Problem Specification for the OECD/NEANSC Burnup Credit Benchmark Phase IV-B : Mixed Oxide (MOX) Fuels

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1. Introduction

Since 1991, the criticality working group of the NEANSC (formerly the NEACRP) has been investigating the methods and data associated with the calculation of burnup credit in criticality safety assessments. During this period, consideration has been given to uranium oxide fuels in both Pressurised Water and Boiling Water Reactors (PWRs and BWRs). These benchmark exercises, denoted as Phases I to III, have covered the calculation of fuel inventory and the calculation of reactivity in storage array and transport flask configurations. The international consensus approach to the benchmarks adopted by the working group generates a great deal of confidence in the assessment methods. Participation in these exercises has produced useful data and a deeper understanding of the issues associated with the calculation of burnup credit.

The next challenge for the burnup credit method lies in its application to mixed oxide (MOX) fuels, i.e. fuel containing a mixture of uranium and plutonium oxides. A comprehensive MOX benchmark study would contain all of the elements of the previous phases, but with the added difficulties associated with the non-unique specification of MOX fuels and the manner in which they would be utilised within existing thermal reactor designs. The definition of a universally attractive benchmark exercise is further complicated by the different incentives for adopting a MOX fuel strategy amongst the member countries of the group participants.

An initial benchmark exercise for MOX fuels has recently been undertaken by the burnup credit working group established by the newly-formed OECD/NEANSC criticality working party (Reference 1). This exercise, which was referred to as Phase IV-A, considered the calculation of infinite PWR fuel pincell reactivity for fresh and irradiated MOX fuels. The benchmark was based upon fuel compositions provided by the benchmark organisers, which were derived using a simplified MOX only representation of the core. This initial exercise considered the impact of different initial plutonium isotopic compositions in the MOX fuel, associated with first generation MOX, weapons plutonium disposition and multiple MOX recycle.

The next step in the proposed benchmark programme is to address the calculation of irradiated MOX fuel compositions. The Phase IV-B benchmark specification proposed here is a first step in comparing methods for the calculation of isotopic inventories for the nuclides of interest to MOX fuel burnup credit. The benchmark participants are requested to perform inventory calculations for two MOX fuel cases appropriate to weapons plutonium disposition and first recycle MOX, using three modelling representations for the reactor core.

2. Parameters and Case Numbers

The spent fuel inventory is required for a total of 6 cases, covering two initial MOX fuel compositions and three calculational models. Participants are requested to provide the inventory of the major actinides and fission products, along with the curium isotopes for specified fuel pins within the MOX assembly.

In the context of this benchmark exercise, the term ‘major actinides’ is taken to represent the following nuclides:

> U-234, U-235, U-236, U-238, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Np-237, Am-241 and Am-243,

consistent with previous benchmark problems.

The term ‘all actinides’ refers to the major actinides plus Am-242^{m} and the specified curium isotopes of Cm-242, Cm-243, Cm-244, Cm-245.

The fission products considered in this exercise are the 15 major fission product absorbers addressed in previous benchmarks, namely:

> Mo-95, Tc-99, Ru-101, Rh-103, Ag-109, Cs-133, Nd-143, Nd-145, Sm-147, Sm-149, Sm-150, Sm-151, Sm-152, Eu-153 and Gd-155.

The selected parameters and case numbers are shown in Table 1.

3. MOX Fuel Compositions

The two initial MOX compositions selected for this study were chosen to represent the range of potential interest in MOX fuels within the working group. The proposed MOX fuels are representative of realistic MOX fuels that would be irradiated in a mixed UO_2-MOX PWR core, alongside UO_2 fuel assemblies with an initial enrichment of 4.3 w/o U-235/U. These MOX fuels consist of:

i. a reference MOX fuel case, appropriate to a typical plutonium vector for material derived from the reprocessing of thermal reactor UO_2 fuels, often referred to as ‘first generation’ MOX, referred to as MOX Case A;

ii. a MOX fuel case appropriate to the disposition of weapons plutonium in MOX, referred to as MOX Case B.

The plutonium isotopic compositions for the different MOX fuel cases are presented in Table 2. Note that the plutonium vector for the reference case, Case A, is different to that adopted in the Phase IV-A exercise. The weapons disposition case plutonium vector is consistent with that used in the Phase IV-A specification. In all cases, the uranium oxide component of the MOX is assumed to be depleted, with a uranium-235 content of 0.25 w/o U-235/U, which is typical of current MOX fuel fabrication. The uranium isotopic composition is shown in Table 3.

Due to the irradiation of the MOX fuel alongside UO_2 fuel assemblies, the MOX fuel design adopts an enrichment pinmap to counter power peaking in the outer MOX pins adjacent to the UO_2 fuel. The MOX fuel assembly geometry adopted for the Phase IV-B exercise is a 17 x 17 PWR fuel assembly with three enrichment zones, as shown in Figure 2. The initial MOX fuel enrichments for these zones for the two MOX fuel cases are shown in Tables 4 and 5.

The pre-irradiation fuel compositions for the two MOX fuel assemblies are shown in Tables 6 and 7 for the MOX fuel cases A and B respectively.

4. <u>Geometry Data</u>

Three calculational models are requested for the Phase IV-B exercise, covering;

i. a supercell calculation for a MOX assembly together with three UO_2 fuel assemblies, as shown in Figure 1, with translational boundary conditions;

ii. a MOX-only core representation, as shown by Figure 2, with reflective boundary conditions;

iii. a simple MOX pincell calculation, using the average MOX fuel composition, with pincell geometry that conserves the fuel-to-moderator ratio of the whole assembly in the previous calculations, ie accounting for 25 guide or instrument tube positions, as shown in Figure 3, with reflective boundary conditions.

The assembly geometry relates to a typical 17 x 17 PWR fuel assembly, as detailed below.

Fuel Pin Pitch:	1.26 cm
Fuel Pin Radius:	0.475 cm
Fuel Pellet Radius:	0.410 cm
Cladding Thickness:	0.065 cm (no airgap between fuel and cladding)

The assembly channel box or water buffer should not be modelled for the above calculations. In particular, the pitch between any two adjacent fuel pins should be constant across the entire supercell, with no variation across the cell boundaries.

The 24 guide tubes and 1 instrument tube shall be modelled as water filled zircalloy tubes with the following dimensions -:

Outer Radius:	0.613 cm
Inner Radius:	0.571 cm
Wall Thickness:	0.042 cm

For the simplified MOX pincell inventory calculations, the pin pitch should be modelled as 1.3127cm.

5. Non-Fissile Material Data

The non-fissile materials are as follows:

Cladding:	Zircalloy-2
Guide Tubes:	Zircalloy-2
Coolant/Moderator:	Light Water, 600 ppm Boron

For the purpose of the benchmark exercise, these materials should be modelled as specified in Table 8. A reduced density zircalloy has been specified for the fuel pin cladding to take account of the air gap between the fuel and cladding. For simplicity, the guide tubes should also be modelled using this reduced density zircalloy composition.

6. UO_2 Fuel Compositions

For the supercell calculations, the adjacent UO_2 fuel assemblies have an initial enrichment of 4.3 w/o U-235/U. The composition of the UO_2 fuel is presented in Table 9.

7. Irradiation Histories

In order to attain a sensible comparison of results, the requested calculations should be performed to attain a constant target burnup for the MOX fuel assembly of 48GWd/teHM. For the supercell calculations it may be necessary to be perform a number of iterations of the calculation to produce the required MOX fuel assembly burnup. The MOX fuel assembly is irradiated over three operating cycles, as shown below.

Cycle 1:	420 days full power, EOC burnup of MOX = 16GWd/teHM
Downtime:	30 days
Cycle 2:	420 days full power, EOC burnup of MOX = 32GWd/teHM
Downtime:	30 days
Cycle 3:	420 days full power, EOC burnup of MOX = 48GWd/teHM
Cooling:	0 years, 5 years

For the supercell calculations, the power of the four-assembly cell should be set to attain the target burnup of the MOX assembly.

8. Material Temperatures

Fuel Temperature:	900K
Cladding Temperature:	620K
Coolant/Moderator Temperature:	575K

9. Specified Format for Submission of Results

The results should be submitted via e-mail to the benchmark organisers, using the address shown on the front page of this specification. In order to facilitate the data manipulation, the participants are requested to submit their results in the following format:

1	Date
2	Institute
3	Contact Person
4	E-mail Address or Telefax Number of the Contact Person
5	Computer Code
6	* Case 1 *
7	Nuclide Density of U-234 for EOC1, EOC2, EOC3, 5 Years Cooling
8	Nuclide Density of U-235 for EOC1, EOC2, EOC3, 5 Years Cooling
9	Nuclide Density of U-236 for EOC1, EOC2, EOC3, 5 Years Cooling
10	Nuclide Density of U-238 for EOC1, EOC2, EOC3, 5 Years Cooling
11	Nuclide Density of Pu-238 for EOC1, EOC2, EOC3, 5 Years Cooling
12	Nuclide Density of Pu-239 for EOC1, EOC2, EOC3, 5 Years Cooling
13	Nuclide Density of Pu-240 for EOC1, EOC2, EOC3, 5 Years Cooling
14	Nuclide Density of Pu-241 for EOC1, EOC2, EOC3, 5 Years Cooling
15	Nuclide Density of Pu-242 for EOC1, EOC2, EOC3, 5 Years Cooling
16	Nuclide Density of Np-237 for EOC1, EOC2, EOC3, 5 Years Cooling
17	Nuclide Density of Am-241 for EOC1, EOC2, EOC3, 5 Years Cooling
18	Nuclide Density of Am-242m for EOC1, EOC2, EOC3, 5 Years Cooling
19	Nuclide Density of Am-243 for EOC1, EOC2, EOC3, 5 Years Cooling
20	Nuclide Density of Cm-242 for EOC1, EOC2, EOC3, 5 Years Cooling
21	Nuclide Density of Cm-243 for EOC1, EOC2, EOC3, 5 Years Cooling
22	Nuclide Density of Cm-244 for EOC1, EOC2, EOC3, 5 Years Cooling
23	Nuclide Density of Cm-245 for EOC1, EOC2, EOC3, 5 Years Cooling
24	Nuclide Density of Mo-95 for EOC1, EOC2, EOC3, 5 Years Cooling
25	Nuclide Density of Tc-99 for EOC1, EOC2, EOC3, 5 Years Cooling
26	Nuclide Density of Ru-101 for EOC1, EOC2, EOC3, 5 Years Cooling
27	Nuclide Density of Rh-103 for EOC1, EOC2, EOC3, 5 Years Cooling
28	Nuclide Density of Ag-109 for EOC1, EOC2, EOC3, 5 Years Cooling
29	Nuclide Density of Cs-133 for EOC1, EOC2, EOC3, 5 Years Cooling
30	Nuclide Density of Nd-143 for EOC1, EOC2, EOC3, 5 Years Cooling

31	Nuclide Density of Nd-145 for EOC1, EOC2, EOC3, 5 Years Cooling
32	Nuclide Density of Sm-147 for EOC1, EOC2, EOC3, 5 Years Cooling
33	Nuclide Density of Sm-149 for EOC1, EOC2, EOC3, 5 Years Cooling
34	Nuclide Density of Sm-150 for EOC1, EOC2, EOC3, 5 Years Cooling
35	Nuclide Density of Sm-151 for EOC1, EOC2, EOC3, 5 Years Cooling
36	Nuclide Density of Sm-152 for EOC1, EOC2, EOC3, 5 Years Cooling
37	Nuclide Density of Eu-153 for EOC1, EOC2, EOC3, 5 Years Cooling
38	Nuclide Density of Gd-155 for EOC1, EOC2, EOC3, 5 Years Cooling
39	In-core k-infinity at EOC1, EOC2, EOC3, 5 Years Cooling
40	Average burnup (GWd/teHM) of pin types 1, 2, 3
41	* Case 2 *
42 to 75	As for items 7 to 40
76	* Case 3 *
77 to 110	As for items 7 to 40
111	* Case 4 *
112 to 145	As for items 7 to 40
146	* Case 5 *
147 to 179	As for items 7 to 39
180	* Case 6 *
181 to 213	As for items 7 to 39
214	Please Describe Your Analysis Environment Here. It will be Included in the Phase IV-B Report. 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 or Substituted Nuclides (if any), Employed Convergence Limits etc. Other Information (if any).

<u>Additional Information</u>

The participants are requested to supply the smeared nuclide number densities for all the fuel pins within the MOX assembly.

EOC (end of cycle) defines the time period immediately after irradiation but before the downtime or cooling period.

The in-core k-infinity calculation is requested for the MOX-UO_2 supercell as a whole, not just for the individual MOX assembly within the supercell.

Table 1: Selected Parameters and Case Numbers

Case #	MOX Type	Calculational Model
1	Case A (First Recycle)	Supercell
2	Case B (Weapons Disposition)	Supercell
3	Case A (First Recycle)	MOX Assembly
4	Case B (Weapons Disposition)	MOX Assembly
5	Case A (First Recycle)	MOX Pincell
6	Case B (Weapons Disposition)	MOX Pincell

Table 2: Plutonium Isotopic Composition in Fresh MOX Fuel

Nuclide	Isotopic Composition, w/o in Pu_{total}	
	MOX Case A	MOX Case B
Pu-238	2.5	0.05
Pu-239	54.7	93.6
Pu-240	26.1	6.0
Pu-241	9.5	0.3
Pu-242	7.2	0.05

Table 3: Uranium Isotopic Compositions in Fresh MOX Fuel

Nuclide	w/o in U_{total}
U-234	0.00119
U-235	0.25000
U-238	99.74881

Table 4: Initial MOX Fuel Enrichments – Case A

MOX Fuel Case A (First Recycle MOX) Enrichment Zones	MOX Fuel Plutonium content, w/o Pu_{total}/[U+Pu]	MOX Fuel Enrichment, w/o $Pu_{fissile}$/[U+Pu]
High	8.866	5.692
Medium	6.206	3.984
Low	4.894	3.142
Average	8.000	5.136

Table 5: Initial MOX Fuel Enrichments – Case B

MOX Fuel Case B (Weapons Disposition) Enrichment Zones	MOX Fuel Plutonium content, w/o Pu_{total}/[U+Pu]	MOX Fuel Enrichment, w/o $Pu_{fissile}$/[U+Pu]
High	4.377	4.110
Medium	3.064	2.877
Low	2.416	2.269
Average	3.950	3.709

Table 6: Initial MOX Fuel Compositions – Case A

Nuclide	Atoms/barn.cm for Given Fuel Pin			
	High	Medium	Low	Average (for pincell calculation)
U-234	2.5718E-7	2.6436E-7	2.6789E-7	2.5952E-7
U-235	5.3798E-5	5.5300E-5	5.6040E-5	5.4287E-5
U-238	2.1194E-2	2.1786E-2	2.2077E-2	2.1387E-2
Pu-238	5.1677E-5	3.6128E-5	2.8473E-5	4.6610E-5
Pu-239	1.1259E-3	7.8717E-4	6.2038E-4	1.0156E-3
Pu-240	5.3500E-4	3.7403E-4	2.9478E-4	4.8255E-4
Pu-241	1.9392E-4	1.3557E-4	1.0685E-4	1.7491E-4
Pu-242	1.4636E-4	1.0233E-4	8.0644E-5	1.3201E-4
O	4.6602E-2	4.6553E-2	4.6529E-2	4.6586E-2

Table 7: Initial MOX Fuel Compositions – Case B

Nuclide	Atoms/barn.cm for Given Fuel Pin			
	High	Medium	Low	Average (for pincell calculation)
U-234	2.6928E-7	2.7281E-7	2.7455E-7	2.7043E-7
U-235	5.6330E-5	5.7069E-5	5.7433E-5	5.6570E-5
U-238	2.2191E-2	2.2482E-2	2.2626E-2	2.2286E-2
Pu-238	5.0917E-7	3.5621E-7	2.8080E-7	4.5941E-7
Pu-239	9.4917E-4	6.6404E-4	5.2345E-4	8.5640E-4
Pu-240	6.0591E-5	4.2389E-5	3.3414E-5	5.4669E-5
Pu-241	3.0169E-6	2.1106E-6	1.6638E-6	2.7221E-6
Pu-242	5.0074E-7	3.5032E-7	2.7615E-7	4.5180E-7
O	4.6524E-2	4.6498E-2	4.6486E-2	4.6515E-2

Table 8: Non-Fissile Material Compositions

Zircalloy-2 (5.8736g/cm^3 – Reduced Density)

Nuclide	Atoms/barn.cm
Zr	3.8657E-2
Fe	1.3345E-4
Cr	6.8254E-5

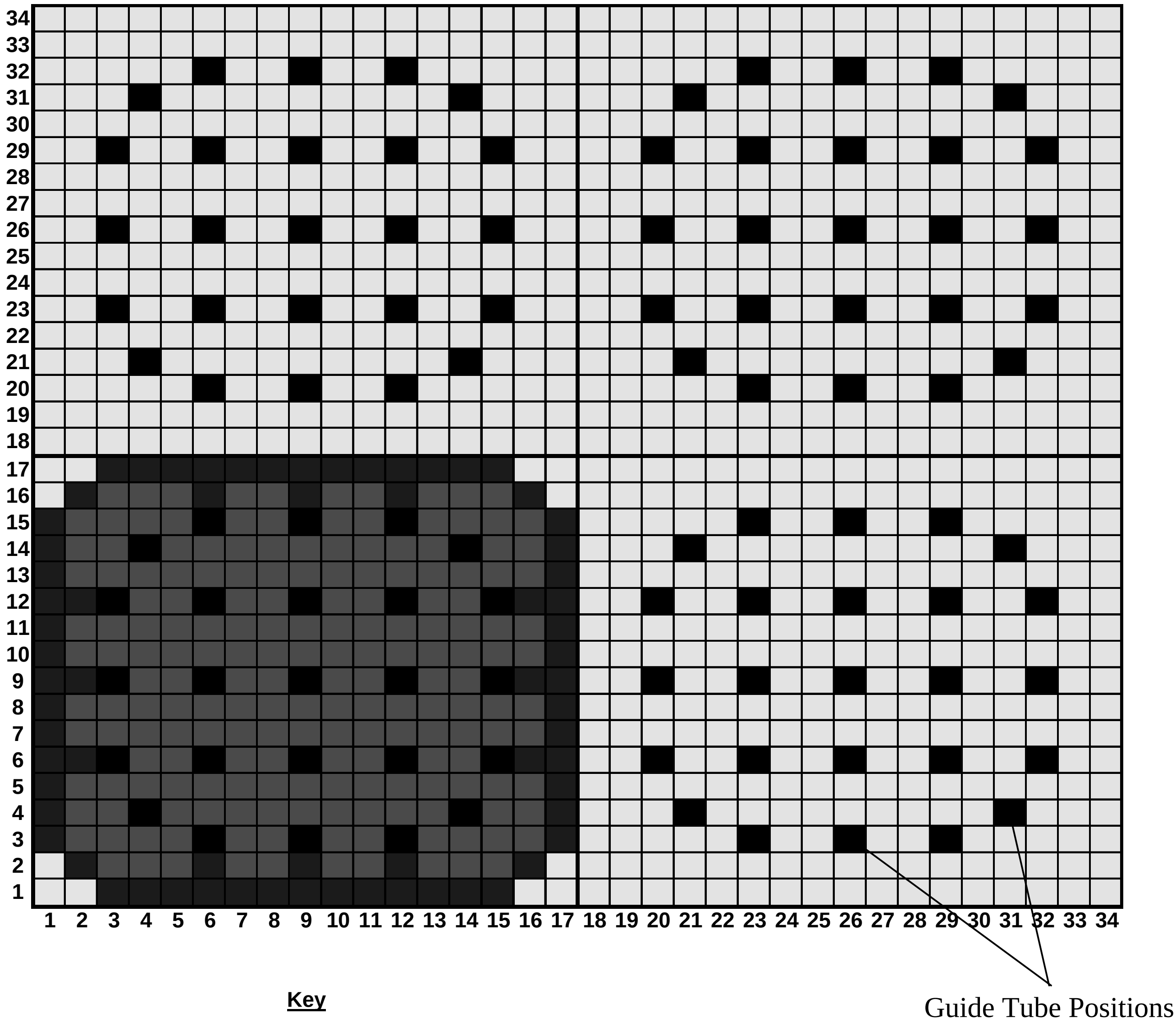
Coolant/Moderator (600ppm Boron, 0.7245g/cm^3)

Nuclide	Atoms/barn.cm
H	4.8414E-2
O	2.4213E-2
B-10	4.7896E-6
B-11	1.9424E-5

Table 9: Initial Composition for 4.3w/o U-235/U UO_2 Fuel

Nuclide	Atoms/barn.cm
U-234	8.1248E-6
U-235	1.0113E-3
U-236	8.0558E-6
U-238	2.2206E-2
O	4.6467E-2

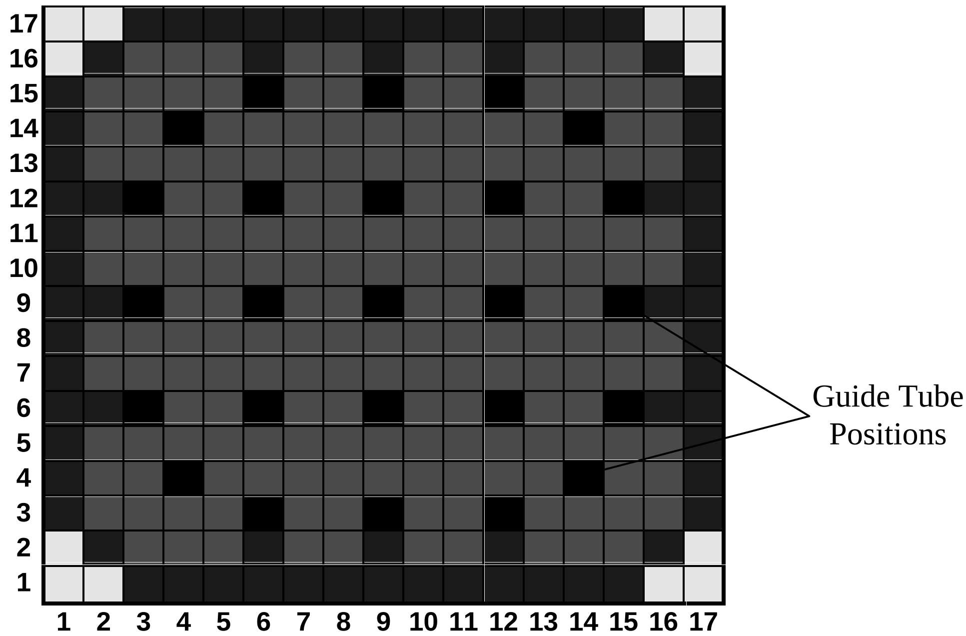
Figure 1. MOX-UO_2 Supercell



Key

- Low Enriched MOX Fuel Pin
- Medium Enriched MOX Fuel Pin
- High Enriched MOX Fuel Pin
- UO2 Fuel Pin (4.3w/o U-235/U Enrichment)

Figure 2. MOX Fuel Assembly



Key

- Low Enriched MOX Fuel Pin

- Medium Enriched MOX Fuel Pin

- High Enriched MOX Fuel Pin

Figure 3. Simplified MOX Pincell