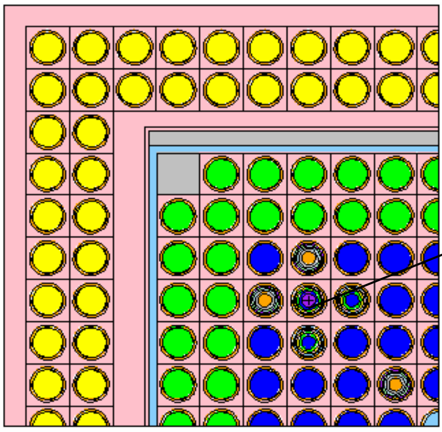
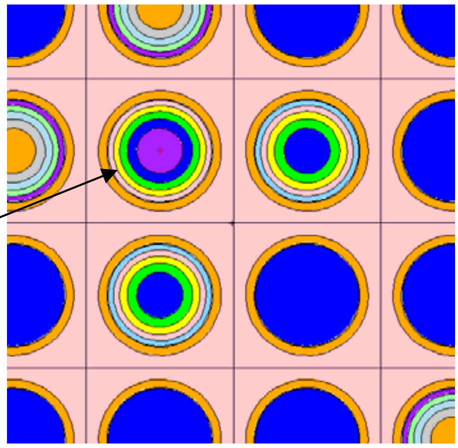


Figure3a: Quarter of GEDEON cluster with 24 depleting mediums

Figure3b: Five depleting mediums for the UOX-Gadolinium rod (+) and the burnup tracer rods





3.2 Modeling of the surrounding of the analyzed rod

The configuration of the cluster containing the rod of interest is completely heterogeneous. Depending on the asymptotic character of the spectrum around the rod, we retain for the study either a 3 X 3 rod cluster (UOX 2 to 5 cycles), or a quarter of an assembly (UOX 6 cycles and MOX 2 and 3 cycles) with reflection or translation boundary conditions, the implicit assumption being that during irradiation, the power distribution in the assembly is flat, in other words far from the peripheral or clustered zone of the core, leading to strong burnup gradients in the studied assembly.

3.3 Length of each time step

This is a very important parameter for the accuracy of the analysis since it sets the degree of reliability of the condensation of the cross-sections for ORIGEN2. The accuracy is thus inversely proportional to the length of the step. Following an analysis concerning the computing time required versus accuracy ratio, we set the MONTEBURNS step length at 1.0 GWd/T, except for the beginning of life where the formation of the major Fission Products (FP) (Xe135 and Sm149) imposes a more frequent actualization. We thus in general obtain 3 to 4 depletion steps between 0 and 1.0 GWd/T. In the exceptional case of rods with gadolinium, the length of the steps is about 0.13 GWd/T.

3.4 Convergence of MCNP4 calculations

After the depletion geometry and the length of burnup steps, the convergence of MCNP4 code is the third parameter which influences the accuracy of the HI concentration. The analysis showed that the treatment of 6000 histories (neutrons) per rod is satisfactory for the follow-up of the concentration, because a critical rod contains approximately 2400 fissions and 3600 captures (from 1 cm) for $\nu = 2.5$. These statistics are sufficient for the disappearance and production of the major HI (8 analyzed HI) although on the cluster, Kinf oscillates by 200 pcm approximately, i.e. 0.2% of fluctuation for the thermal flux, the main producer of fissions.

Tests carried out for higher convergences (more then 6000 histories per rod) did not give significant variations for the HI (< 0.3%). On the other hand, the tests carried out for less than 3000 histories/rod lead to a loss accuracy of the HI concentrations of about 1 %.

3.5 Importance fraction (IF)

The condensation of the cross-sections into 1 group (ORIGEN2) is activated according to the concentration of the isotope of interest and its contribution to either fissions or captures of the depleted medium. In general, the cross sections are re-condensed (from the reaction rates of MCNP4 calculation) if the atomic or mass densities or reactions rates (captures or fission) are higher than 10^{-5} of the corresponding total value of the medium. Preliminary tests carried out for 10^{-4} or 10^{-3} (reduced MONTEBURNS calculation time) showed small variations in the HI densities, obtained by indirect effect: whereas the significant studied HI have concentrations higher than 10^{-3}, the non re-condensed FP cross-sections can induce variations in their own concentration and thus on the burnup value indicated.

The retained value of 10^{-5} is asymptotic for the analyzed PWR rods (HI and FP burnup tracers).

3.6 Fission energy

This includes the kinetic energy of the FP, of n and γ prompts, of β and γ decay and radioactive capture. We set at 200 MeV the fission energy of isotope U235 for burnup lower than 60.0 GWd/T. The other isotopes are modeled from the energy set for U235 (for PU239 for example we obtain an energy of 208 MeV using MONTEBURNS). For a burnup higher than 60.0 GWd/T we set the fission energy of U235 at 202 MeV. This variation is induced by the drop in the kinf of the rod (Fissions/Captures ratio) and the concentration of the FP and radioactive actinides. This parameter directly affects the concentrations because it depends linearly on burnup and thus the consumption of the fissile isotopes and the production of Pu (proportional to the fluence).

3.7 Cross-section libraries

Our actual reference is the JEF2.2 libraries. We have cross-sections for 20 HI and 20 major FP. However, exact modeling (340 potentially up to date isotopes) requires the use of the minor FP and other actinides of the Endf-BVI evaluation. Thus all modeling (13 rods) is obtained starting from 40 JEF2.2 isotopes (HI+FP) which affects the reactivity and thus the spectrum, and from 300 isotopes (actinides+ minor FP) of Endf-BVI origin. A modeling (UOX rod-3 cycles) carried out completely by Endf-BVI is presented (§4.) in order to indicate the impact of the libraries.

The impact on Keff of limiting the isotopes in MCNP4 to the main 340 was evaluated at less than 0.1%, thus negligible compared to the total uncertainty.

The obtained sensitivities (§3.) are shown in table 1.

Table 1: Optimisation of the depletion parameters

Parameter	Standard values	No standard values	No std values Order of deviation (HI densities)
Convergence	6000 hist./rod	3000 hist./rod	1%
Depletion steps	1.0 GWd/T	2.0 GWd/t	1%
Geometry	Quarter of assembly	3x3 cluster	1%
Depleting mediums	Studied rod: 5	Studied rod: <3	<1%
Update of isotopes	$IF=10^{-5}$	$IF=10^{-3}$	1%

4. Calculation/Measurement comparisons

The key parameter for a good comparison is the exactitude of the energy produced for the studied rod (burnup). The energy released by the experiments is accompanied by an uncertainty of about 1% (UOX), which induces a more or less significant error according to the burnup obtained. For low burnup (less than 30.0 GWd/T) the U235 concentration is still significant but the concentrations of Pu239/Pu240/Pu241 are rather low and in ascending phase. On the other hand, for high burnup (> 60.0 GWd/T), the remaining amount of U235 is half of the amount of Pu239 produced (quasi asymptotic amount). Any error in burnup thus affects U235 much more that Pu239 expressed as a percentage of the C/M variation because the comparison is carried out on the remaining fraction of the isotope and not on the consumed fraction: for example between a burnup of 60.0 GWd/T and 71.0 GWd/T the remaining fraction of U235 is approximately 14% and 7% and the consumptions of the same isotope are 86 % and 93 % respectively. One notes that for very high burnup, the comparison of the remaining fraction of the HI in the process of disappearing becomes delicate and the C/M result is very sensitive to the degree of accuracy of the MONTEBURNS model with respect to burnup.

The comparisons on the 11 depleted rods in PWRs (without Gadolinium) gave variations in the fissile isotopes (U235, Pu239 and Pu241) of less than 3% on average (table 2), which is considered as satisfactory. However one can observe a systematic over-production of Pu239 which could be explained by U238 capture. A simulation with a U238 capture reduced by 1% shows a reduction in the positive variation for Pu239. The simulation was carried out on a UOX rod with 71.0 GWd/T.

An under-production of U236 can also be seen, which probably indicates that the capture of U235 is too low.

The comparison with GEDEON-1 (2 analyses) gives good C/M results for the isotopic evolution (table 2) and fission rates measured in the Gadolinium rods and their immediate neighbours.

On the two analyzed rods (disappeared poison fraction) we obtained variations of -2.5% and -1.0% for the Gd155 and Gd157 isotopes respectively. One thus observes for these two isotopes light under-capture. The burnup is indicated by the fissile isotopes U235 and Pu239, representative of very low burnup (low densities for Nd and Cs). The C/M deviations on the fission rate stay at less than 2% throughout depletion.

The differences obtained by using JEFF2.2 or ENDF_B6 for the heavy isotopes are in fact very slight for the fissile isotope concentrations (< 1%), and show a slightly higher reactivity for JEF2.2 of approximately 300 pcm throughout depletion.

The results obtained with the no standard options for an UOX rod are shown in table 3.

Table 2: C/M comparisons for PWR UOX and MOX fuel rods.

ISOTOPES	UOX 9 analyses < 71.0 GWd/t	MOX 2 analyses < 47.2 GWd/t	GEDEON-1 2 analyses < 6.34 GWd/t
U234	0.971	0.918	
U235	0.986	1.014	1.010
U236	0.957	0.987	0.980
PU238	0.908	0.965	
PU239	1.019	1.030	1.000
PU240	1.021	1.018	
PU241	0.996	1.000	
PU242	0.964	0.985	
Gd155			1.025
Gd157			1.010
No of depleted mediums	6 to 9	8	24

Table 3: C/M comparisons –No standard options

ISOTOPES	C/M (%) 5 rings 3 cycles* JEF2.2 IF=10^{-7}	C/M (%) 1 ring 3 cycles JEF2.2 IF=10^{-5}	C/M (%) 1 ring 3 cycles JEF2.2 IF =10^{-3}	C/M (%) 1 ring 3 cycles ENDF- BVI IF =10^{-3}
234U/238U	-1.6	-0.5	-0.8	-1.0
235U/238U	-0.9	-0.9	-0.9	-1.3
236U/238U	-4.2	-4.0	-4.1	-0.5
238Pu/238U	-10.5	-9.6	-10.5	-11.9
239Pu/238U	0.1	1.3	1.3	0.3
240Pu/U238	0.8	0.8	0.8	0.5
241Pu/U238	-2.5	-2.3	-1.9	-1.5
242Pu/U238	-6.6	-6.4	-6.4	-6.6

* UOX rod - burnup = 39.4 GWd/T

5. Uncertainties

5.1 Length of burnup steps

For fuels without gadolinium we retained a step of 1.0 GWd/T and for UOX rods with gadolinium 0.13 GWd/T. If, for the heavy isotopes, this splitting is largely sufficient, one can accept that for gadolinium this length of step is not optimal taking into consideration the rate of disappearance of the odd isotopes Gd155 and Gd157 between 0 and 6.34 GWd/T. We will thus retain for these two gadolinium isotopes an uncertainty of 1%.

5.2 Libraries

In general, data (cross sections and other data) are evaluated with 1% uncertainty. Nevertheless, this value reflects the static (BOL) impact on reactivity and not the cumulative impact after significant burnup. In addition, the qualification of the MCNP4/JEF2.2 showed that there is no systematic effect on reactivity (this can be explained by compensation of errors) but C/M variations for some isotopes such as U236 and Pu239 can indicate the sources of these compensations, in our case the isotopes U235 and U238. Referring to our argument on the remaining fraction of the fissile isotopes and taking account of the sensitivity of the reactivity of the rod at U235 and U238 concentration, one can conclude that this parameter is significant for the variations in density of the HI and the final reactivity.

Following a simulation starting from the Endf-BVI libraries (table 3), we estimate this uncertainty at 2% (between libraries) for the isotopes U235, Pu238, Pu239, Pu240, Pu241 and Pu242 and 4% for U236.

5.3 The yields of the FP burnup tracers and their capture

We will retain for our evaluation an uncertainty of 1%.

5.4 Burnup measurements

These are given with an accuracy of about 1%.

However the effect on the concentrations of the fissile isotopes is not linear. Whereas the concentration of Pu239 is quasi-stable during the 2nd half of irradiation, that of U235 is very sensitive: a variation of 1% in the energy produced induces a 4% variation in C/M, in particular for very high burnup (UOX rod, burnup=71.0 GWd/T).

We will retain for this parameter an uncertainty of 4% for U235 and only 2% for the other heavy isotopes.

5.5 Thermal conditions

The state point is relatively well known and in all cases is lower than 50°C for fuel and 5°C for water. The modification of the capture which results from this and the modification of the neutron spectrum can induce an effect of 2% on the concentrations of the heavy isotopes.

5.6 Overall uncertainty

Finally, after a quadratic combination (independent effects), we consider a total uncertainty of 5% for U235-U236, and 4% for the other HI, for high burnup (>50.0 GWd/T).
For a burn up lower than 50.0 GWd/T, the total uncertainty to be retained for any heavy isotope is 4% and 5% for U236.

6. Conclusion

The analysis of fuel irradiated by MONTEBURNS showed that the simulation carried out using 40 JEF2.2 isotopes (main HI+FP) and 300 Endf-BVI isotopes (other actinides and fission products) for the 13 irradiated rods is very satisfactory. The average C/M variations for the fissile isotopes (U235, Pu239 and Pu241) is less than 3% and for the significant even isotopes (U236, Pu240, Pu242) less than 5%.

The maximum uncertainty (calculation + MONTEBURNS options + libraries+ experiment) is 5% for U235-U236 and 4% for the other heavy isotopes (1σ). The basic components of uncertainty are the burnup, the libraries and the thermal condition of the fuel rod.

A "fast" scheme with a significant MONTEBURNS time saving is possible within the framework of the sensitivity studies. In this case, one can retain a single ring for the fuel rod, 2.0 GWd/T for the burnup step, 10^{-3} for the importance fraction and reduced MCNP4 convergence. Compared to the reference calculation, the time saving is of a factor of 20 approximately.

This work shows that MONTEBURNS is able to accurately model the depletion of UOX and MOX fuels up to 71.0 GWd/T and 47.2 GWd/T respectively. As the reference scheme depends on the continuous energy libraries used and on the exact representation of the real geometry only, it is also able to model any configuration representative of the future PWR, BWR, HTR and VHTR reactors with the same accuracy.

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