Specification for CB 6 Benchmark on VVER-440 Final Disposal

(Similar to the OECD/NEA/NSC WPNCS EGBUC Phase VII benchmark aimed at UO_2 PWR spent fuel compositions for long-term disposal)

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1. Introduction

The proposed benchmark intends to acquire VVER-440 spent fuel data similar to those resulted from OECD/NEA/NSC WPNCS EGBUC Phase VII benchmark aimed at determination of UO_2 PWR spent fuel compositions for long-term disposal (/1/,/2/). It is focused on prediction of spent fuel isotopic compositions and corresponding k_{eff} values in a cask configuration over the time duration relevant to long-term spent fuel disposal.

As in the Phase VII benchmark, the current VVER-440 benchmark is divided into two sets of calculations:

- Decay calculations for provided VVER-440 UO_2 discharged fuel compositions
- k_{eff} calculations for a conceptual cask model

Participants are requested to perform **decay calculations** for the fuel compositions and criticality calculations for the fuel in the cask model for selected post-irradiation time steps up to 1 000 000 years. Despite of the fact that the physical condition of the fuel will change over such a long time period, there is interest in the change in isotopic compositions over this duration, as well as interest in the relative behavior of k_{eff} over this duration. The resulting isotopic compositions and k_{eff} values as a function of time will be analyzed but not compared with any measured data.

2. Decay Calculations

Based on the given discharge fuel composition (see Tab.1, 2nd column), the isotopics of the 'benchmark resulted nuclides' (see Tab.1, 3rd column) should be found by the decay calculations for cooling times of the cases from 2 to 30 as listed in Tab 2. The discharge isotopics are provided for spent fuel of the **simplified 'Gd-2' VVER-440 fuel assembly (no enrichment zoning, no burnable absorber Gd_2O_3 in fuel) with ZrNbHf shroud of 1.5 mm; the initial enrichment and final burnup are 4.25 wt% ^{235}U and 50 MWd/kg$_U$, respectively.**

Table 1: Discharge VVER-440 fuel composition (4.25 initial wt% ^{235}U, 50 MWd/kg_U) for calculating time-dependent spent fuel isotopics

Isotope	Atom density [atom/b·cm]	Benchmark resulted nuclides	important contributors to	
			actinide+FP burnup credit	dose rate
C-14	1.764E-09	x		x
O-16	4.526E-02**)		x	
Cl-36	1.000E-06 *)	x		x
Ca-41	1.000E-06 *)	x		x
Ni-59	1.000E-06 *)	x		x
Se-79	4.750E-07	x		x
Zr-93	5.963E-05	x		x
Rb-93	1.584E-12			
Sr-90	4.559E-05	x		x
Sr-93	2.364E-10			
Y-93	1.983E-08			
Y-95	3.915E-10			
Nb-93m	5.816E-11	x		x
Nb-94	5.968E-11	x		x
Nb-95	1.953E-06			
Mo-93	5.635E-15	x		x
Mo-95	5.669E-05	x	x	
Mo-99	1.819E-07			
Mo-101	6.354E-10			
Tc-99m	1.474E-08			
Tc-99	6.204E-05	x	x	x
Tc-101	6.187E-10			
Ru-101	6.179E-05	x	x	
Ru-103	2.449E-06			
Rh-103	3.226E-05	x	x	
Pd-107	1.785E-05	x		x
Pd-109	9.208E-09			
Ag-109	5.862E-06	x	x	
Sn-126	1.226E-06	x		x
Sb-126	2.462E-10	x		x
Sb-126m	3.256E-13	x		x
Sb-129	2.031E-09			
Te-129m	6.676E-08			
I-129	9.665E-06	x		x

I-133	6.308E-08			
I-135	1.911E-08			
Xe-133	3.659E-07			
Xe-135	8.799E-09			
Cs-133	6.542E-05	x	x	
Cs-135	2.829E-05	x		x
Cs-137	7.107E-05	x		x
Pr-143	6.786E-07			
Pr-147	2.171E-10			
Pr-149	2.057E-11			
Nd-143	4.206E-05	x	x	
Nd-145	3.563E-05	x	x	
Nd-147	2.543E-07			
Nd-149	1.013E-09			
Pm-147	7.019E-06			
Pm-149	4.752E-08			
Pm-151	8.920E-09			
Sm-147	4.109E-06	x	x	
Sm-149	1.157E-07	x	x	
Sm-150	1.556E-05	x	x	
Sm-151	8.173E-07	x	x	x
Sm-152	5.996E-06	x	x	
Sm-153	4.072E-08			
Sm-155	2.505E-11			
Eu-151	1.114E-09	x	x	
Eu-152	2.258E-09			
Eu-153	6.380E-06	x	x	
Eu-155	3.206E-07			
Gd-155	3.958E-09	x	x	
Pb-210	8.468E-19	x		x
Rn-222	2.574E-23			
Ra-226	3.977E-18	x		x
Ra-228	6.868E-22	x		x
Ac-227	1.762E-17	x		x
Th-226	7.251E-23			
Th-229	1.574E-14	x		x
Th-230	3.335E-13	x		x
Th-232	1.007E-11	x		x

Th-231	1.149E-15			
Pa-231	8.481E-13	x		x
U-230	6.922E-20			
U-232	8.633E-12	x		x
U-233	1.899E-11	x	x	x
U-234	9.592E-08	x	x	x
U-235	1.900E-04	x	x	x
U-236	1.304E-04	x	x	x
U-237	2.720E-07			
U-238	2.081E-02	x	x	x
U-239	1.352E-08			
U-240	1.406E-20			
Np-235	5.917E-13			
Np-236	9.290E-12			
Np-236m	2.499E-13			
Np-237	1.724E-05	x	x	x
Np-238	4.793E-08			
Np-239	1.948E-06			
Np-240	5.974E-11			
Pu-236	3.190E-11			
Pu-237	1.765E-11			
Pu-238	8.021E-06	x	x	x
Pu-239	1.600E-04	x	x	x
Pu-240	6.755E-05	x	x	x
Pu-241	4.363E-05	x	x	x
Pu-242	1.946E-05	x	x	x
Pu-243	5.074E-09			
Pu-244	7.004E-10			
Pu-245	4.501E-14			
Pu-246	3.462E-16			
Am-239	1.498E-16			
Am-240	6.530E-14			
Am-241	1.775E-06	x	x	x
Am-242	3.615E-09			
Am-242m	4.051E-08	x	x	x
Am-243	5.557E-06	x	x	x
Cm-242	5.547E-07			
Cm-243	2.012E-08			

Cm-244	2.348E-06			
Cm-245	1.335E-07	x		x
Cm-246	1.408E-08	x		x

**) it is provided for criticality calculations only
*) The nuclide does not exist in the calculated discharge inventory for the VVER-440 assembly

Table 2: Cooling times for calculating and reporting isotopic compositions

Time case number	Time [y]	Time case number	Time [y]
1	0	16	1000
2	1	17	2000
3	2	18	5000
4	5	19	8000
5	10	20	10000
6	20	21	15000
7	40	22	20000
8	60	23	25000
9	80	24	30000
10	100	25	40000
11	120	26	45,000
12	150	27	50000
13	200	28	100000
14	300	29	500000
15	500	30	1000000

3. K_{eff} Calculations

Criticality calculations should be performed for a conceptual VVER-440 cask model loaded with the VVER-440 spent fuel assemblies the fuel isotopics of which result from the decay calculations corresponding to the times listed in Table 2. The cask model to be used is described below - it is identical to the cask used in CB4 calculational benchmark (/3/,/4/). The model of FA for the calculations is a conservative simplification of 'Gd-2' VVER-440 FA design supposing no enrichment zoning and no burnable absorbers; the burnup profiles are uniform.

k_{eff} values will be calculated using actinide and fission product approach for the fuel description which include ^{16}O and the nuclides identified in fourth column of Table 1 as 'important contributors to actinide+FP burnup credit': ^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{242m}Am, ^{243}Am, ^{95}Mo, ^{99}Tc, ^{101}Ru, ^{103}Rh, ^{109}Ag, ^{133}Cs, ^{143}Nd, ^{145}Nd, ^{147}Sm, ^{149}Sm, ^{150}Sm, ^{151}Sm, ^{152}Sm, ^{151}Eu, ^{153}Eu and ^{155}Gd.

3.1. Geometry and material data

The conceptual cask fully loaded with VVER-440 fuel assemblies is the criticality model for k_{eff} calculations. The fuel pin cell dimensions and geometry of the cask unit including the

assembly are shown in Figures 1and 2, respectively. Cross-section views of the cask model for use in criticality calculations are provided in the following Figures 3 and 4. The cask is completely flooded with pure water. The temperature for cask components is 300 K.

Specification of VVER-440 Fuel Pin Cell (of Hexagonal Section) in FA (see Fig.1 and 2):

Fresh Fuel Composition	9.73461E-4 ^{235}U 2.16545E-2 ^{238}U 4.526E-02 ^{16}O
Central pellet hole	Smeared with Fuel
Fuel Cell Pitch	1.23 cm
Fuel Radius	0.38 cm
Cladding Inner Radius	0.3865 cm
Outer Radius	0.4535 cm
Material	1% wt. Nb, 98.99% wt. Zr, 0.01% wt. Hf, ρ_{eff} = 6.44 g/cm^3
Gap between fuel and cladding	He
Active Fuel Length	244 cm
Moderator	Pure Water (spacer grids neglected)
Axial Burnup Distribution	Uniform
Radial Burnup Distribution	Uniform
Number Densities of Nuclides in Fuel	Case Dependent (for the cases specified in Table 2 use the values for nuclides mentioned in 4th column of Table 1 as resulted from the decay calculations, for the case with fresh fuel use the fresh fuel composition)

Specification of the Model of the VVER-440 Fuel Assembly of Hexagonal Section (see Fig.3):

Number of Fuel Pins in the Assembly	126
Fuel Assembly Length	320 cm
Lower Fuel Endplug+FA Hardware Layer (of Hexagonal Section)	
Outer Dimension (Inscribed Diameter)	14.5 cm
Thickness	47.2 cm
Upper Fuel Endplug+FA Hardware Layer (of Hexagonal Section)	
Outer Dimension (Inscribed Diameter)	14.5 cm
Thickness	28.8 cm

Number Densities of Nuclides in Fuel Endplug+FA Hardware [atoms/b·cm] :

4.51906E-02	H
2.25953E-02	O-16
5.27527E-03	Cr
4.16061E-04	Mn-55
1.92374E-02	Fe
2.59655E-03	Ni

Assembly Shroud (of Hexagonal Section)

Length	244 cm
Outer Dimension (Inscribed Diameter)	14.5 cm

Thickness	1.5 mm
Material	2.5% wt. Nb, 97.47% wt. Zr, 0.03% wt. Hf, ρ_{eff} = 6.44 g/cm^3

Central Instrumental Tube (Cylindrical)

Length	244 cm
Outer Diameter	10.3 mm
Inner Diameter	8.8 mm
Material	1% wt. Nb, 98.99% wt. Zr, 0.01% wt. Hf, ρ_{eff} = 6.44 g/cm^3

Specification of Cask Lattice Unit (of Hexagonal Section) (Fig.3)

Fuel Assembly (of Hexagonal Section)	See Description Above	
Outer Dimension (Inscribed Diameter)	14.5 cm	
Length	320 cm	

Water Channel (of Hexagonal Section)

	Pure Water	
Inner Dimension (Inscribed Diameter)	14.5 cm	
Outer Dimension (Inscribed Diameter)	15.0 cm	

Storage Tube (of Hexagonal Section)

Length	320 cm	
Inner Dimension (Inscribed Diameter)	15.0 cm	
Outer Dimension (Inscribed Diameter)	16.0 cm	
Material		
	7.2010E-2	Fe
	1.6262E-2	Cr
	1.7099E-3	Mn-55

Water Channel (of Hexagonal Section)

	Pure Water	
Inner Dimension (Inscribed Diameter)	16.0 cm	
Outer Dimension (Inscribed Diameter)	16.3 cm	

Intervening Plates (of Hexagonal Section)

Length	320 cm	
Inner Dimension (Inscribed Diameter)	16.3 cm	
Outer Dimension (Inscribed Diameter)	17.5 cm	
Material	5.8573E-2	Al-27
	1.3379E-3	Mg
	2.3677E-4	Mn-55

Pitch of the Units	17.5 cm

Specification of Cask Model (Finite Cylindrical System) (Fig.3, Fig.4)

Radial Description (from the center to the surface, Fig.3, Fig.4):

Finite Array of the Units
The Unit Description See Above
Number of Units Placed in the Cask 84

Cast Iron Cylindrical Body

	7.0475E-2	Fe
	1.1933E-2	C-12
	4.9870E-4	Mn-55
Inner Radius	90 cm	
Outer Radius	127 cm	

Axial Description (from the bottom to the top, Fig. 4):

Lower Cast Iron Lid (bottom)
Outer Radius 127 cm
Material - see above the cask body
Thickness 40 cm
Cylindrical Cask Body
Radial description - see above
Finite Array of Units Length 320 cm
Upper Cast Iron Lid (top)
Outer Radius 127 cm
Material - see above the cask body
Thickness 40 cm

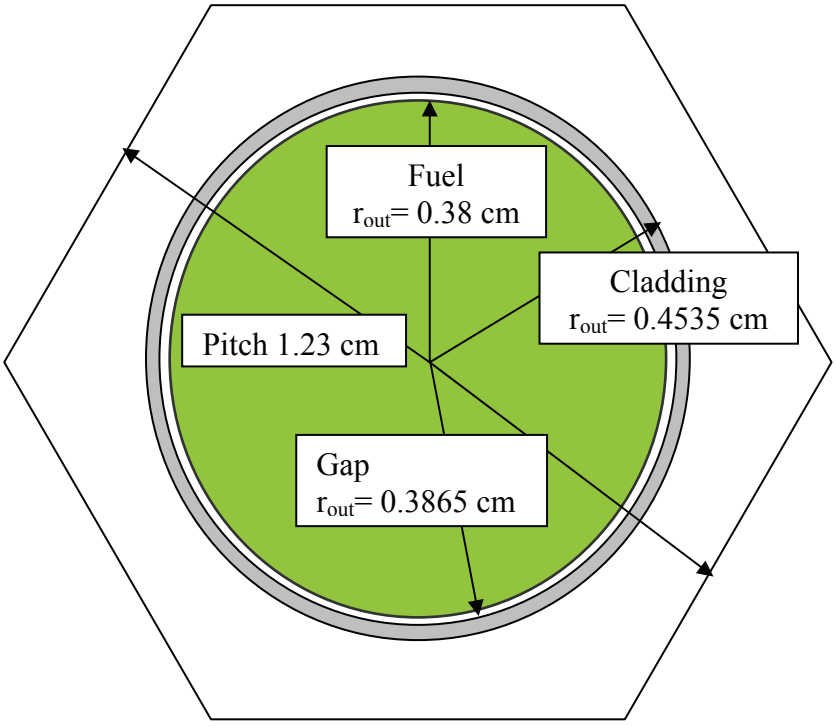
Inside the cask cavity (from the bottom to the top):

Finite Array of the Units
Water Gap
Pure Water
Thickness 4 cm

Note:
Looking at the pictures the colors of the same material regions in Fig.1,2,3 and 4 may differ from one to another due to possibility of gray scale reproducing .

3.2. Pictures

Fig.1 Fuel pin cell dimensions



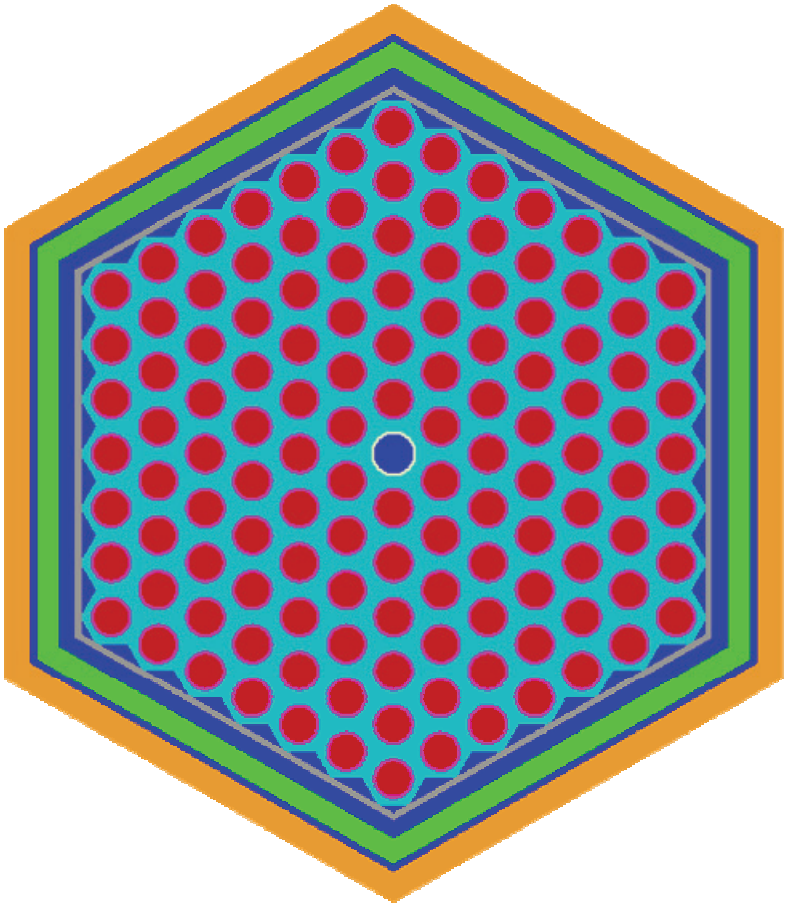
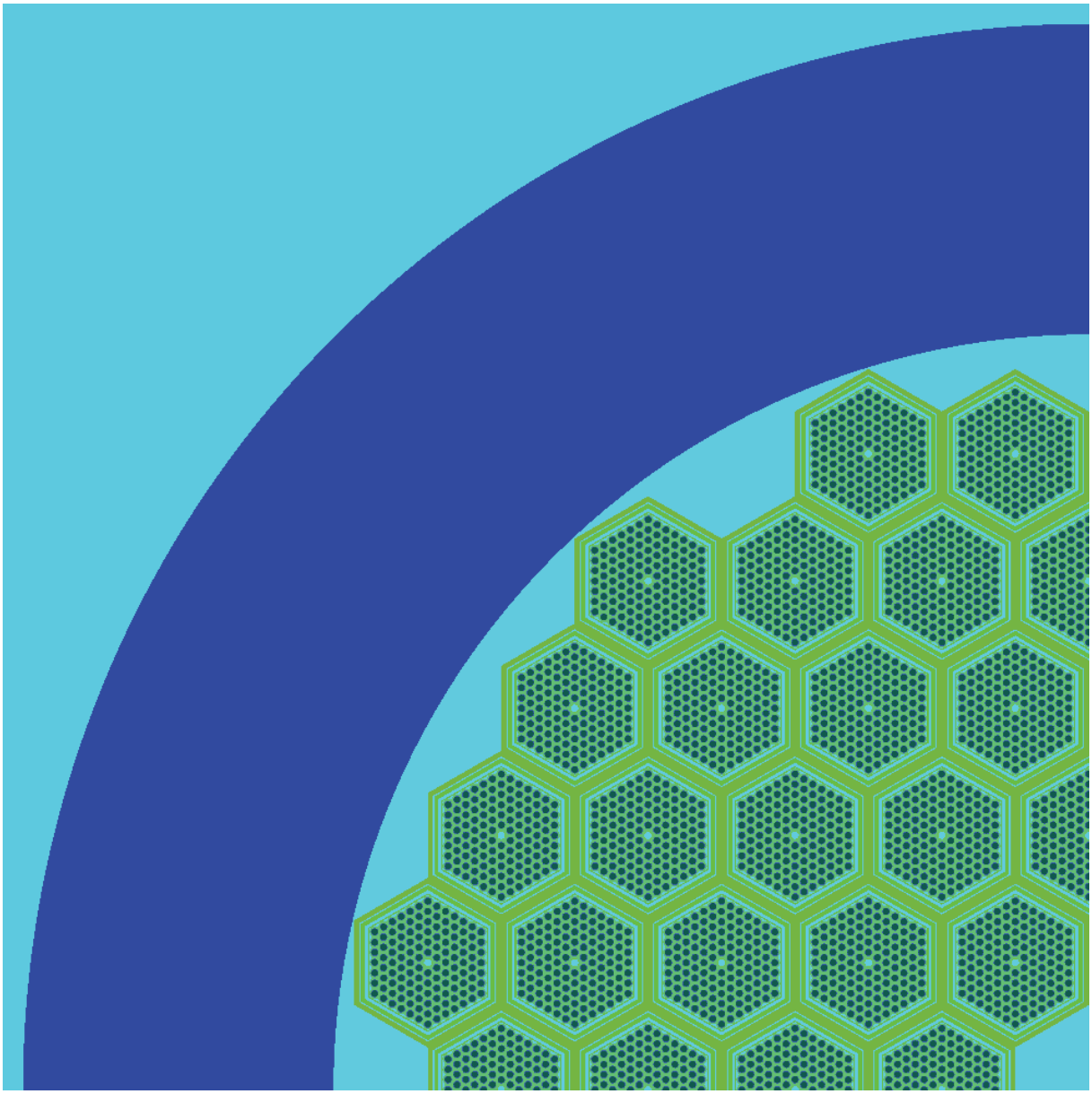


Fig. 2 Cross Section of Cask Unit - FA in storage tubes surrounded with intervening plates

Fig. 3 Horizontal Cask Cross Section (quarter of x-y slice at z=100 cm)



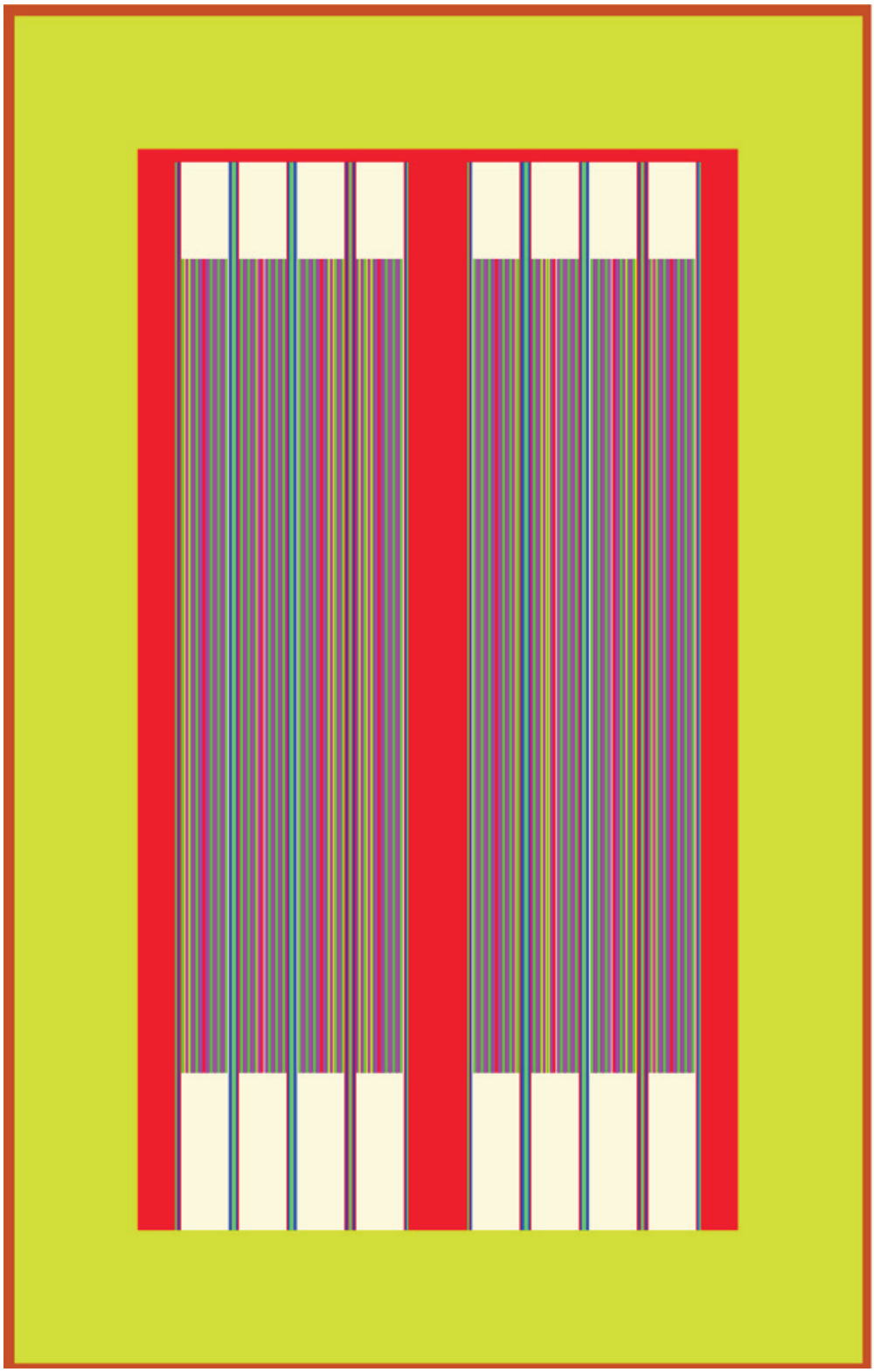


Fig. 4 Cask Lateral Cross Section (z-x slice at y=0)

4. Parameters required

4.1. Fuel compositions

Provide atom densities, in [atom/barn·cm], for the light element, actinide, and fission product nuclides designated as 'Benchmark resulted nuclides' in Table 1, 3rd column, for each of the time case numbers 2-30 listed inTable 2.

4.2. k_{eff} calculations

Provide k_{eff} values of the fully loaded flooded cask for fresh fuel and for isotopic compositions resulted from the decay calculations (for 31 cases: 1 fresh fuel composition and 30 decay-time steps according to the Table 2). If the k_{eff} values are calculated using a Monte Carlo transport code the values of estimated standard deviation will be reported. The reported values should contain four significant digits.

5. Requested Information and Results

Forward the results via e-mail to NRI at Rez, Czech Republic to haf@nri.cz or mar@nri.cz . The results should be provided in two files according to the format instructions provided below.

5.1. Spent fuel composition results

The "spent fuel composition results" file should be composed of:

Line No. / Contents

1. "VVER-440 assembly: 4.25 wt% ^{235}U enrichment and 50 MWd/kg$_U$ burnup"
2. Date
3. Institute
4. Contact Person
5. E-mail address of the contact person
6. Computer Code
7. *Time case 2*
8. Nuclide density (atom/barn·cm) of ^{14}C
9. Nuclide density (atom/barn·cm) of ^{36}Cl
10. Nuclide density (atom/barn·cm) of ^{41}Ca
11. Nuclide density (atom/barn·cm) of ^{59}Ni
12. Nuclide density (atom/barn·cm) of ^{79}Se
13. Nuclide density (atom/barn·cm) of ^{93}Zr
14. Nuclide density (atom/barn·cm) of ^{90}Sr
15. Nuclide density (atom/barn·cm) of ^{93m}Nb
16. Nuclide density (atom/barn·cm) of ^{94}Nb
17. Nuclide density (atom/barn·cm) of ^{93}Mo
18. Nuclide density (atom/barn·cm) of ^{95}Mo
19. Nuclide density (atom/barn·cm) of ^{99}Tc
20. Nuclide density (atom/barn·cm) of ^{101}Ru
21. Nuclide density (atom/barn·cm) of ^{103}Rh

22. Nuclide density (atom/barn·cm) of ^{107}Pd
23. Nuclide density (atom/barn·cm) of ^{109}Ag
24. Nuclide density (atom/barn·cm) of ^{126}Sn
25. Nuclide density (atom/barn·cm) of ^{126}Sb
26. Nuclide density (atom/barn·cm) of ^{126m}Sb
27. Nuclide density (atom/barn·cm) of ^{129}I
28. Nuclide density (atom/barn·cm) of ^{133}Cs
29. Nuclide density (atom/barn·cm) of ^{135}Cs
30. Nuclide density (atom/barn·cm) of ^{137}Cs
31. Nuclide density (atom/barn·cm) of ^{143}Nd
32. Nuclide density (atom/barn·cm) of ^{145}Nd
33. Nuclide density (atom/barn·cm) of ^{147}Sm
34. Nuclide density (atom/barn·cm) of ^{149}Sm
35. Nuclide density (atom/barn·cm) of ^{150}Sm
36. Nuclide density (atom/barn·cm) of ^{151}Sm
37. Nuclide density (atom/barn·cm) of ^{152}Sm
38. Nuclide density (atom/barn·cm) of ^{151}Eu
39. Nuclide density (atom/barn·cm) of ^{153}Eu
40. Nuclide density (atom/barn·cm) of ^{155}Gd
41. Nuclide density (atom/barn·cm) of ^{210}Pb
42. Nuclide density (atom/barn·cm) of ^{226}Ra
43. Nuclide density (atom/barn·cm) of ^{228}Ra
44. Nuclide density (atom/barn·cm) of ^{227}Ac
45. Nuclide density (atom/barn·cm) of ^{229}Th
46. Nuclide density (atom/barn·cm) of ^{230}Th
47. Nuclide density (atom/barn·cm) of ^{232}Th
48. Nuclide density (atom/barn·cm) of ^{231}Pa
49. Nuclide density (atom/barn·cm) of ^{232}U
50. Nuclide density (atom/barn·cm) of ^{233}U
51. Nuclide density (atom/barn·cm) of ^{234}U
52. Nuclide density (atom/barn·cm) of ^{235}U
53. Nuclide density (atom/barn·cm) of ^{236}U
54. Nuclide density (atom/barn·cm) of ^{238}U
55. Nuclide density (atom/barn·cm) of ^{238}Pu
56. Nuclide density (atom/barn·cm) of ^{239}Pu
57. Nuclide density (atom/barn·cm) of ^{240}Pu
58. Nuclide density (atom/barn·cm) of ^{241}Pu
59. Nuclide density (atom/barn·cm) of ^{242}Pu
60. Nuclide density (atom/barn·cm) of ^{237}Np
61. Nuclide density (atom/barn·cm) of ^{241}Am
62. Nuclide density (atom/barn·cm) of ^{242m}Am
63. Nuclide density (atom/barn·cm) of ^{243}Am
64. Nuclide density (atom/barn·cm) of ^{245}Cm
65. Nuclide density (atom/barn·cm) of ^{246}Cm
66. *Time case 3*
67. As for items 8 to 65

and so on for the following Time cases from 4 to 30.

As for the last record of the file, please, describe your analysis environment here. It will be included in the benchmark report. The description should include:
Institute and country, participants, neutron data library, neutron data processing code or method, description of your code system, omitted nuclides if any, omitted cases if any, other related information.

5.2. k_{eff} values

The "keff results" file should be composed of:

Line No.	Contents
1	"keff calculation"
2	Date
3	Institute
4	Contact Person
5	E-mail address of the contact person
6	Computer Code
7	"actinide and fission products "
8	k_{eff} ("±" standard deviation, if applicable) value for fresh fuel
9 to 38	k_{eff} ("±" standard deviation, if applicable) values for cases 31 through 60 (see Section 4.2 for case description).
39	Please describe your analysis environment here. It will be included in the benchmark report. The description should include: Institute and country, participants, description of your code system, neutron data library, neutron data processing code or method, neutron energy groups, geometry modeling (3-D, 2-D etc.), omitted nuclides if any, omitted cases if any, other related information.

6. Schedule

Submission of the benchmark results for evaluation is expected by the end of 2010. A preliminary evaluation related to AER Group E participant contributions will be made in July 2010.

7. Reference

/1/ John C. Wagner, Georgeta Radulescu (ORNL, USA), 'Specification for Phase VII Benchmark UO2 Fuel: Study of spent fuel compositions for long-term disposal', November, 2008

/2/ John C. Wagner, preliminary results of the Phase VII Benchmark, Eighteenth Meeting of the Expert Group on Burnup Credit Criticality (OECD/NEA/NSC EGBUC) 26 October 2009, Cordoba, Spain

/3/ L. Markova, 'Specification of the CB4 Burnup Credit Benchmark', 6th Meeting of AER Working Group E on Physical Problems on Spent Fuel, Radwaste and Decommissioning of Nuclear Power Plants, Trnava, Slovak Republic, April 24-25, 2001

/4/ L. Markova, 'Final Evaluation of CB4 VVER Benchmark', 6th meeting of the Working Party on Nuclear Criticality Safety (OECD/NEA/NSC WPNCS) & 11th meeting of Expert Group on Burnup Credit Criticality Safety (EGBUC), Issy-les-Moulieaux, Paris, September 9, 2002