Problem Specification for the OECD/NEANSC Burnup Credit Benchmark Phase IV-A : 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.

Experience from the earlier benchmark exercises has shown that the first step in any benchmark programme must not be overly ambitious if it is to succeed in establishing some common ground between the participants. In recognition of this, it is proposed that the initial MOX burnup credit benchmark, denoted as Phase IV-A, should be centred upon a simplified MOX fuel configuration. A full discussion of the key issues concerning burnup credit for MOX fuels can be found in Reference 1. It is our current intention that these issues will be investigated by future MOX benchmarking exercises.

The Phase IV-A benchmark exercise concerns the calculation of infinite PWR fuel pincell reactivity for fresh and irradiated MOX fuels. The fuel compositions have been derived by the benchmark co-ordinators, BNFL, using the WIMS7 reactor lattice code. The nuclear data was provided by the 172-group WIMS ‘1996’ nuclear dataset, which is based upon JEF2.2 evaluations. These calculations used a simplified MOX only representation of the core, and irradiated the fuel in a single cycle at a power of 35MW/teHM, with a constant boron loading of 500ppm in the core coolant. A comprehensive description of the calculational method adopted can be found in Reference 2.

2. Parameters and Case Numbers

The neutron multiplication factor is required for a total of 63 cases, covering various combinations of initial MOX fuel composition, burnup, cooling and spent fuel representation (i.e. “actinide only” or “fission product” burnup credit). The selected parameters and case numbers are shown in Table 1.

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 the specified curium isotopes.

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 simple pincell model means that the completion of the exercise is estimated to require approximately 1 day of effort for the criticality assessor.

3. Geometry Data

The geometry for the Phase IV-A exercise is an infinite PWR fuel cell lattice, analogous to that used in the Phase I-A exercise for PWR UO_2 fuel, as shown in Figure 1.

Fuel Pin Pitch:	1.33cm square pin array
Fuel Pellet Radius:	0.412cm
Cladding Thickness:	0.063cm (no airgap between fuel and clad)

4. Material Data

The pincell materials shown in Figure 4 are as follows:

Cladding:	Zircalloy
Pincell Moderator:	Water
Fuel:	Mixed Oxide Fuel (as defined in Section 5)

For the purposes of the benchmark exercise, the non-fissile material compositions should be modelled as specified in Table 1.

5. MOX Fuel Compositions

The original proposal for the MOX benchmarking exercise (Reference 1) suggested that three different MOX fuels should be considered, which were chosen to represent

the range of potential interest within the group for MOX fuels. The proposed MOX fuels were representative 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;

iii. a MOX fuel case appropriate to future MOX fuels that might be produced using the plutonium recovered from the reprocessing of irradiated MOX, i.e. the 'later generation' of MOX fuel from a plutonium recycling strategy, referred to as MOX Case C.

The plutonium isotopic compositions for these MOX fuels are presented in Table 2. in all cases, the uranium oxide component of the MOX is assumed to be depleted, with a uranium-235 content of 0.25w/o U-235/U, which is typical of current MOX fuel fabrication. The uranium isotopic composition is shown in Table 3. The initial MOX fuel enrichments for the three MOX cases are shown in Table 4.

The fuel compositions for the requested calculations are shown in Tables 5, 6 and 7 for the MOX fuel cases A, B and C respectively. These compositions will also be provided to the participants in floppy disk or CD format, in order to ease the handling of the various fuel compositions in the calculations.

6. Specified Format for Submission of Results

The results should be submitted via e-mail to the benchmark organisers, using the e-mail 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 to 68	Multiplication Factors for the Requested Cases
69	Please Describe Your Analysis Environment Here. It will be Included in the Phase IV-A 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 Limit or Statistical Errors for the Eigenvalue Calculations,
Other Information (if any).

References

1. "Proposal for the OECD/NEANSC Burnup Credit Benchmark Programme - Phase IV : Mixed Oxide (MOX) Fuels for PWR and BWR", R L Bowden and P R Thorne, Draft Version 1, June 1996. Presented at the OECD/NEANSC Criticality Working Group Meeting, Paris, June 1996.

2. CR5172 Rev 1 "Derivation of Isotopic Number Densities for the Specification of the OECD/NEANSC Burnup Credit Benchmark, Phase IV-A (MOX Fuels)", R L Bowden and G J O'Connor, July 1997.

Table 1. Non-Fissile Material Compositions

Zircalloy

Nuclide	Atoms/barn.cm
Zr	4.2982E-2
Fe	1.4838E-4
Cr	7.5891E-5

Water

Nuclide	Atoms/barn.cm
H	6.67294E-2
O	3.33662E-2

Table 2. Plutonium Isotopic Compositions in Fresh MOX Fuel

Nuclide	Isotopic Composition, w/o in Pu_{total}		
	MOX Case A	MOX Case B	MOX Case C
Pu-238	1.8	0.05	4.0
Pu-239	59.0	93.6	36.0
Pu-240	23.0	6.0	28.0
Pu-241	12.2	0.3	12.0
Pu-242	4.0	0.05	20.0

Table 3. Uranium Isotopic Compositions in Fresh MOX Fuel

Nuclide	w/o in U_{total}
U-234	0.00119
U-235	0.25000
U-236	99.74881

Table 4. Initial MOX Fuel Enrichments

MOX Fuel Type	MOX Fuel Plutonium Content, w/o Pu_{total}/[U+Pu]	MOX Fuel Enrichment, w/o $Pu_{fissile}$/[U+Pu]
Case A	5.6	3.987
Case B	4.0	3.756
Case C	8.0	3.840

Table 5. Specified Calculations

MOX Case	Cooling Time (years)	Fission Products Modelled?	Actinides Modelled	Burnup (GWd/teHM)			
				Fresh	20	40	60
A	1	Yes	Major	Case 1	Case 2	Case 3	Case 4
		No	Major		Case 5	Case 6	Case 7
			All		Case 8	Case 9	Case 10
	5	Yes	Major		Case 11	Case 12	Case 13
		No	Major		Case 14	Case 15	Case 16
			All		Case 17	Case 18	Case 19
B	1	Yes	Major	Case 20	Case 21	Case 22	Case 23
		No	Major		Case 24	Case 25	Case 26
			All		Case 27	Case 28	Case 29
	5	Yes	Major		Case 30	Case 31	Case 32
		No	Major		Case 33	Case 34	Case 35
			All		Case 36	Case 37	Case 38

Table 5 (cont)

MOX Case	Cooling Time (years)	Fission Products Modelled?	Actinides Modelled	Burnup (GWd/teHM)			
				Fresh	20	40	60
C	1	Yes	Major	Case 39	Case 40	Case 41	Case 42
			All		Case 43	Case 44	Case 45
		No	Major		Case 46	Case 47	Case 48
			All		Case 49	Case 50	Case 51
	5	Yes	Major		Case 52	Case 53	Case 54
			All		Case 55	Case 56	Case 57
		No	Major		Case 58	Case 59	Case 60
			All		Case 61	Case 62	Case 63

Table 6. Material Compositions for MOX Case A

Nuclide	Atoms/barn.cm for Given Fuel Burnup and Cooling Time						
	Fresh	20GWd/teHM		40GWd/teHM		60GWd/teHM	
		1 Year Cooling	5 Years Cooling	1 Year Cooling	5 Years Cooling	1 Year Cooling	5 Years Cooling
U-234	2.7999E-7	6.3600E-7	1.3530E-6	7.7718E-7	1.5879E-6	9.1664E-7	1.8564E-6
U-235	5.8570E-5	4.2219E-5	4.2287E-5	2.9018E-5	2.9070E-5	1.9181E-5	1.9223E-5
U-236	-	3.7252E-6	3.8580E-6	6.1753E-6	6.2984E-6	7.5360E-6	7.6448E-6
U-238	2.3074E-2	2.2732E-2	2.2732E-2	2.2365E-2	2.2365E-2	2.1986E-2	2.1986E-2
Pu-238	2.4700E-5	2.2785E-5	2.2389E-5	2.5504E-5	2.5364E-5	2.9509E-5	2.9410E-5
Pu-239	8.0623E-4	5.9182E-4	5.9176E-4	4.5028E-4	4.5024E-4	3.6327E-4	3.6325E-4
Pu-240	3.1298E-4	3.1445E-4	3.1491E-4	2.9067E-4	2.9250E-4	2.5605E-4	2.5961E-4
Pu-241	1.6533E-4	1.8251E-4	1.5056E-4	1.8125E-4	1.4953E-4	1.6525E-4	1.3633E-4
Pu-242	5.3981E-5	7.0592E-5	7.0592E-5	9.1733E-5	9.1733E-5	1.1211E-4	1.1211E-4
Np-237	-	1.6134E-6	1.6134E-6	3.0746E-6	3.0746E-6	4.1997E-6	4.1997E-6
Am-241	-	1.8432E-5	5.0375E-5	2.2303E-5	5.4028E-5	2.1568E-5	5.0491E-5
Am-243	-	1.3528E-5	1.3528E-5	2.4023E-5	2.4023E-5	3.2566E-5	3.2566E-5
O-16	4.8992E-2	4.8992E-2	4.8992E-2	4.8992E-2	4.8992E-2	4.8992E-2	4.8992E-2
Cm-242	-	3.2217E-7	6.4678E-10	6.7186E-7	1.3488E-9	8.4273E-7	1.6918E-9
Cm-243	-	2.8535E-8	2.6018E-8	1.1090E-7	1.0111E-7	1.8772E-7	1.7116E-7
Cm-244	-	4.1736E-6	3.5812E-6	1.3749E-5	1.1798E-5	2.8565E-5	2.2194E-5
Cm-245	-	3.0261E-7	3.0261E-7	1.6967E-6	1.6967E-6	3.9227E-6	3.9227E-6
Mo-95	-	2.3101E-5	2.3261E-5	4.4441E-5	4.4599E-5	6.3363E-5	6.3520E-5
Tc-99	-	2.8609E-5	2.8610E-5	5.3736E-5	5.3736E-5	7.5064E-5	7.5064E-5
Ru-101	-	2.9847E-5	2.9847E-5	5.7774E-5	5.7774E-5	8.3092E-5	8.3092E-5
Rh-103	-	2.9106E-5	2.9111E-5	4.9708E-5	4.9714E-5	6.3144E-5	6.3149E-5
Ag-109	-	6.5892E-6	6.5892E-6	1.1408E-5	1.1408E-5	1.5024E-5	1.5024E-5
Cs-133	-	3.1181E-5	3.1181E-5	5.7100E-5	5.7100E-5	7.7818E-5	7.7818E-5
Nd-143	-	2.1008E-5	2.1008E-5	3.8610E-5	3.8610E-5	5.2176E-5	5.2176E-5
Nd-145	-	1.4896E-5	1.4896E-5	2.8038E-5	2.8038E-5	3.9157E-5	3.9157E-5
Sm-147	-	2.7653E-6	5.9794E-6	5.2265E-6	9.3872E-6	6.8435E-6	1.1221E-5
Sm-149	-	3.5704E-7	3.5704E-7	3.3504E-7	3.3504E-7	3.0728E-7	3.0728E-7
Sm-150	-	6.6564E-6	6.6564E-6	1.3820E-5	1.3820E-5	2.0276E-5	2.0276E-5
Sm-151	-	1.3380E-6	1.2968E-6	1.5043E-6	1.4580E-6	1.5866E-6	1.5379E-6
Sm-152	-	3.8440E-6	3.8439E-6	6.2143E-6	6.2143E-6	7.5692E-6	7.5692E-6
Eu-153	-	3.2743E-6	3.2743E-6	7.5074E-6	7.5074E-6	1.0848E-5	1.0848E-5
Gd-155	-	7.5755E-8	2.5948E-7	1.4403E-7	5.0261E-7	2.2005E-7	7.7899E-7

Table 7. Material Compositions for MOX Case B

Nuclide	Atoms/barn.cm for Given Fuel Burnup and Cooling Time						
	Fresh	20GWd/teHM		40GWd/teHM		60GWd/teHM	
		1 Year Cooling	5 Years Cooling	1 Year Cooling	5 Years Cooling	1 Year Cooling	5 Years Cooling
U-234	2.8452E-7	2.2995E-7	2.6895E-7	2.1773E-7	3.6734E-7	2.6275E-7	5.7503E-7
U-235	5.9518E-5	4.0882E-5	4.0948E-5	2.5627E-5	2.5670E-5	1.4759E-5	1.4791E-5
U-236	-	3.9723E-6	4.0436E-6	6.5755E-6	6.6585E-6	7.8389E-6	7.9160E-6
U-238	2.3447E-2	2.3103E-2	2.3103E-2	2.2715E-2	2.2715E-2	2.2300E-2	2.2300E-2
Pu-238	4.8972E-7	1.1910E-6	1.2270E-6	4.5563E-6	4.7086E-6	9.6242E-6	9.8070E-6
Pu-239	9.1194E-4	5.7376E-4	5.7369E-4	3.7279E-4	3.7275E-4	2.7573E-4	2.7570E-4
Pu-240	5.8276E-5	1.6882E-4	1.6879E-4	1.9642E-4	1.9672E-4	1.8198E-4	1.8321E-4
Pu-241	3.8689E-6	7.4303E-5	6.1297E-5	1.1078E-4	9.1391E-5	1.1209E-4	9.2467E-5
Pu-242	4.8161E-7	8.9143E-6	8.9143E-6	3.0626E-5	3.0626E-5	5.6427E-5	5.6427E-5
Np-237	-	1.5675E-6	1.5675E-6	3.0228E-6	3.0228E-6	4.1080E-6	4.1080E-6
Am-241	-	5.9894E-6	1.8995E-5	1.0955E-5	3.0345E-5	1.2034E-5	3.1652E-5
Am-243	-	1.2867E-6	1.2867E-6	6.8336E-6	6.8336E-6	1.5293E-5	1.5293E-5
O-16	4.8965E-2	4.8965E-2	4.8965E-2	4.8965E-2	4.8965E-2	4.8965E-2	4.8965E-2
Cm-242	-	7.5157E-8	1.5088E-10	3.0247E-7	6.0723E-10	4.9610E-7	9.9596E-10
Cm-243	-	5.1466E-9	4.6925E-9	4.0239E-8	3.6690E-8	9.5010E-8	8.6628E-8
Cm-244	-	2.6410E-7	2.2662E-7	2.6910E-6	2.3090E-6	9.2627E-6	7.9480E-6
Cm-245	-	1.3681E-8	1.3681E-8	2.3729E-7	2.3729E-7	1.0624E-6	1.0624E-6
Mo-95	-	2.3871E-5	2.4036E-5	4.5718E-5	4.5879E-5	6.4917E-5	6.5075E-5
Tc-99	-	2.8946E-5	2.8946E-5	5.4176E-5	5.4176E-5	7.5371E-5	7.5371E-5
Ru-101	-	2.9955E-5	2.9955E-5	5.8079E-5	5.8079E-5	8.3707E-5	8.3707E-5
Rh-103	-	2.8121E-5	2.8126E-5	4.6580E-5	4.6585E-5	5.7355E-5	5.7360E-5
Ag-109	-	5.7370E-6	5.7370E-6	1.0105E-5	1.0105E-5	1.3457E-5	1.3457E-5
Cs-133	-	3.1383E-5	3.1383E-5	5.7177E-5	5.7177E-5	7.7393E-5	7.7393E-5
Nd-143	-	2.0862E-5	2.0862E-5	3.7501E-5	3.7501E-5	4.9110E-5	4.9110E-5
Nd-145	-	1.4826E-5	1.4826E-5	2.7866E-5	2.7866E-5	3.8801E-5	3.8801E-5
Sm-147	-	2.6881E-6	5.8102E-6	4.9973E-6	8.9723E-6	6.3962E-6	1.0505E-5
Sm-149	-	2.7823E-7	2.7823E-7	2.5523E-7	2.5523E-7	2.3274E-7	2.3274E-7
Sm-150	-	6.6563E-6	6.6563E-6	1.3926E-5	1.3926E-5	2.0464E-5	2.0464E-5
Sm-151	-	1.0732E-6	1.0402E-6	1.1467E-6	1.1114E-6	1.1985E-6	1.1616E-6
Sm-152	-	3.8212E-6	3.8212E-6	5.9493E-6	5.9493E-6	7.0762E-6	7.0762E-6
Eu-153	-	3.2199E-6	3.2199E-6	7.4656E-6	7.4656E-6	1.0705E-5	1.0705E-5
Gd-155	-	5.8022E-8	2.0452E-7	1.1923E-7	4.2851E-7	1.8106E-7	6.5902E-7

Table 8. Material Compositions for MOX Case C

Nuclide	Atoms/barn.cm for Given Fuel Burnup and Cooling Time						
	Fresh	20GWd/teHM		40GWd/teHM		60GWd/teHM	
		1 Year Cooling	5 Years Cooling	1 Year Cooling	5 Years Cooling	1 Year Cooling	5 Years Cooling
U-234	2.7318E-7	1.5063E-6	3.6143E-6	1.9068E-6	3.9071E-6	2.1766E-6	4.1510E-6
U-235	5.7145E-5	4.1669E-5	4.1734E-5	2.9739E-5	2.9794E-5	2.0961E-5	2.1009E-5
U-236	-	3.6788E-6	3.8787E-6	6.0137E-6	6.1853E-6	7.3406E-6	7.4879E-6
U-238	2.2513E-2	2.2161E-2	2.2161E-2	2.1796E-2	2.1796E-2	2.1428E-2	2.1428E-2
Pu-238	7.8503E-5	6.7431E-5	6.5740E-5	6.3615E-5	6.2454E-5	6.2619E-5	6.1686E-5
Pu-239	7.0356E-4	5.6858E-4	5.6852E-4	4.8007E-4	4.8003E-4	4.2049E-4	4.2046E-4
Pu-240	5.4493E-4	4.7278E-4	4.7425E-4	4.0401E-4	4.0879E-4	3.4474E-4	3.5312E-4
Pu-241	2.3257E-4	2.4534E-4	2.0240E-4	2.3568E-4	1.9443E-4	2.1323E-4	1.7590E-4
Pu-242	3.8610E-4	3.7523E-4	3.7523E-4	3.6946E-4	3.6946E-4	3.6386E-4	3.6386E-4
Np-237	-	1.6899E-6	1.6899E-6	3.1985E-6	3.1985E-6	4.3720E-6	4.3720E-6
Am-241	-	2.5361E-5	6.8303E-5	3.0694E-5	7.1945E-5	3.0366E-5	6.7687E-5
Am-243	-	4.0530E-5	4.0530E-5	6.4516E-5	6.4516E-5	7.8878E-5	7.8878E-5
O-16	4.9031E-2	4.9031E-2	4.9031E-2	4.9031E-2	4.9031E-2	4.9031E-2	4.9031E-2
Cm-242	-	4.1769E-7	8.3855E-10	8.4517E-7	1.6895E-9	1.0431E-6	2.0941E-9
Cm-243	-	3.8856E-8	3.5428E-8	1.4606E-7	1.3318E-7	2.4454E-7	2.2297E-7
Cm-244	-	1.1769E-5	1.0098E-5	3.4867E-5	2.9918E-5	6.0098E-5	5.1568E-5
Cm-245	-	9.0845E-7	9.0845E-7	4.5435E-6	4.5435E-6	9.6412E-6	9.6412E-6
Mo-95	-	2.2735E-5	2.2892E-5	4.3787E-5	4.3944E-5	6.2588E-5	6.2743E-5
Tc-99	-	2.8403E-5	2.8403E-5	5.3414E-5	5.3414E-5	7.4849E-5	7.4849E-5
Ru-101	-	2.9798E-5	2.9798E-5	5.7667E-5	5.7667E-5	8.3006E-5	8.3006E-5
Rh-103	-	2.9664E-5	2.9669E-5	5.1912E-5	5.1917E-5	6.7750E-5	6.7756E-5
Ag-109	-	6.9595E-6	6.9595E-6	1.2094E-5	1.2094E-5	1.6067E-5	1.6067E-5
Cs-133	-	3.1031E-5	3.1031E-5	5.6923E-5	5.6923E-5	7.7931E-5	7.7931E-5
Nd-143	-	2.1064E-5	2.1064E-5	3.9138E-5	3.9138E-5	5.3831E-5	5.3831E-5
Nd-145	-	1.4931E-5	1.4931E-5	2.8137E-5	2.8137E-5	3.9433E-5	3.9433E-5
Sm-147	-	2.7739E-6	6.0029E-6	5.2757E-6	9.4928E-6	7.0109E-6	1.1512E-5
Sm-149	-	4.0641E-7	4.0641E-7	4.0019E-7	4.0019E-7	3.8076E-7	3.8076E-7
Sm-150	-	6.6678E-6	6.6678E-6	1.3785E-5	1.3785E-5	2.0207E-5	2.0207E-5
Sm-151	-	1.4686E-6	1.4235E-6	1.7611E-6	1.7070E-6	1.9357E-6	1.8762E-6
Sm-152	-	3.8100E-6	3.8100E-6	6.3411E-6	6.3411E-6	8.0271E-6	8.0271E-6
Eu-153	-	3.3404E-6	3.3404E-6	7.5293E-6	7.5293E-6	1.0865E-5	1.0865E-5
Gd-155	-	8.5534E-8	2.8847E-7	1.6237E-7	5.5419E-7	2.5211E-7	8.6971E-7
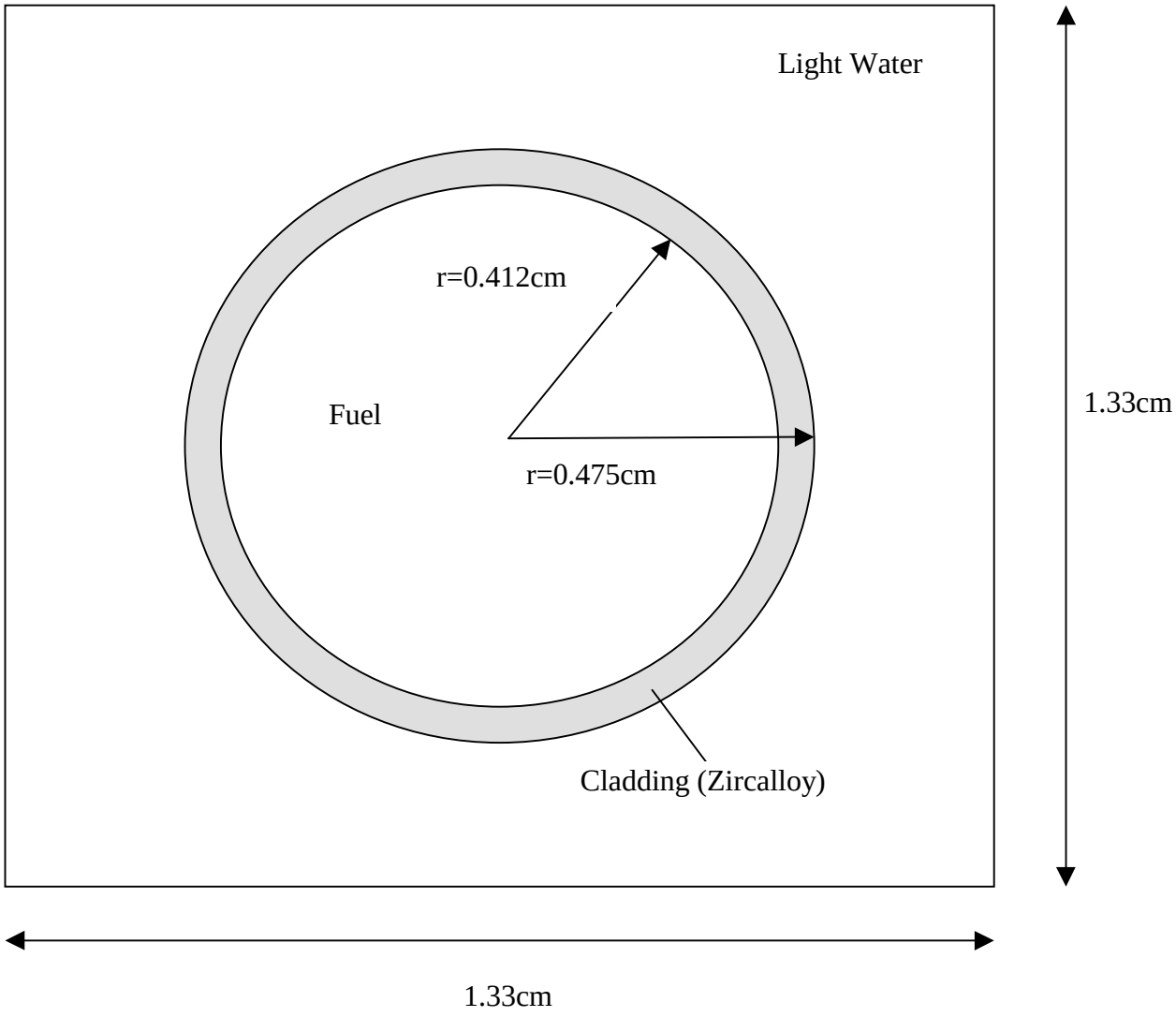
Figure 1. Geometry of MOX Fuel Pincell for PWR