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DEPLETION CALCULATION BENCHMARK DEVOTED TO FUEL CYCLE ISSUES

Specification for Phase 1

JT00167269

English - Or. English

Specification for the Phase 1 of a Depletion Calculation Benchmark devoted to Fuel Cycles

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1 INTRODUCTION

In the past, many reactor system benchmarks have been done but only a few concerning the fuel cycle, particularly with MOx fuel. Nowadays there is an emphasis on reactor systems linked with the associated fuel cycle (Generation IV for example).

Benchmarks devoted to depletion calculations have already been undertaken but they were restricted to a specific issue of fuel cycle:

- Burnup credit benchmark (working party on nuclear criticality safety (WPNCS**)** [1]: the nuclide densities calculations focused mainly on the 15 most poisoning fission products and for a short cooling time (5 years)
- Benchmark on decay heat calculation: this benchmark focus on decay heat calculation due to 235 uranium fissions [2].

The proposed benchmark investigates a broader range of isotopes, physics quantities and fuel types. The objective is to compare existing depletion calculations obtained with various codes and data libraries (DARWIN/CESAR, FISPIN, FISPACT, SRAC, ORIGEN,..), applied to fuel and back-end cycle configurations : transport, reprocessing, interim storage and waste repository. We propose to focus on nuclide densities of the most important nuclides implied in fuel cycle: Actinides, Fission Products and Activation Products and also on associated fuel cycle quantities: masses, neutron emission rate and decay heat.

Detected discrepancies between participants will enable us to improve the calculation schemes (self-shielding, subdivisions in fuel or moderator, …), to improve the knowledge of burnup chains used in depletion calculations (maybe to recommend a chain for fuel cycle applications) and to improve the knowledge on nuclear data (capture cross-sections, branching ratio, fission yields, decay constants) involved in fuel cycle studies.

The following specification is devoted to the FIRST PHASE of the Benchmark. The aim of this phase is to constitute a reference case on an UOx fuel. We propose to use the experimental information given by Japanese Post Irradiation Experiment from the TAKAHAMA-3 PWR ; thus we can compare the calculation and experimental results for the major actinides and verify for well known isotopes how good our predictions are. The list of available experimental results and associated uncertainties are given in Appendix A.

This experiment has been already used in French nuclear data studies [3] and it was shown that the trends given by this experiment are consistent with the trends given by spent fuel experiments performed in France [4]. This experiment was also used by JAERI for the validation of the SWAT burnup code system [5].

2 SPECIFICATION

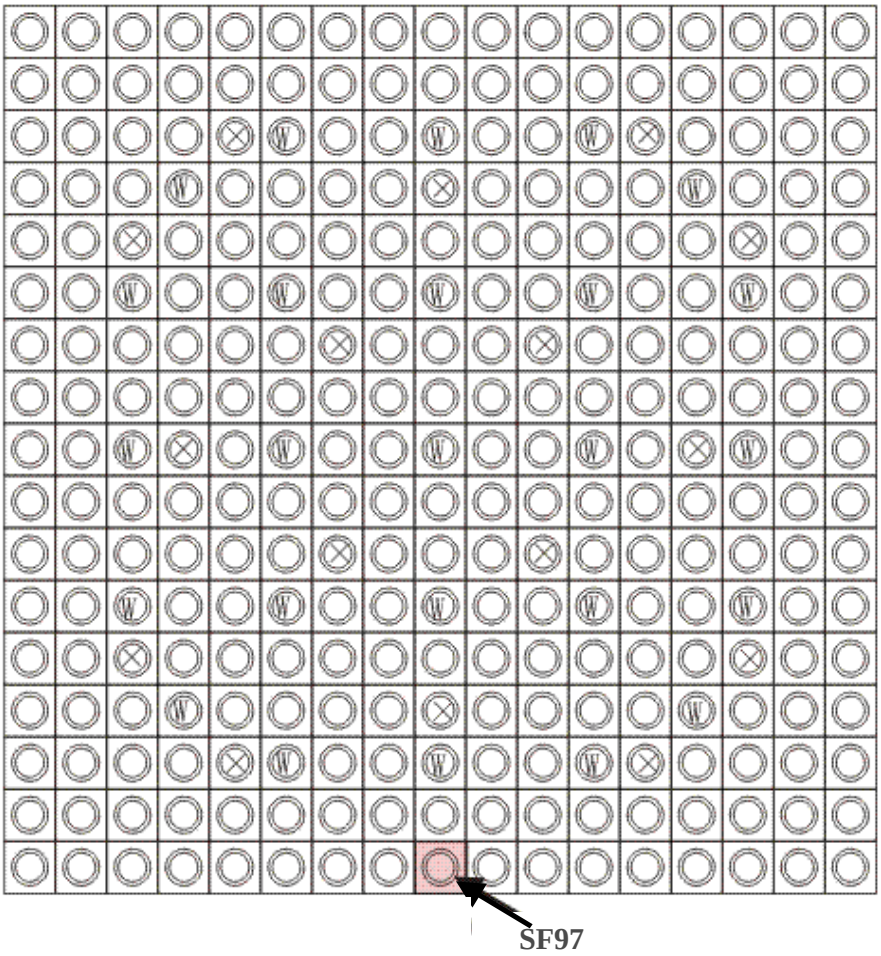
The specification of the benchmark is based on the data included in the SFCOMPO database originally developed at JAERI and now maintained at the NEA databank [6], [7], [8].

2.1 Outline of the TAKAHAMA experiment

TAKAHAMA-3 is a 17x17 PWR operated by Kansai Electric Power Company in Japan. The PIE was conducted under the auspices of Science and Technology Agency of Japan. From two fuel assemblies, named NT3G23 and NT3G24, 16 samples were taken and isotopic composition was measured for irradiated UO2 and UO2-Gd2O3 fuel.

We propose to make two calculations : a simple **cell calculation** or/and an **assembly calculation** where the analysed sample is explicitly described.

For the assembly calculation, the studied sample, named SF97, is coming from a UO2 spent fuel pin located in the peripheral row of the assembly. This assembly is the NT3G24 assembly loaded with 248 UO2 fuel pins , 4.1%wt U235 enriched, 16 UO2-GD2O3 pins (2.6% wt U235 and 6% wt Gd) and 25 water holes. However, the SFCOMPO database is not fully complete and additional assumptions have to be made concerning the experimental conditions (water gap dimension, temperature, boron contents) for the cell and assembly calculations.



W : Position of Control Rod (fill with coolant)
X : Gd Fuel Rod

Figure 1 : Position of the SF97 spent fuel in the NT3G24 assembly

The fuel pin has been cut in many sections (Figure 2) ; we selected the SF97-4 sample located at core mid-height.

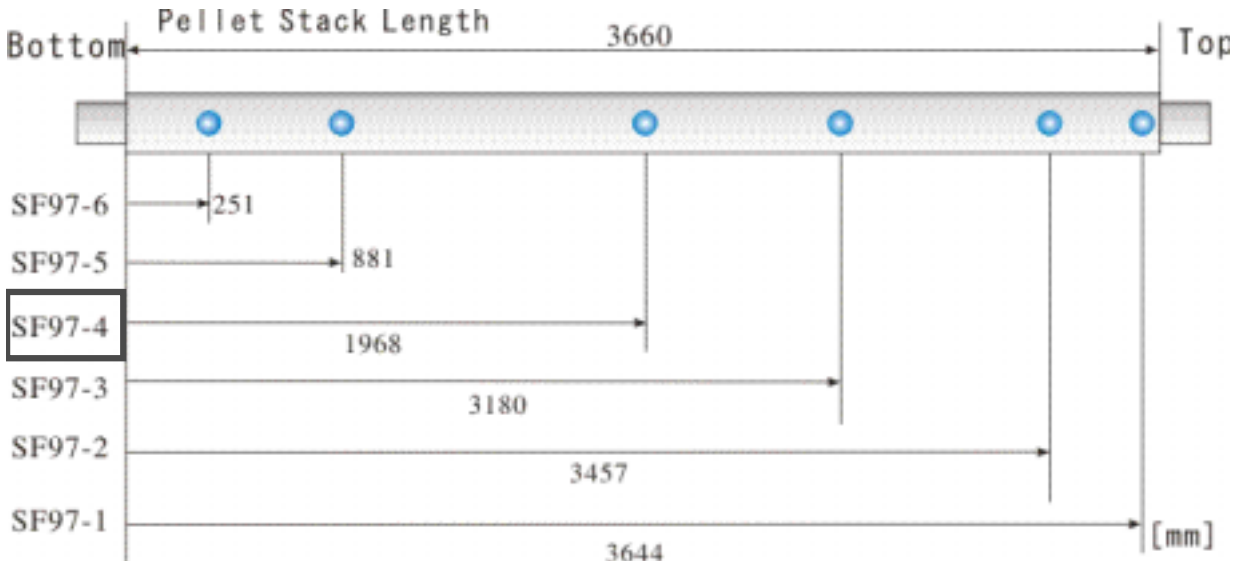


Figure 2 : Position of the SF97 spent fuel in the NT3G24 assembly

2.2 Geometry description

2.2.1 Cell calculation

The pincell model assumes an equivalent volume ratio of fuel to moderator with the whole fuel assembly, including the water gap. The Figure 3 shows the geometry and associated dimensions for this model.

The proposed boundary condition is the reflection (infinite lattice).

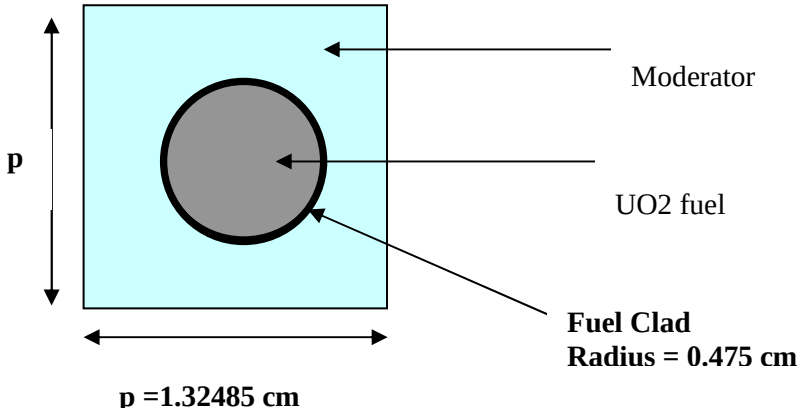


Figure 3 : Cell calculation geometry

The value of the equivalent cell radius is 0.7475 cm.

2.2.2 Assembly calculation

We propose to represent the UOx assembly, as shown in Figure 1, with reflective boundary conditions.

The assembly geometry relates to a typical 17 x 17 PWR fuel assembly, as detailed below and on Figure 4 to Figure 6.

Fuel Pin Pitch: 1.265 cm
Fuel Pin Radius: 0.475 cm
Fuel Pellet Radius: 0.4025 cm
Cladding Thickness: 0.0725 cm (no air gap between fuel and cladding)

The 24 guide tubes and 1 instrument tube shall be modelled as water filled zircalloy tubes with the following dimensions (see figure 6):

Outer Radius: 0.613 cm
Inner Radius: 0.573 cm

The half water gap is 0.0538 cm thick.

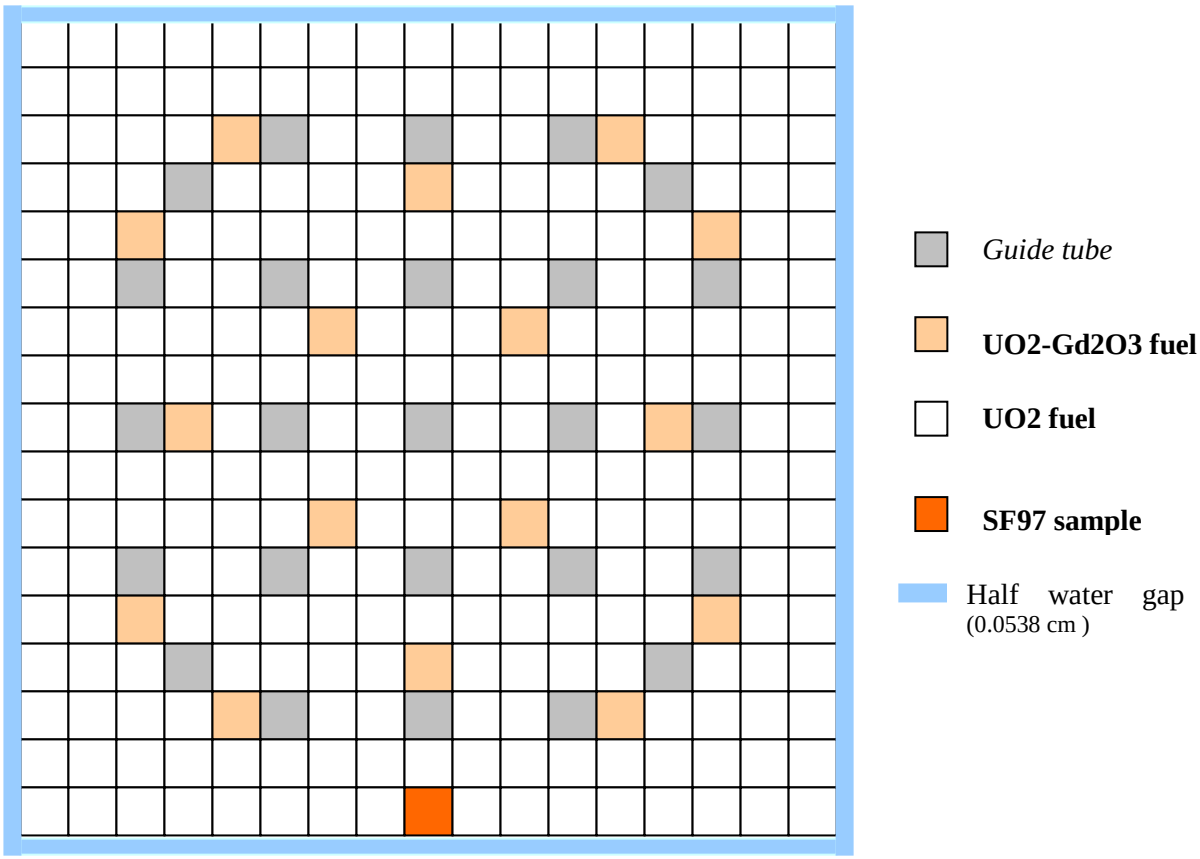


Figure 4 : Assembly geometry

The geometry of the various cells is defined in Figure 5 and Figure 6.

UO2 FUEL CELL or UO2-Gd2O3 FUEL CELL

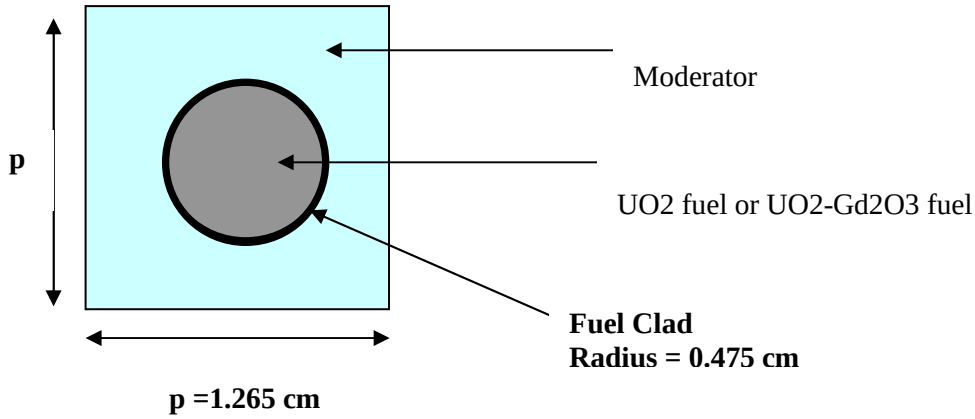


Figure 5 : Fuel cell geometry for the assembly calculation

GUIDE TUBE CELL

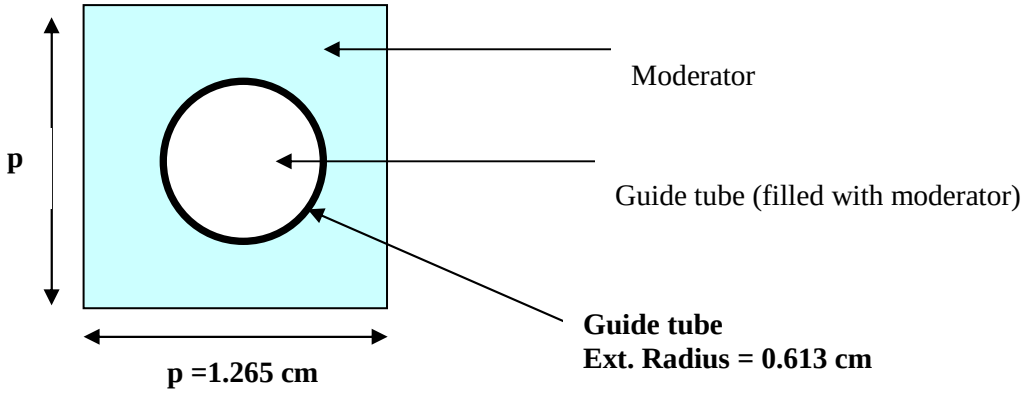


Figure 6 : Guide tube geometry for the assembly calculation

2.3 UO2 fuel composition (densities in atom/barn.cm)

The ***UO2 fuel*** has an initial enrichment of 4.1 wt % 235U. The composition to be used in the benchmark is presented in Table 1.

Table 1: Initial Composition for UO2 Fuel

Nuclide	Atoms/barn.cm
U-234	9.1361E-06
U-235	9.3472E-04
U-238	2.1523E-02
O	4.4935E-02

This fuel composition is suitable for both the cell and the assembly calculation.

2.4 UO2-Gd2O3 fuel composition (densities in atom/barn.cm)

The ***UO2-Gd2O3 fuel*** is composed of 2.6% wt U235 and 6% wt Gd. The composition is presented in Table 2 and must be used for the assembly calculation.

Table 2: Initial Composition for UO2-Gd2O3 Fuel

Nuclide	Atoms/barn.cm
U-234	4.2940E-06
U-235	5.6226E-04
U-238	2.0549E-02
Gd-154	4.6173E-05
Gd-155	2.9711E-04
Gd-156	4.1355E-04
Gd-157	3.1518E-04
Gd-158	4.9786E-04
Gd-160	4.3764E-04
O	4.5243E-02

2.5 Non-fissile material composition (densities in atom/barn.cm)

For the purpose of the benchmark exercise, these non-fissile materials should be modelled as specified in Table 3 to 5. A reduced density zircalloy has been used for the fuel pin cladding to take account of the air gap between the fuel and cladding.

The guide tubes should be modelled using the composition given in Table 4.

Table 3: Fuel clad Composition

Nuclide	Atoms/barn.cm
Fe (natural)	1.3225E-04
Cr (natural)	6.7643E-05
Zr (natural)	3.8310E-02

Table 4: Guide Tube Composition

Nuclide	Atoms/barn.cm
Fe (natural)	1.4838E-04
Cr (natural)	7.5891E-05
Zr (natural)	4.2982E-02

Table 5: Coolant/Moderator Composition

Nuclide	Atoms/barn.cm
H	4.8132E-02
O	2.4066E-02
B10	3.6487E-06
B11	1.4686E-05

These compositions are suitable for both the cell and the assembly calculation.

2.6 Impurities content for UOx fuels

In this benchmark, we propose to compare the activation products masses coming from initial impurities. The proposed values for the impurities content are specified in Table 6.

Table 6: Initial fuel impurities (atomes/tones Heavy Metal lnitial (tHMI))

H1	2.0491E+23
H2	3.0741E+19
B10	6.2931E+21
B11	2.5331E+22
C12	5.6257E+24
C13	6.2571E+22
N14	4.8610E+23
N15	1.7857E+21
Cl35	3.6473E+23
Cl37	1.1663E+23
Ca40	4.9532E+24
Ca42	3.3058E+22
Ca43	6.8978E+21
Ca44	1.0658E+23
Ca46	2.0438E+20
Ca48	9.5547E+21
Fe54	3.5435E+23
Fe56	5.6040E+24
Fe57	1.3441E+23
Fe58	1.7106E+22
Co59	1.3896E+23
Ni58	2.3817E+24
Ni60	9.1052E+23
Ni61	3.9421E+22
Ni62	1.2524E+23
Ni64	3.1746E+22
Cu63	7.4286E+23
Cu65	3.3110E+23
Zr90	3.8493E+23
Zr91	8.3944E+22
Zr92	1.2831E+23
Zr94	1.3003E+23
Zr96	2.0949E+22

Nb93	7.3465E+23
Mo92	3.1677E+23
Mo94	1.9745E+23
Mo95	3.3982E+23
Mo96	3.5604E+23
Mo97	2.0385E+23
Mo98	5.1507E+23
Mo100	2.0556E+23
Sn112	5.5781E+21
Sn114	3.7379E+21
Sn115	2.0702E+21
Sn116	8.3557E+22
Sn117	4.4165E+22
Sn118	1.3928E+23
Sn119	4.9341E+22
Sn120	1.8741E+23
Sn122	2.6626E+22
Sn124	3.3296E+22

REMARK : Do not forget to take into account the oxygen isotopes in your activation calculation.

2.7 Other Parameters for depletion calculation

Fuel temperature: 900 K
Clad temperature: 600 K
Moderator temperature: 576 K

2.8 Irradiation histories

The assembly was irradiated 3 cycles and the SF97 experimental fuel pin reached an average burnup of roughly 46 GWd/t. Table 7 presents the proposed irradiation cycles and the associated power to be modelled.

Table 7: Irradiation history

Start	Stop	Days	Status	Power (W/gU)
26/01/90	15/02/91	385	Full power	38.6
15/02/91	14/05/91	88	Downtime	0
14/05/91	19/06/92	402	Full power	38.6
19/06/92	20/08/92	62	Downtime	0
20/08/92	30/09/93	406	Full power	38.6

2.9 Cooling:

The results are to be compared at discharge (zero cooling), 5, 50, 100 and 300 years cooling.

3 NUCLIDES AND ADDITIONAL QUANTITIES REQUIRED FOR COMPARISON

Please forward the results by electronic mail to Dr Bénédicte ROQUE at CEA/CADARACHE **benedicte.roque@cea.fr**

The required quantities are :

- Masses of the nuclides specified in the table above in **grams/tHMl**
- Neutron emission : (alpha,n) emission, spontaneous fission and total emission in **neutrons/seconde/tHMl**
- Decay heat : alpha, beta and gamma decay heat and total decay heat in **Watts/tHMl**

The required quantities shall be forwarded using the following tables (you can copy the Tables in Microsoft Excel and send it as an attached file to the e-mail).

Please do not forget to specify the geometry (cell or assembly calculation) you have used.

Table 8: Masses of activation products

MASSES OF ACTIVATION PRODUCTS (g/tHMI)					
Nuclide	**Discharge**	**5 years**	**50 years**	**100 years**	**300 years**
Cl36					
Ca41					
Mn53					
Mn54					
Fe55					
Fe60					
Co60					
Ni59					
Ni63					
Mo93					

Some nuclides are produced both by fission reaction and activation reaction. We propose to evaluate separately the two contributions in the table above. ***If your fuel cycle code does not separate the two contributions, please replace the two lines FP and AP in the table above by only one line with FP+AP.***

Table 9: Masses of fission and activation products

MASSES OF FISSION AND ACTIVATION PRODUCTS (g/ tHMI)						
nuclide		**Discharge**	**5 years**	**50 years**	**100 years**	**300 years**
H3	**FP (fission)**					
	AP (activation)					
Be10	**FP**					
	AP					
C14	**FP**					
	AP					
Zr93	**FP**					
	AP					
Nb94	**FP**					
	AP					
Sn119m	**FP**					
	AP					
Sn121m	**FP**					
	AP					
Sn126	**FP**					
	AP					
Sb125	**FP**					
	AP					

Table 10 : Masses of fission products

MASSES OF FISSION PRODUCTS (g/ tHMI)					
Nuclide	**Discharge**	**5 years**	**50 years**	**100 years**	**300 years**
Se79					
Kr85					
Rb85					
Rb87					
Sr88					
Sr90					
Nb93m					
Mo95					
Mo97					
Tc99					
Ru101					
Ru106					
Rh103					
Pd107					
Ag108m					
Ag109					
Ag110m					
I127					
I129					

Xe130					
Xe131					
Xe132					
Xe134					
Xe136					
Cs133					
Cs134					
Cs135					
Cs137					
Ba136					
Ba138					
La139					
Ce140					
Ce144					
Nd142					
Nd143					
Nd144					
Nd145					
Nd146					
Nd148					
Nd150					
Pm147					
Sm146					
Sm147					
Sm148					
Sm149					
Sm150					
Sm151					
Sm152					
Sm154					
Eu153					
Eu154					
Eu155					
Gd154					
Gd155					
Gd156					
Ho166m					

Table 11 : Masses of actinides

MASSES OF ACTINIDES (g/ tHMI)					
Nuclide	**Discharge**	**5 years**	**50 years**	**100 years**	**300 years**
U232					
U233					
U234					
U235					
U236					
U238					
Np236					
Np237					
Pu236					
Pu238					
Pu239					
Pu240					
Pu241					
Pu242					
Pu243					
Pu244					
Am241					
Am242m					
Am243					
Cm242					
Cm243					
Cm244					
Cm245					
Cm246					
Cm247					
Cm248					
Ra226					
Ra228					
Ac227					
Th229					
Th230					
Th232					
Cf252					

Table 12 : Neutron emission rate

NEUTRON EMISSION RATE (neutrons/s/ tHMI)					
	Discharge	**5 years**	**50 years**	**100 years**	**300 years**
(α,n) emission rate					
Spontaneous Fission emission rate					
Total emission rate					

Table 13 : Decay heat

DECAY HEAT (Watts/ tHMI)					
	Discharge	**5 years**	**50 years**	**100 years**	**300 years**
Alpha Decay Heat					
Beta Decay Heat					
Gamma Decay Heat					
Total Decay Heat					

4 OPTIONAL CALCULATIONS

Additional but optional calculations are suggested; they concern sensitivity calculations linked to the assumptions made on irradiation parameters.

These assumptions concern :

1) The half water gap thickness

The studied fuel rod is near the water gap; therefore the sensitivity of the fuel inventory to this parameter needs to be investigated. We propose to evaluate the sensitivity with two calculations :

- an assembly calculation with **no** water blade
- an assembly calculation considering that **the uncertainty** on the water blade thickness is **45%** (the new value of the water gap is then 0.078 cm)

2) The boron content

Two assumptions are made in the calculation. The first one is that a mean value is used during all the irradiation and the second one is the value itself. Concerning the first assumption, studies [5] and [9] have shown that considering a constant boron content does not induce significant bias on the studied isotopes.

We therefore propose to focus on the second assumption. In the benchmark, it is suggested to use a mean value of 456 ppm; this is the value usually used in French calculations. The reference [8] gives a detailed boron history for the 5, 6 and 7 cycles of irradiation but no information for the previous cycles. The calculation of a mean value with these data gives a value of 484 ppm.

We suggest to use **an uncertainty of 10%** on the mean value of boron content in order to evaluate the sensitivity of fuel inventory to this parameter.

The new concentration of the moderator, corresponding to this uncertainty, is given in Table 14:

Table 14 : Moderator concentration for sensitivity study on boron content

Nuclide	Atoms/barn.cm
H	4.8126E-02
O	2.4063E-02
B10	4.0141E-06
B11	1.6157E-05

3) The fuel and moderator-coolant temperature

It has been shown that a variation in the **cladding temperature** has no influence on the evolution of the isotopic inventory [9]. Therefore no sensitivity studies are needed for this parameter.

The **fuel temperature** is an important parameter in fuel inventory prediction [9]. However, a variation of 50°C in the fuel temperature leads to a degree of uncertainty of about 1% at 60 GWd/t for 239Pu. For the purpose of the benchmark we propose to assume that the bias generated by this parameter in negligible.

The **temperature** variation of the **moderator** results both in a thermal spectrum shift and in a variation in density. The isotopes for which the fuel inventory is 'deviated' are mainly 239Pu and 241Pu.

The temperature for the studied sample is determined assuming that the increase of temperature is proportional to the integrated power in the axial direction and that the axial power distribution has a cosine shape. Therefore the calculation of moderator-coolant temperature, at the height of the sample, depends on the difference ΔT between the inlet and outlet temperature of the core and on the precise knowledge of the sample height. The information given in reference [8] indicates ΔT= 37°C and a sample height of 1968 mm (the thickness of the dissolved pellet is 0.5 mm). We propose to use, for sensitivities calculation, an uncertainty of 5°C for ΔT and to assume that the uncertainty on the sample height is negligible ; this involved an uncertainty on the moderator coolant temperature of 3°C leading to the concentration presented in Table 15 :

Table 15 : Moderator concentration for sensitivity study on temperature moderator

Nuclide	Atoms/barn.cm
H	4.8126E-02
O	2.4063E-02
B10	4.0141E-06
B11	1.61573E-05

4) The power history

The benchmark specification proposes to use a constant power irradiation of 38.6 W/g. This assumption leads to bias for isotopes depending on the power history such as Xe135, Sm149 and also for isotopes strongly depending on the final burnup value (isotopes of the end of the depletion chain such as Pu242).

In order to evaluate the sensitivity to this parameters we suggest two calculations.

The first one uses a mean value of the specific power for each cycle. The values were calculated using the reference [8] ; the value for the third cycle is adjusted in order to reach the same burnup as the one used in the benchmark. The proposed power history is the following :

Table 16 : Detailed power history for sensitivity calculation

Start	Stop	Days	Status	Power (W/gU)
26/01/90	15/02/91	385	Full power	39.26
15/02/91	14/05/91	88	Downtime	0
14/05/91	19/06/92	402	Full power	41.86
19/06/92	20/08/92	62	Downtime	0
20/08/92	30/09/93	406	Full power	34.75

The second study, devoted to evaluate the sensitivity of the irradiated sample to the final burnup, proposes to perform a calculation with a constant power value of 39.4 W/g leading to an increase in the burnup of roughly 2%. The corresponding irradiation history is :

Table 17 : New power value for sensitivity calculations

Start	Stop	Days	Status	Power (W/gU)
26/01/90	15/02/91	385	Full power	39.6
15/02/91	14/05/91	88	Downtime	0
14/05/91	19/06/92	402	Full power	39.6
19/06/92	20/08/92	62	Downtime	0
20/08/92	30/09/93	406	Full power	39.6

5 OTHER REQUESTED INFORMATION

Please, describe your analysis environment. The description should include:

Institute and Country,
Participants,
Neutron data library,
Neutron data processing code or method,
Neutron energy groups,
Description of your code system,
Geometry modelling,
Omitted nuclides if any,
Omitted cases if any.

6 COMPLEMENTARY INFORMATION

After the results collection and in case of high discrepancies between participants, complementary data will be asked such as reaction rates, decay data used in depletion chain, detailed depletion chain, fission yields, branching ratio.

7 SCHEDULE

February 2004 :	Distribution of draft specification PHASE 1 UOx fuel
March 2004 :	Comments on the specification PHASE-1
End of June 2004 :	Distribution of the final specification PHASE-1
End of August 2004 :	Gathering of results from all participants by CEA
September 2004 :	Presentation of the results and first analyse
September 2004:	Distribution of draft specification Phase-II –MOx fuel calculation

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[9] *Qualification of the APOLLO2 Assembly code using PWR-UO2 isotopics assays. The importance of Irradiation history and thermomechanics on Fuel inventory prediction.* Chabert C. Santamarina A., Dorel R., Biron D. Poinot-Salanon C. Int. Conf. PHYSOR 2000, Pittsburgh, May 7-12 2000

APPENDIX A : List of available chemical results in SFCOMP and associated chemical analysis uncertainties

U234	1 %	determined by Isotopic Dilution Mass spectrometry
U235	0.1 %	
U236	2 %	
U238	0.1 %	
Pu238	0.5 %	
Pu239	0.3 %	
Pu240	0.3 %	
Pu241	0.3 %	
Pu242	0.3 %	
Np237	10 %	determined by alpha-ray measurement
Am241	2 %	determined by alpha and mass spectrometry
Am242m	10 %	
Am243	0.5 %	
Cm242	10 %	
Cm243	2 %	
Cm244	2 %	
Cm245	2 %	
Cm246	0.5 %	
Cm247	10 %	
Nd143	0.1 %	determined by Isotopic Dilution Mass spectrometry
Nd144	0.1 %	
Nd145	0.1 %	
Nd146	0.1 %	
Nd148	0.1 %	
Nd150	0.1 %	
Cs137	3 %	determined by gamma-ray spectrometry
Cs134	3 %	
Eu154	3 %	
Ce144	10 %	
Sb125	10 %	
Ru106	5 %	
Sm147	0.1 %	determined by Isotopic Dilution Mass spectrometry
Sm148	0.1 %	
Sm149	0.1 %	
Sm150	0.1%	
Sm151	0.1 %	
Sm152	0.1 %	
Sm154	0.1 %	