Codes And Methods Improvements for VVER comprehensive safety assessment

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WP4 - Task 4.2

D4.3 – Definitions of tests cases for the verification phases of the multi-parametric library generator

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Version 1 – 11/02/2021

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Summary

The H2020 CAMIVVER project aims to develop and improve codes and methods for VVER comprehensive safety assessment.

In the Work Package 4 (WP4), Task 4.1 is intended to the creation of a multi-parametric neutron data library generator prototype based on APOLLO3®. Task 4.2, for its part, is dedicated to the verification of the consistency of the prototype generator based on APOLLO3®. The activity carried out within Task 4.2 is organised in two parts: first one is the definition and selection of test cases (VVER and PWR) to be used and the parameters to be compared and second one is the result comparison on the basis of the selected configurations. The present document fits in the first part of Task 4.2 and corresponds to Deliverable 4.3 *(Definitions of tests cases for the verification phases of the multi-parametric library generator*) of the CAMIVVER project.

The aim of this document is to summarize in a common document available to all the partners the data (assembly and reflector descriptions) to be used on the activities carried out within WP4 (Verification and Validation process of the neutron library generator prototype based on APOLLO3® and developed within Task 4.1) and WP5 (core and transient calculation).

The deliverable is completed by indications on the activities of verification to be carried out within Task 4.2: Calculation options for deterministic/stochastic comparison, methods and dataset for depletion comparison, methods and dataset for state-point comparison, output expectation, PWR and VVER tests cases selection.

Validation and verification of the prototype's development will be performed against five VVER assemblies, three PWR assemblies and three rods type

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CAMIVVER - D4.3 - Definitions of tests cases for the verification phases of the multi-parametric library generator

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AVERTISSEMENT / CAUTION

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The deliverable is completed by indications on the activities of verification to be carried out within Task 4.2: Calculation options for deterministic/stochastic comparison, methods and dataset for depletion comparison, methods and dataset for state-point comparison, output expectation, PWR and VVER tests cases selection.

Validation and verification of the prototype's development will be performed against the following assemblies:

- Khmelnitsky-2 390GO with and without dysprosium rod;
- Khmelnitsky-2 13AU and 30AV5 (no rod);
- Kozloduy-6 profiled UOX (3.3%/3.0%) with and without B_4C rod;
- Kozloduy-6 UOX 4.4% (no rod);
- PWR UOX 3.7% with and without AIC rod;
- KAIST UOX 3.3%, UOX gadolinium and MOX heterogeneous (no rod).

Table of Contents

1. Introduction

The H2020 CAMIVVER project aims to develop and improve codes and methods for VVER comprehensive safety assessment.

In the Work Package 4 (WP4), Task 4.1 is intended to the creation of a multi-parametric neutron data library generator prototype based on APOLLO3®. Task 4.2, for its part, is dedicated to the verification of the consistency of the prototype generator based on APOLLO3®. The activity carried out within Task 4.2 is organised in two parts: first one is the definition and selection of test cases (VVER and PWR) to be used and the parameters to be compared and second one is the result comparison on the basis of the selected configurations.

The present document corresponds to Deliverable 4.3 *(Definitions of tests cases for the verification phases of the multi-parametric library generator*) of the CAMIVVER project. The aim of this document is to summarize in a common document available to all the partners the data (assembly and reflector descriptions) to be used on the activities carried out within WP4 (Verification and Validation process of the neutron library generator prototype based on APOLLO3® and developed within Task 4.1) and WP5 (core and transient calculation). The data here summarized are -in coherence with the VVER data shown in Deliverable 3.2 (*Definition report with specification for NPP with VVER 1000 reactor with respect to selected transients*) and the core model and boundary conditions presented in D5.1 (*Description of the core reference test cases – Part 1*).

The present document collects assembly and reflector data for the VVER cases (chapter 2) as well as for the PWR cases (chapter 3).

In order to complete the deliverable, chapters 4 and 5 bring some indications on the activities of verification to be carried out within Task 4.2. In particular as indicated in [1], for the PWR assemblies cases the verification of the results obtained with APOLLO3® prototype will be carried out by comparing against the results obtained by the French industrial multi-parametric neutron data libraries generator based on APOLLO2 and reference stochastics calculations based on TRIPOLI-4® and SERPENT Monte-Carlo codes. As for VVER assembly's cases, verification will be ensured by comparing results against calculations based on reference stochastics codes (TRIPOLI-4® and SERPENT) only as well as for the reflector part (either PWR and VVER cases). A schedule for verification and validation is proposed in chapter 4. Finally, chapter 5 describes physical data expected during the V&V process.

The selection of assembly described here has been done for the sake of consistency with the proposed activities in WP5 [1], where benchmarks require neutron data libraries generated by the APOLLO3® based prototype.

Data compiled and presented within this document should be used to set up models for the 2D lattice transport calculations. Additional information, required to generate the multi-parametric data libraries (e.g. water density variation range, xenon level range, burn-up points, etc.) and for determining the feedbacks during core calculations are provided in the present document. Concerning core calculation, specific data (e.g. boundary conditions) will be available by D3.2 and D5.1.

Some of the data reported in chapter 4 (e.g. information about possible calculation scheme, branching points, etc.) is not definitive and should be treated as it. Some changes will very likely emerge during the discussions foreseen within tasks 4.1 and 4.3.

2. Assemblies and reflectors description for VVER Benchmarks

Both benchmarks selected in the CAMIVVER project are VVER-1000 reactors: the OECD NEA benchmark Kozloduy-6 (see [2][3][4][5]) and the AER Symposium proposed benchmark Khmelnitsky-2 (see [6][7]) provide useful data for this process of verification and validation. As indicated in [8], small core configurations will be considered for WP5 activities. However full core model may be considered for the following phase of the project and small description is added in Appendix.

Several different assemblies' types in terms of technology and fuel mapping configuration will be integrated to the tests cases base. The following sections are dedicated to the description of the VVER assemblies. The data required for deterministic and stochastic assembly modelling and calculations are summarized hereafter. They are extracted from the available literature and share among partners within WP3. The best level of data accuracy will be provided in accordance with information collected on different documents.

2.1. Nominal conditions

The nominal conditions for Kozloduy-6 and Khmelnitsky-2 are specified in Table 1. These conditions are the ones that will be used during the fuel depletion calculation. Information for branches calculations is provided in chapter 4.

	Kozloduy-6	**Khmelnitsky-2**
Reactor power [MWth]	3000	
Linear power [W/cm]	166.2	
Specific power [MW/MTHM][1]	36.8577	
Reactor pressure [MPa]	15.7	
Moderator temperature [K]	574	560
Moderator density [g/cm^3]	0.725	0.7526
Fuel temperature [K]	900	
Cladding temperature [K]	600	
Boron concentration [g/kg] [2]	3.431	
Boron concentration [ppm]	600	

Table 1: VVER nominal conditions - [4][7]

[1] Megawatt per metric ton of heavy metal loaded.

[2] $CB_{ppm} = CB_{g/kg} \times 174.88$ [7]

2.2. Fuel assembly design

Figures below describe 2D assembly configurations from Kozloduy-6 and Khmelnitsky-2 benchmarks. In particular, five different assembly types and two different fuel types, UOX (UO_2 enriched with ^{235}U) and UOX gadolinium (5% Gd_2O_3 and UO_2 enriched with ^{235}U), are defined:

- six homogeneous UOX assemblies (four for Kozloduy-6 UOX 2%, 3%, 3.3% and 4.4% and two for Khmelnitsky-2 UOX 1.3% and 2.2%, see Figure 1 and Figure 2);
- three homogeneous UOX gadolinium assemblies (for Khmelnitsky-2 see Figure 3, Figure 4 and Figure 5);
- two heterogeneous profiled UOX assemblies (for Kozloduy-6 see Figure 6 and Figure 7);
- two heterogeneous UOX gadolinium assemblies with zoning ring and corners (for Khmelnitsky-2 see Figure 8 and Figure 9);
- and one heterogeneous UOX gadolinium with zoning ring (for Khmelnitsky-2 see Figure 10).

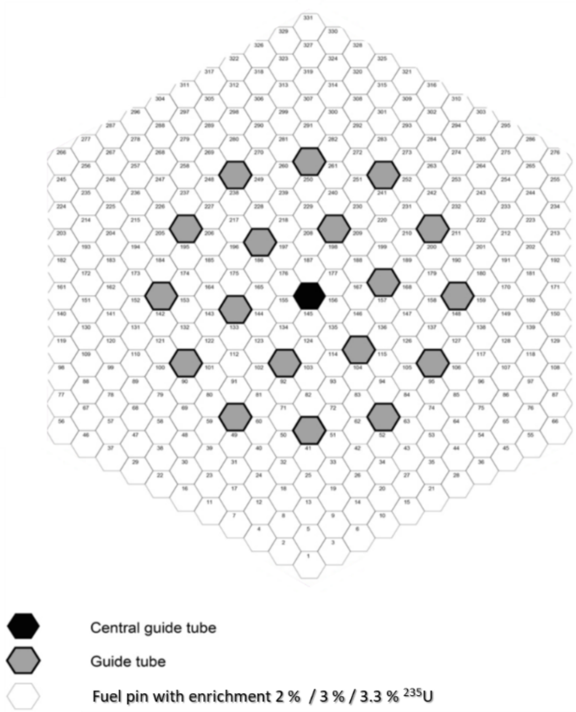


Figure 1: Kozloduy-6 fuel assembly type UOX 2%, 3%, 3.3% and 4.4%

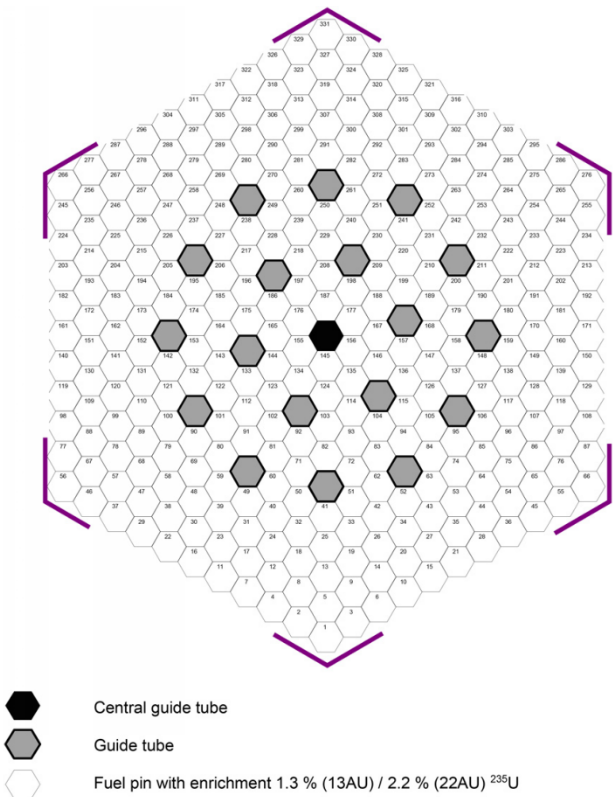


Figure 2: Khmelnitsky-2 fuel assembly type 13AU and 22AU [7]

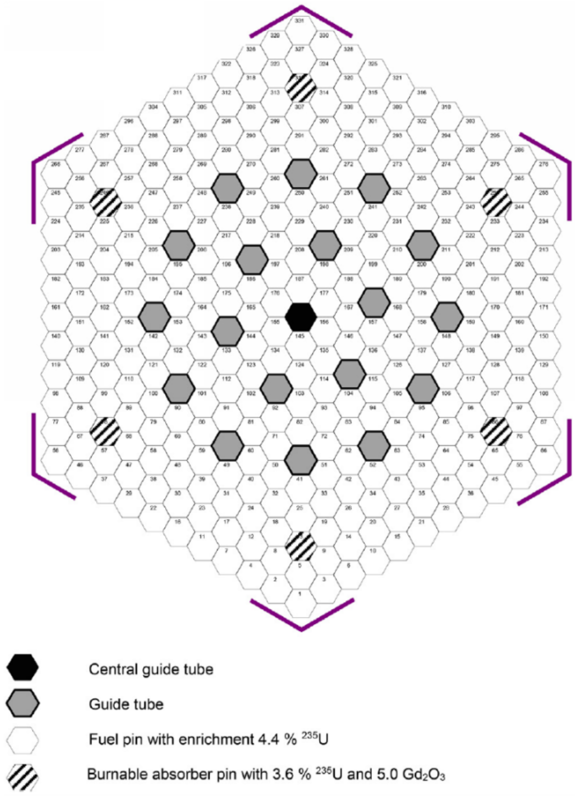


Figure 3: Khmelnitsky-2 fuel assembly type 439GT [7]

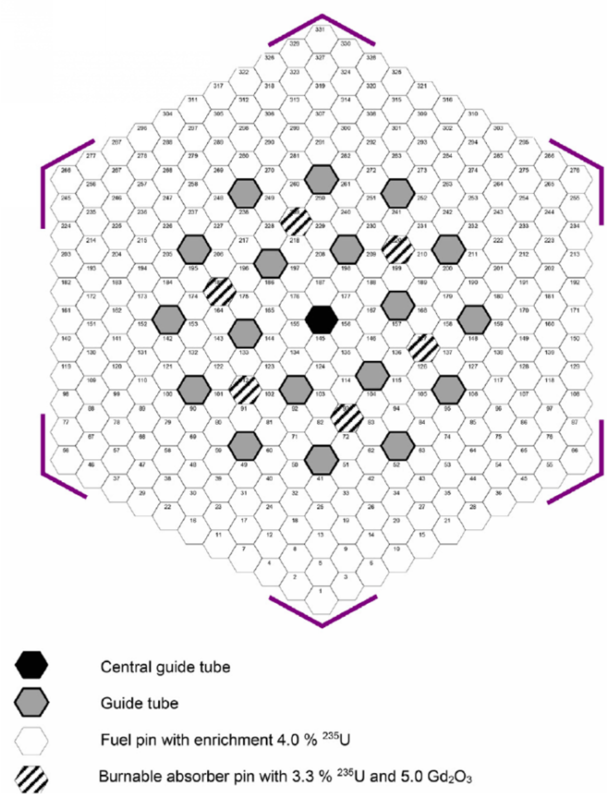


Figure 4: Khmelnitsky-2 fuel assembly type 398GO [7]

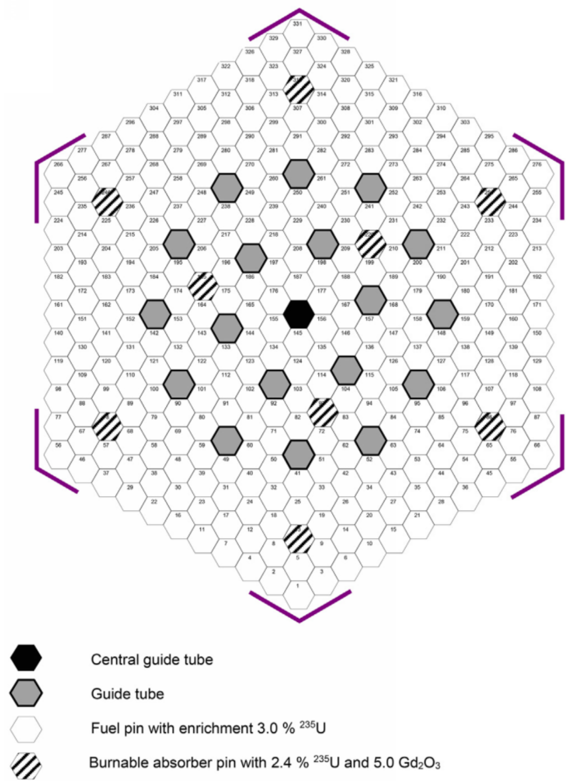


Figure 5: Khmelnitsky-2 fuel assembly type 30AV5 [7]

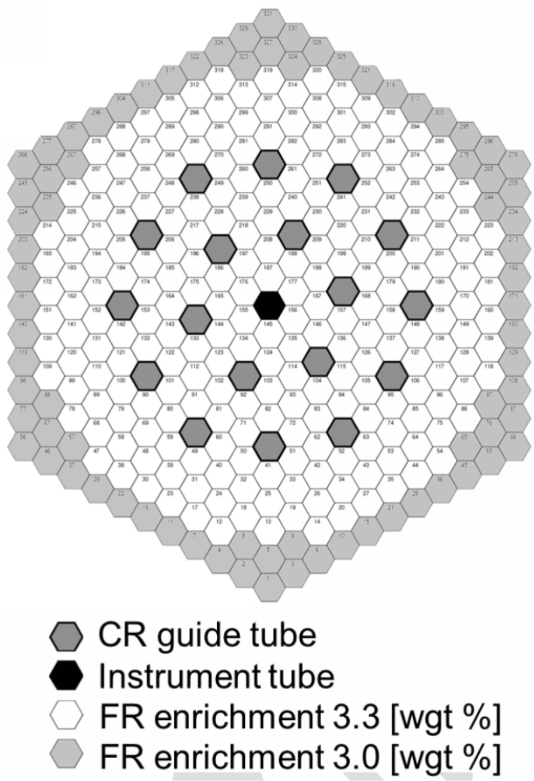


Figure 6: Kozloduy-6 profiled fuel assembly 2D assembly layout

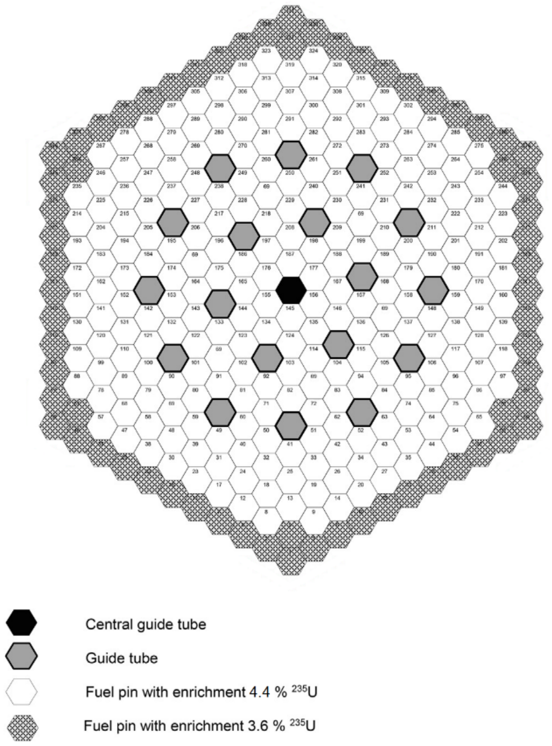


Figure 7: Kozloduy-6 profiled fuel assembly 2D assembly layout

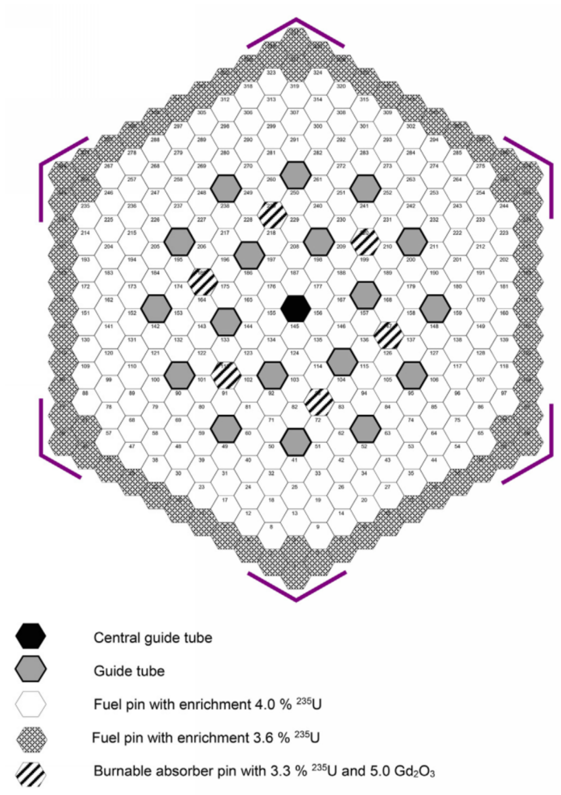


Figure 8: Khmelnitsky-2 fuel assembly type 390GO [7]

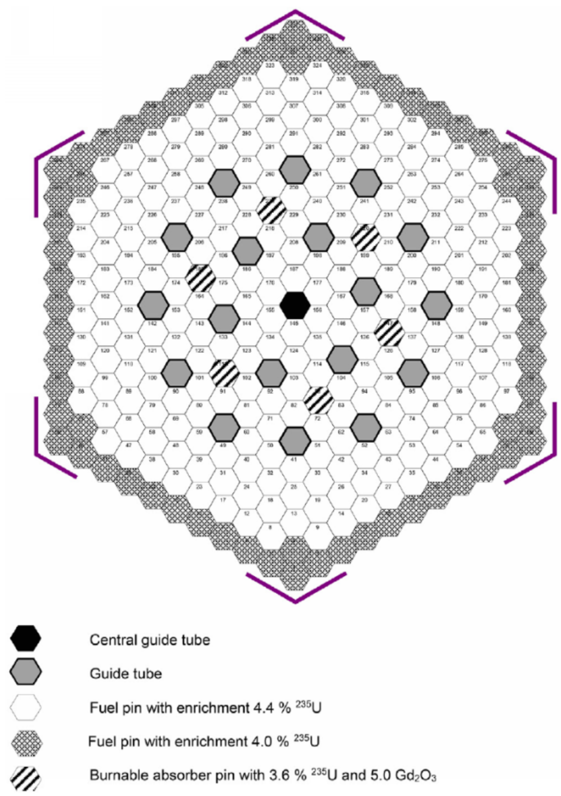


Figure 9: Khmelnitsky-2 fuel assembly type 430GO [7]

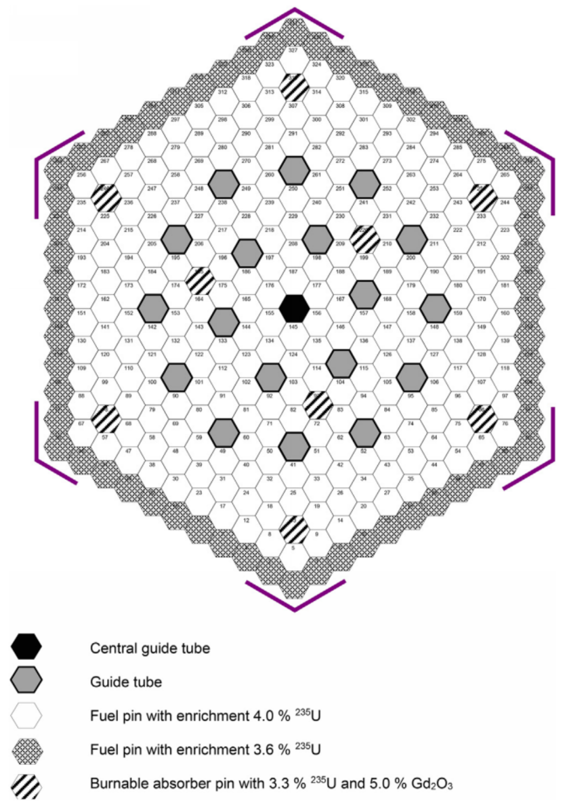


Figure 10: Khmelnitsky-2 fuel assembly type 39AWU [7]

Geometrical data for 2D lattice description of assemblies are available in Table 2, Table 3, Table 4 and Table 5. Material expansion is not considered in lattice calculation and so no expansion laws will be provided in this document.

	Kozloduy-6	Khmelnitsky-2
Number of fuel rods	312	
Number of central guide tube	1	
Number of guide tubes per assembly	18	
Fuel assembly lattice pitch [cm]	23.6	
Fuel assembly wrench size [cm]	23.4	23.48
Active height [cm]	353 (cold state) / 355 (hot state)	

Table 2: Assembly data - [2][4][7]

2.2.1. Cells description

Figure 11 and Figure 12 give a look at the fuel cell while Figure 13 and Figure 14 show detail for respectively control rod cells and central tube cell details.

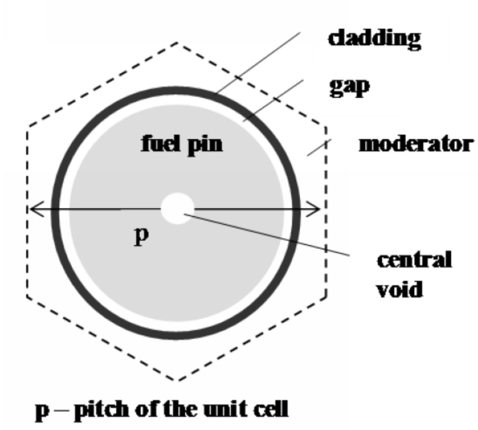


Figure 11: Kozloduy-6 fuel cell [2]

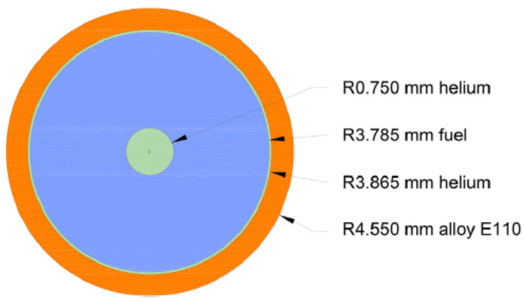


Figure 12: Khmelnitsky-2 fuel cell [7]

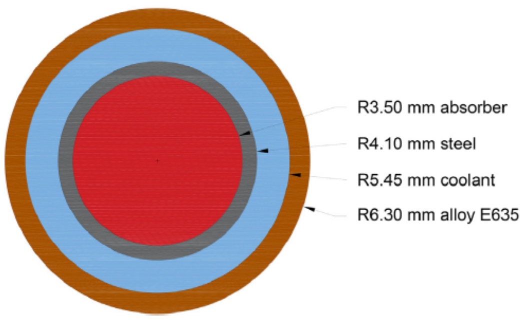


Figure 13: Khmelnitsky-2 guide tube with control rod cell [7]

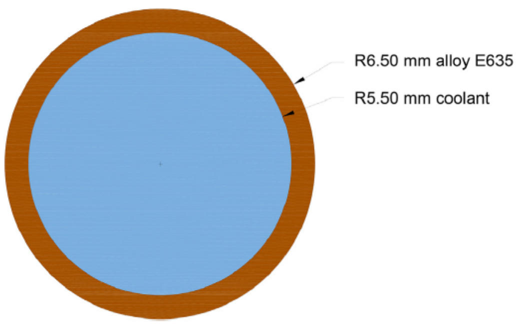


Figure 14: Khmelnitsky-2 central tube [7]

	Kozloduy-6	**Khmelnitsky-2**
Unit cell pitch [cm]	1.275	
Fuel rod grid	Triangular	
Fuel pellet diameter [cm]	0.756	0.757
Fuel pellet material	UO_2 / profiled UO_2	UO_2 or UO_2 + Gd_2O_3
Central void diameter [cm]	0.14 [3]	0.15
Central void material	He	
Cladding inner diameter [cm]	0.772	0.773
Cladding outer diameter [cm]	0.91	
Cladding material	Alloy E110 (Zr+1%Nb)	
Gap material	He	

Table 3: Fuel cell data - [2][4][5][7]

	Kozloduy-6	**Khmelnitsky-2**
Guide tube inner diameter [cm]	1.10	1.09
Guide tube outer diameter [cm]	1.26	
Guide tube material	Steel 08X18H10T	Alloy E635
Absorber number	18, fill in the guide tubes	
Absorber (control rods) pellet diameter [cm]	0.70	
Absorber material	B_4C	B_4C or Dy_2O_3 TiO_2
Absorber cladding outer diameter [cm]	0.82	
Cladding material	Steel 06X18H10T	Steel
Central inner diameter [cm]	0.96	1.1
Central tube outer diameter [cm]	1.12	1.3
Cladding material	Alloy E110 (Zr+1%Nb)	Alloy E635

Table 4: Guide tube, control rod and central tube data - [2][4][7]

NB: It has been decided to smear the gap in the clad. The consequences are the modification on the clad inner diameter (equal to fuel pellet diameter) and the decrease of clad material density.

[3] In reference [5], two central void diameters are defined for the same fuel technology, 2.35 mm and 1.4 mm as different documents contradict each other. Despite of this unclear definition, central void diameter of 1.4 mm will be considered in the Task 4.2 but both central void diameters will be used to generate two sets of libraries for WP5 as discussed during the WP4/WP5 meeting of 05/02/2021.

2.2.2. Stiffening plate and spacer grid

The fuel assembly design used in Khmelnitsky-2 is composed of stiffening plates in each corner improving the mechanical stability of the assembly. A 2D scheme of a stiffener is presented in Figure 15. The modelling of the stiffening plates in deterministic codes like APOLLO3® may be discussed as part of the actions of task 4.1. Different options may be considered (real geometry or smeared in moderator associated to corner's cells). The option retained for the modelling in the prototype will not be detailed in this deliverable.

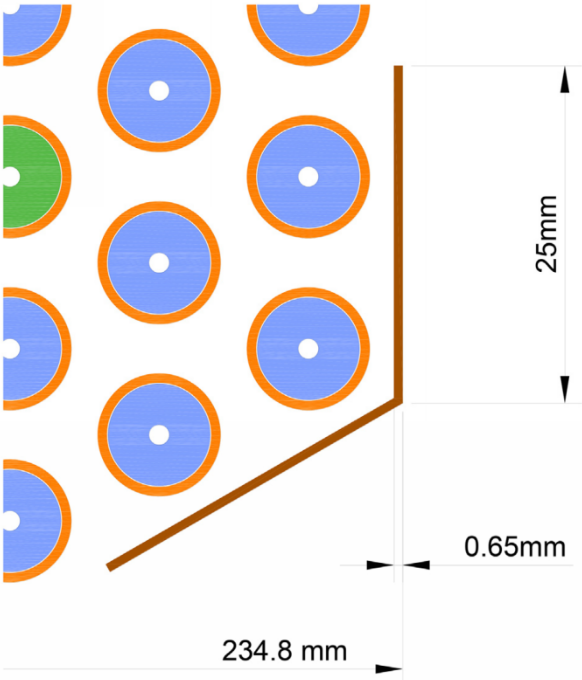


Figure 15: Corner stiffener geometry [7]

	Kozloduy-6	Khmelnitsky-2
Number of corner stiffeners in Fuel Assembly (FA)	None	6
Width [cm]		2.5
Thickness [cm]		0.065
Material		Alloy E635

Table 5: Stiffening plate data - [7][5]

3D spacer grids cannot be explicitly modelled on 2D lattice calculation. In order to take into account their impact on core calculation, spacer grids may be modelled as an additional thickness of fuel cladding preserving alloy mass (as proposed in [7]) or smeared in the moderator (as indicated in [3]). Once again the choice of the modelling option to be implemented in the prototype will be discussed within Task 4.1. Spacer grids data are compiled in Table 6.

	Kozloduy-6	**Khmelnitsky-2**
Number of spacer grids in FA	13	14
Axial pitch [cm]	25.5	25.5
Width [cm]	3.0	2.0
Mass [kg]	0.654	0.55
Volume	1.2% of the FA volume	
Material	Steel 08X18H10T	Alloy E110 (Zr+1%Nb)

Table 6: Spacer grid data - [5][7]

The actions carried out in WP4 and WP5 are exclusively code-to-code benchmarks so in this case the detailed modelling of stiffening plates and spacer grid becomes less critical. Nevertheless, it is crucial to verify the correctness of the implementation of these features in the prototype in order to prepare - industrial applications. The smearing feature must be validated on one test-case including spacer grids. A more explicit grid model will be tested within task 4.4, different approaches are under discussion at this time.

2.3. Fuel composition

2.3.1. Kozloduy-6

NB: Atomic density has been calculated using the industrial version of APOLLO2 code.

	Fuel with enrichment 2.0% ^{235}U **Figure 1**	**Fuel with enrichment 3.0% ^{235}U** **Figure 1**	**Fuel with enrichment 3.3% ^{235}U** **Figure 1**
Fuel density [g/cm^3]	10.6	10.6	10.6
Fuel composition [w/o]			
U235	2.0	3.0	3.3
U238	97.9946	96.9946	96.6946
U234	0.0054	0.0054	0.0054
Fuel composition [10^{24} at/cm^3]			
U235	4.788116e-04	7.182066e-04	7.900237e-04
U238	2.316416e-02	2.292744e-02	2.285642e-02
U234	1.298335e-06	1.298315e-06	1.298309e-06
O16	4.728855e-02	4.729388e-02	4.729548e-02

Table 7: Kozloduy-6 fuel composition data [2][3][5]

	Fuel with enrichment 3.6% ^{235}U **Figure 7**	**Fuel with enrichment 4.4% ^{235}U** **Figure 7**
Fuel density [g/cm^3]	10.6	10.6
Fuel composition [w/o]		
U235	3.6	4.4
U238	96.3946	95.5946
U234	0.0054	0.0054
Fuel composition [10^{24} at/cm^3]		
U235	8.618401e-04	1.053347e-03
U238	2.278540e-02	2.259603e-02
U234	1.298303e-06	1.298288e-06
O16	4.729708e-02	4.730135e-02

Table 8: Kozloduy-6 fuel composition data [2][3][5]

2.3.2. Khmelnitsky-2

NB: Atomic density has been extracted from Excel file provided by [7].

13AU and 22AU Types	Fuel with enrichment 1.3% ^{235}U Figure 2	Fuel with enrichment 2.2% ^{235}U Figure 2
Fuel density [g/cm^3]	10.2605	10.2605
Fuel composition [w/o]		
U235	1.3	2.2
U238	98.7	97.8
U234	0.0	0.0
Fuel composition [10^{24} at/cm^3] [4]		
U235	3.01261e-04	5.09820e-04
U238	2.25838e-02	2.23776e-02
O16	4.57701e-02	4.57747e-02

Table 9: Khmelnitsky-2 fuel composition data for 13AU (1.3% ^{235}U) and 22AU (2.2% ^{235}U) assembly types [7]

[4] See Excel file attached to [7]

430GO Type **Figure 9**	**Fuel with enrichment 4.4% ^{235}U**	**Fuel with enrichment 4.0% ^{235}U**	**Burnable absorber with UO_2 (3.6% ^{235}U) and 5.0% Gd_2O_3**
Fuel density [g/cm^3]	10.2605	10.2605	10.2279
	Fuel composition [w/o]		
U235	4.4	4.0	3.6
U238	95.6	96.0	96.4
U234	0.0	0.0	0.0
	Fuel composition [10^{24} at/cm^3] [4]		
U235	1.01961e-03	9.26920e-04	7,90006e-04
U238	2.18734e-02	2.19651e-02	2,08874e-02
O16	4.57861e-02	4.57840e-02	4,59036e-02
Gd152			3,51766e-06
Gd154			3,78440e-05
Gd155			2,55262e-04
Gd156			3,50791e-04
Gd157			2,66479e-04
Gd158			4,20283e-04
Gd160			3,65230e-04

Table 10: Khmelnitsky-2 fuel composition data for 430GO assembly type [7]

390GO and 39AWU Types Figure 8 and Figure 10	**Fuel with enrichment 4.0% ^{235}U**	**Fuel with enrichment 3.6% ^{235}U**	**Burnable absorber with UO_2 (3.3% ^{235}U) and 5.0% Gd_2O_3**
Fuel density [g/cm^3]	10.2605	10.2605	10.2279
Fuel composition [w/o]			
U235	4.0	3.6	3.3
U238	96.0	96.4	96.7
U234	0.0	0.0	0.0
Fuel composition [10^{24} at/cm^3] [4]			
U235	9.2692e-04	8.34233e-04	7.24175e-04
U238	2.19651e-02	2.20568e-02	2.09525e-02
O16	4.57840e-02	4.57820e-02	4.59021e-02
Gd152			3.51766e-06
Gd154			3.78440e-05
Gd155			2.55262e-04
Gd156			3.50791e-04
Gd157			2.66479e-04
Gd158			4.20283e-04
Gd160			3.65230e-04

Table 11: Khmelnitsky-2 fuel composition data for 390GO and 39AWU assembly types [7]

30AV5 Type Figure 5	Fuel with enrichment 3.0% ^{235}U	Burnable absorber with UO_2 (2.4% ^{235}U) and 5.0% Gd_2O_3
Fuel density [g/cm^3]	10.2605	10.2279
	Fuel composition [w/o]	
U235	3.0	2.4
U238	97.0	97.6
U234	0.0	0.0
	Fuel composition [10^{24} at/cm^3] [4]	
U235	6.95201e-04	5.26680e-04
U238	2.21942e-02	2.11478e-02
O16	4.57789e-02	4.58977e-02
Gd152		3.51766e-06
Gd154		3.78440e-05
Gd155		2.55262e-04
Gd156		3.50791e-04
Gd157		2.66479e-04
Gd158		4.20283e-04
Gd160		3.65230e-04

Table 12: Khmelnitsky-2 fuel composition data for 30AV5 assembly [7]

398GO Type Figure 4	Fuel with enrichment 4.0% ^{235}U	Burnable absorber with UO_2 (3.3% ^{235}U) and 5.0% Gd_2O_3
Fuel density [g/cm^3]	10.2605	10.2279
	Fuel composition [w/o]	
U235	4.0	3.3
U238	96.0	96.7
U234	0.0	0.0
	Fuel composition [10^{24} at/cm^3] [4]	
U235	9.2692e-04	7.24175e-04
U238	2.19651e-02	2.09525e-02
O16	4.57840e-02	4.59021e-02
Gd152		3.51766e-06
Gd154		3.78440e-05
Gd155		2.55262e-04
Gd156		3.50791e-04
Gd157		2.66479e-04
Gd158		4.20283e-04
Gd160		3.65230e-04

Table 13: Khmelnitsky-2 fuel composition data for 398GO assembly [7]

439GT Type **Figure 3**	**Fuel with enrichment 4.4% ^{235}U**	**Burnable absorber with UO_2 (3.6% ^{235}U) and 5.0% Gd_2O_3**
Fuel density [g/cm^3]	10.2605	10.2279
	Fuel composition [w/o]	
U235	4.4	3.6
U238	95.6	96.7
U234	0.0	0.0
	Fuel composition [10^{24} at/cm^3] [4]	
U235	1.01961e-03	7.90006e-04
U238	2.18734e-02	2.08874e-02
O16	4.57861e-02	4.59036e-02
Gd152		3.51766e-06
Gd154		3.78440e-05
Gd155		2.55262e-04
Gd156		3.50791e-04
Gd157		2.66479e-04
Gd158		4.20283e-04
Gd160		3.65230e-04

Table 14: Khmelnitsky-2 fuel composition data for 439GT assembly [7]

2.4. Reflector design

In addition to the assembly description, the different reflector descriptions are here indicated. Temperature conditions in reflector parts are summarized in Table 15.

Top reflector	[K]	592.05
Radial reflector	[K]	Nominal moderator temperature, see Table 1
Bottom reflector	[K]	560.15

Table 15: Reflector temperature conditions [4]

2.4.1. Radial reflector

During the first discussion of the CAMIVVER project, several VVER small core configurations have been proposed to be calculated in WP5 [8].

These small VVER core configurations have been chosen for having simple and quite fast configuration which makes code-to-code comparisons under transient conditions much more convenient and affordable.

2.4.1.1. Kozloduy-6 minicore

As indicated in [8] one of the proposed VVER small core is the one shown in Figure 16 with an arrangement of 7 fuel assembly (FA), where the central position may include a control rod (CR).

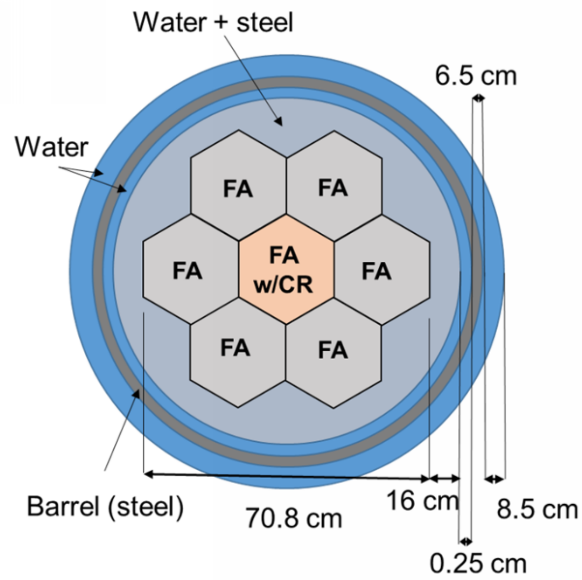


Figure 16 : Mini-core configuration based on Kozloduy-6 [8]

For generating the cross section for the reflector zone more options have to be investigated due to the impact that this choice may have on the core results. One option is the one shown in Figure 17 where the classical 1D approach is used. A more interesting option for cross-section calculation is to consider a 2D model of the reflector zone consistent with Figure 16 and with the reference Monte-Carlo calculations. The homogenized compositions are shown in Table 16.

Concerning the reflector modelling options, a discussion is needed to select the options for the benchmark as for instant 1D vs 2D geometry modelling and the treatment of the baffle zone (homogeneous vs. heterogeneous configuration). The thicknesses in Table 16 correspond to one of the slab that can be used to model the reflector.

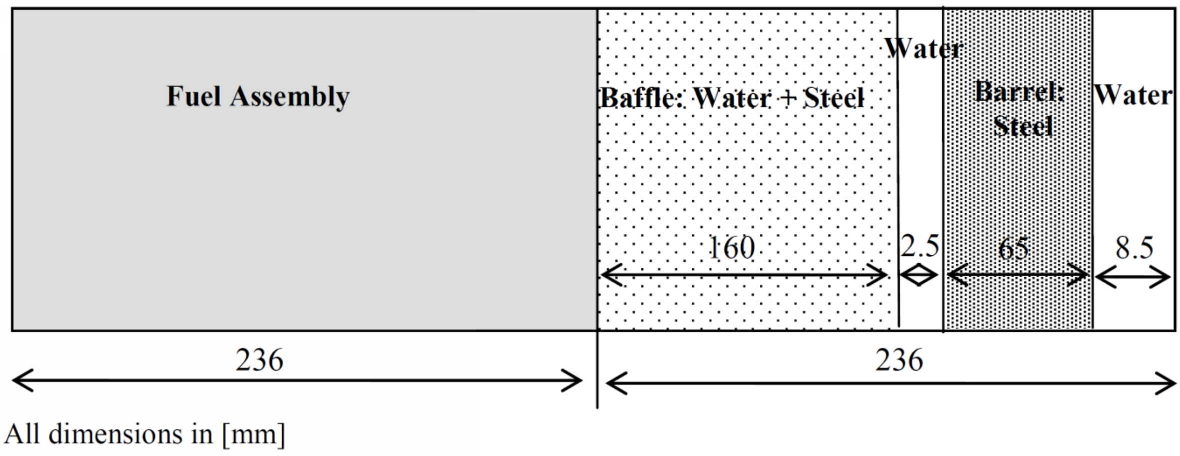


Figure 17: Kozloduy-6 mini-core radial reflector cross-section [2]

Layer	Composition		Thickness [cm]
	Material	Volume fraction (%)	
Baffle	Water	34.95	16
	Steel 08X18H10T	65.05	
Water_1	Water	100	0.25
Barrel	Steel 08X18H10T	100	6.5
Water_2	Water	100	0.85

Table 16: Kozloduy-6 mini-core radial reflector data [2]

2.4.1.2. Water reflector

As indicated in [8] another proposed VVER small core is the one shown in Figure 18.

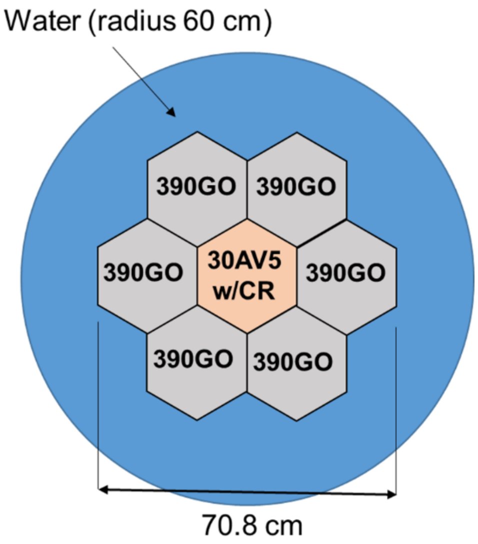


Figure 18: Mini-core configuration based on Khmelnitsky-2 [8]

For this case, a homogenized water reflector will be considered. Moderator composing this reflector is defined in Table 17.

Moderator Density: 0.7526 g/cm^3	
Elements	Atomic density [10^{24} at/cm^3]
B-10	6.67409e-06
B-11	2.68640e-05
H_2O	2.51578e-02

Table 17: Water reflector data – Boron concentration 600 ppm

2.4.2. Axial reflector

Axial layers from bottom to top are: two lower homogeneous mixture layers, fuel pin lower plug, fuel region, upper plenum and two upper homogeneous layers (Figure 19). The compositions of homogeneous mixture layers are shown in 2.5.3. Axial reflector data are enable for Kozloduy-6 but Khmelnitsky-2's axial reflector can be assumed similar to Kozloduy-6's one.

2.4.2.1. Top reflector

For the top reflector, zone a 1D model may be adopted as indicated in Table 18. The VVER top reflector model is the one shown in Figure 19.

Layer	Material	Thickness [cm]
Layer 1	Upper plenum	22.2
Layer 2	Reflector_Mix_T1	4.5
Layer 3	Reflector_Mix_T2	5.3

Table 18: Khmelnitsky-2 top reflector data [7]

2.4.2.2. Bottom reflector

For the bottom reflector, zone a 1D model may be adopted as indicated in Table 19. The VVER bottom reflector model is the one shown in Figure 19.

Layer	Material	Thickness [cm]
Layer 1	Lower plug	2.3
Layer 2	Reflector_Mix_B1	1.7
Layer 3	Reflector_Mix_B2	25

Table 19: Khmelnitsky-2 bottom reflector data [7]

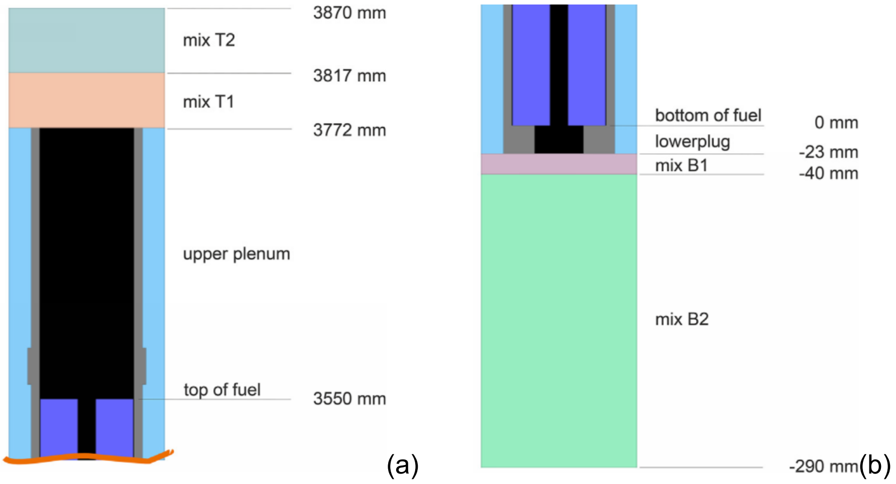


Figure 19: Axial layout of the fuel pin model Khmelnitsky-2 [7] – upper (a) and lower (b)

2.5. Material

2.5.1. Structural

NB: Kozloduy's atomic density has been calculated using the industrial version of APOLLO2 code. Khmelnitsky's atomic density has been extracted from Excel file provided by [7].

Khmelnitsky-2 – Alloy E110 (Zr+1%Nb) [7] Density: 6.4516 g/cm^3			
Elements	Wt%	Atomic density [10^{24} at/cm^3]	
Zr	98.97	Zr-90	2.20052e-02
		Zr-91	4.74596e-03
		Zr-92	7.17541e-03
		Zr-94	7.11667e-03
		Zr-96	1.12260e-03
Nb	1.00	Nb-93	4.18189e-04
Hf	0.03	Hf-174	1.07216e-08
		Hf-176	3.48463e-07
		Hf-177	1.22523e-06
		Hf-178	1.78690e-06
		Hf-179	8.87146e-07
		Hf-180	2.27225e-06

Table 20: Khmelnitsky-2 – Alloy E110

Kozloduy-6 – Alloy E110 (Zr+1%Nb) [3] Central tube density : 6.52 g/cm^3			
Elements	Wt%	Atomic density [10^{24} at/cm^3]	
Zr	98.97	Zr-90	2.191687e-02
		Zr-91	4.779539e-03
		Zr-92	7.305624e-03
		Zr-94	7.403600e-03
		Zr-96	1.192755e-03
Nb	1.00	Nb-93	4.226374e-04
Hf	0.03	Hf-174	1.055923e-08
		Hf-176	3.471349e-07
		Hf-177	1.227511e-06
		Hf-178	1.800349e-06
		Hf-179	8.988550e-07
		Hf-180	2.315113e-06

Table 21: Kozloduy-6 – Alloy E110 for central tube

Kozloduy-6 – Alloy E110 (Zr+1%Nb) [3] Fuel clad density : 6.48 g/cm^3			
Elements	Wt%	Atomic density [10^{24} at/cm^3]	
Zr	98.97	Zr-90	2.178241e-02
		Zr-91	4.750217e-03
		Zr-92	7.260804e-03
		Zr-94	7.358179e-03
		Zr-96	1.185437e-03
Nb	1.00	Nb-93	4.200446e-04
Hf	0.03	Hf-174	1.049445e-08
		Hf-176	3.450052e-07
		Hf-177	1.219980e-06
		Hf-178	1.789304e-06
		Hf-179	8.933405e-07
		Hf-180	2.300909e-06

Table 22: Kozloduy-6 – Alloy E110 for fuel clad

Khmelnitsky-2 – Alloy E635 (Zr+1%Nb) [7] Density: 6.55 g/cm^3			
Elements	Wt%	Atomic density [10^{24} at/cm^3]	
Zr	98.47	Zr-90	2.22279e-02
		Zr-91	4.79400e-03
		Zr-92	7.24805e-03
		Zr-94	7.18871e-03
		Zr-96	1.13396e-03
Nb	1.00	Nb-93	4.24567e-04
Hf	0.03	Hf-174	1.08851e-08
		Hf-176	3.53778e-07
		Hf-177	1.24392e-06
		Hf-178	1.81416e-06
		Hf-179	9.00677e-07
		Hf-180	2.30690e-06
Fe	0.50	Fe-54	2.13900e-05
		Fe-56	3.23508e-04
		Fe-57	7.34371e-06
		Fe-58	9.53218e-07

Table 23: Khmelnitsky-2 – Alloy E635

Khmelnitsky-2 – Steel [7] Density: 7.90 g/cm^3			
Elements	Wt%	Atomic density [10^{24} at/cm^3]	
Cr	18.00	Cr-50	7.15598e-04
		Cr-52	1.37996e-02
		Cr-53	1.56476e-03
		Cr-54	3.89503e-04
Mn	1.50	Mn-55	1.29896e-03
Ni	11.00	Ni-58	6.06990e-03
		Ni-60	2.33812e-03
		Ni-61	1.01636e-04
		Ni-62	3.24061e-04
		Ni-64	8.25287e-05
Fe	69.50	Fe-54	3.46068e-03
		Fe-56	5.43253e-02
		Fe-57	1.25461e-03
		Fe-58	1.66965e-04

Table 24: Khmelnitsky-2 – Steel

Kozloduy-6 – Steel 06X18H10T [3] Density: 7.86 g/cm³			
Elements	Wt%	Atomic density [10^{24} at/cm^3]	
Cr	18.5	Cr-50	7.317579e-04
		Cr-52	1.411122e-02
		Cr-53	1.600099e-03
		Cr-54	3.982986e-04
Ti	0.6	Ti-46	4.894742e-05
		Ti-47	4.414167e-05
		Ti-48	4.373823e-04
		Ti-49	3.209764e-05
		Ti-50	3.073305e-05
C	0.06	C	2.366485e-04
Mn	2.0	Mn-55	1.723178e-03
Si	0.8	Si-28	1.243528e-03
		Si-29	6.314335e-05
		Si-30	4.162321e-05
S	0.02	S-32	2.802777e-05
		S-33	2.243875e-07
		S-34	1.266608e-06
		S-36	5.904940e-09
P	0.035	P-31	5.348689e-05
Ni	10.5	Ni-58	5.764637e-03
		Ni-60	2.220527e-03
		Ni-61	9.652481e-05
		Ni-62	3.077633e-04
		Ni-64	7.837824e-05

Fe	67.485	Fe-54	3.343235e-03
		Fe-56	5.248164e-02
		Fe-57	1.212030e-03
		Fe-58	1.612989e-04

Table 25: Kozloduy-6 – Steel 06X18H10T

Kozloduy-6 – Steel 08X18H10T [3] Density: 7.86 g/cm^3			
Elements	Wt%	Atomic density [10^{24} at/cm^3]	
Cr	18.5	Cr-50	7.317579e-04
		Cr-52	1.411122e-02
		Cr-53	1.600099e-03
		Cr-54	3.982986e-04
Ti	0.6	Ti-46	4.894742e-05
		Ti-47	4.414167e-05
		Ti-48	4.373823e-04
		Ti-49	3.209764e-05
		Ti-50	3.073305e-05
C	0.08	C	3.155314e-04
Mn	2.0	Mn-55	1.723178e-03
Si	0.8	Si-28	1.243528e-03
		Si-29	6.314335e-05
		Si-30	4.162321e-05
S	0.02	S-32	2.802777e-05
		S-33	2.243875e-07
		S-34	1.266608e-06
		S-36	5.904940e-09
P	0.035	P-31	5.348689e-05
Ni	10.5	Ni-58	5.764637e-03
		Ni-60	2.220527e-03
		Ni-61	9.652481e-05
		Ni-62	3.077633e-04
		Ni-64	7.837824e-05

Fe	67.465	Fe-54	3.342244e-03
		Fe-56	5.246609e-02
		Fe-57	1.211670e-03
		Fe-58	1.612511e-04

Table 26: Kozloduy-6 – Steel 08X18H10T

2.5.2. Absorber material

NB: Kozloduy's atomic density has been calculated using the industrial version of APOLLO2 code. Khmelnitsky's atomic density has been extracted from Excel file provided by [7].

Khmelnitsky-2 – B_4C [7] Density: 1.8 g/cm^3		
Elements	Wt%	Atomic density [10^{24} at/cm^3]
B-10	14.43	1.56170e-02
B-11	63.84	6.28602e-02
C	21.74	1.96193e-02

Table 27: Khmelnitsky-2 – B4C

Kozloduy-6 – B_4C [3] Density: 1.7 g/cm^3		
Elements	Wt%	Atomic density [10^{24} at/cm^3]
B-10	14.3511	1.474865e-02
B-11	63.9135	5.936517e-02
C	21.7354	1.854157e-02

Table 28: Kozloduy-6 – B4C

Khmelnitsky-2 – Dy_2O_3 TiO_2 [7] Density: 5.1 g/cm^3			
Elements	Wt%	Atomic density [10^{24} at/cm^3]	
O	18.00	O-16	3.45542e-02
Ti	12.00	Ti-46	6.35214e-04
		Ti-47	5.72848e-04
		Ti-48	5.67612e-03
		Ti-49	4.16546e-04
		Ti-50	3.98837e-04
Dy	70.00	Dy-156	7.40890e-06
		Dy-158	1.25687e-05
		Dy-160	3.08131e-04
		Dy-161	2.49905e-03
		Dy-162	3.37039e-03
		Dy-163	3.29379e-03
		Dy-164	3.73885e-03

Table 29: Khmelnitsky-2 – Dysprosium

2.5.3. Mixture

Upper plenum [7]	
Material	Vol%
Moderator	56
Steel	2
Alloy E365	11.8
Helium	30.2

Table 30: Upper reflector, first layer

Reflector_Mix_T1 [7]	
Material	Vol%
Moderator	56
Steel	1.9
Alloy E365	30.6
Helium	11.5

Table 31: Upper reflector, second layer

Reflector_Mix_T2 [7]	
Material	Vol%
Moderator	98.9
Steel	1.1

Table 32: Upper reflector, third layer

Lower plug [7]	
Material	Vol%
Moderator	58
Steel	7
Alloy E365	35

Table 33: Lower reflector, first layer

Reflector_Mix_B1 [7]	
Material	Vol%
Moderator	57
Steel	33
Alloy E365	10

Table 34: Lower reflector, second layer

Reflector_Mix_B2 [7]	
Material	Vol%
Moderator	67
Steel	33

Table 35: Lower reflector, third layer

3. Assemblies and reflectors description for PWR Benchmarks

In addition to VVER configurations and in agreement with the CAMIVVER work programme [1], PWR configurations are investigated in WP4 (for verifying the prototype results) and on WP5 for coupled calculations carried out within Task 5.3.

As indicated in [8], two PWR mini core calculations have been proposed:

- a 32 assembly small core configuration – as described in ref. [12][13] and based on [14]. This case will be the starting configuration for the Task 5.3 activities.
- a 52 assembly small core configuration based on the KAIST benchmark problem suite (see [9][10] and [11] for the reflector updated model). This case will be initially analysed within Task 4.4 because it is small enough to perform fast direct whole-reactor calculations without spatial homogenization. Besides it is suited to investigate the homogenization options of the traditional two-step calculation schemes, especially the methodology for reflector homogenization [11]. A 3D option will be investigated in a second phase of WP5.

With the two cases indicated above, six different assemblies' types in term of fuel configuration (UOX and MOX with and without gadolinium burnable absorber) are integrated to the tests cases base. Several reflector options (in particular water and heavy reflector cases) will complete the test cases. The following sections are dedicated to the description of these cases giving the data required for deterministic and stochastic calculations. The best level of data accuracy will be provided in accordance with information found on different documents. The data described here may evolve during the project on the basis of the first comparisons. Any further change will be discussed during the WP4 and WP5 meetings and updated data will be agreed among the partners.

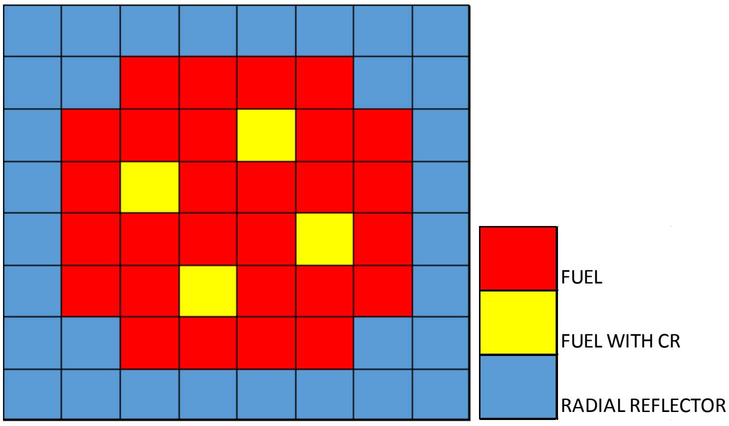
In addition other PWR assembly cases may be considered as indicated in [1].

3.1. The 32 assembly small core configuration

The 32 assembly small core configuration proposed for starting activities on Task 5.3 is here briefly described. As indicated in [12][13], Framatome has performed some efforts for compiling missing data in reference [14].

The data described here may evolve during the project on the basis of the first comparisons. They should then be considered as a "working horse" data to start related activities on WP4 and WP5. Any change will be discussed during the WP4 and WP5 meetings and updated data will be agreed among the partners.

The PWR minicore is composed of lattice (8x8) of assemblies as indicated in Figure 20.



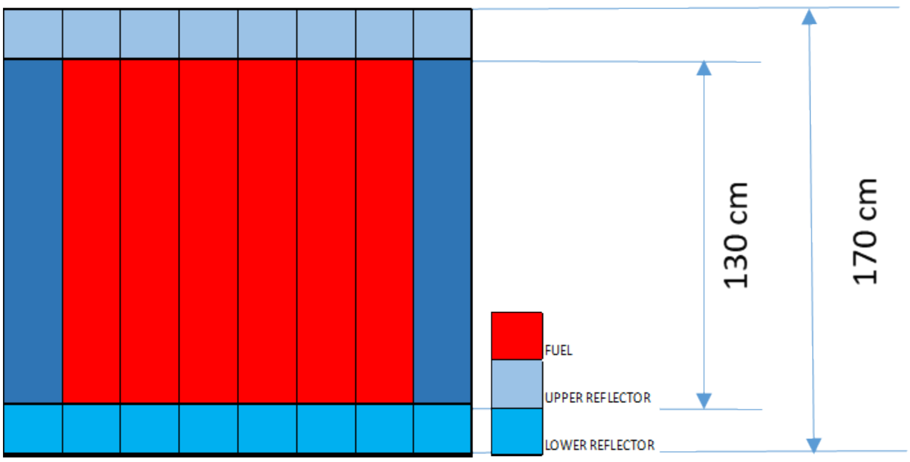


Figure 20 : PWR minicore radial and axial mapping

3.1.1. Nominal conditions

The nominal conditions are specified in Table 49. These conditions will be used during the depletion calculation. More detailed information for branches calculations is provided in [12] and [13].

Reactor power [MWth]	100
Linear power [W/cm]	91.05
Specific power [MW/MTHM][1]	16.86
Reactor pressure [MPa]	15.5
Moderator temperature [K]	577.75
Moderator density [g/cm^3]	0.717
Fuel temperature [K]	833.15
Cladding temperature [K]	577.75
Boron concentration [ppm][2]	600

Table 36: PWR minicore nominal conditions

3.1.2. Fuel assembly design

The core is composed by a single UOX 3.7% U235 enriched assembly type described in Figure 21.

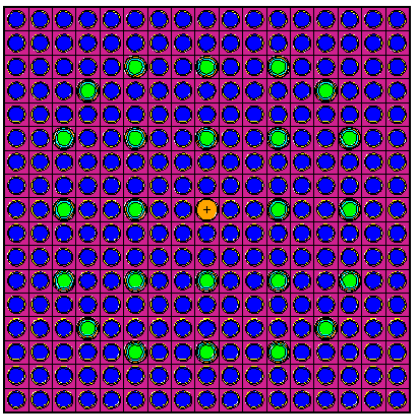


Figure 21 : UOX 3.7% 2D assembly layout

Geometrical data for 2D lattice description of assemblies are available in Table 37, Table 38 and Table 39. Material expansion is not considered in lattice calculation and so no expansion law will be provided in this document.

	32 PWR minicore
Number of fuel rods	264
Number of guide tubes	25
Assembly pitch [cm]	21.504
Assembly water blade [cm]	0.084
Active height [cm]	130.00
Total height [cm]	170.00

Table 37: PWR minicore assembly data

3.1.2.1. Cells description

	32 PWR minicore
Unit cell pitch [cm]	1.26
Fuel pellet diameter [cm]	0.8192
Fuel pellet material	UOX 3.7
Cladding inner diameter [cm]	0.836
Cladding outer diameter [cm]	0.950
Cladding material	Zircaloy
Gap material	He

Table 38: PWR minicore fuel cell data

	32 PWR minicore
Guide tube inner diameter [cm]	1.14
Guide tube outer diameter [cm]	1.22
Guide tube material	Zircaloy
Absorber number	24, fill in the guide tubes except central one
Absorber (control rods) pellet diameter [cm]	0.870
Absorber material	AIC
Absorber cladding inner diameter [cm]	0.878
Absorber cladding outer diameter [cm]	0.972
Cladding material	Zircaloy

Table 39: PWR minicore guide tube data

NB: It has been decided to smear the gap in the clad. The consequences are the modification on the clad inner diameter (equal to fuel pellet diameter) and the decrease of clad material density.

3.1.1. Fuel composition

NB: Atomic density has been calculated using the industrial version of APOLLO2 code.

	Fuel with enrichment 3.7% (UOX 3.7)
Fuel density [g/cm^3]	10.245
	Fuel composition [10^{24} at/cm^3]
U234	7.61072e-06
U235	8.56113e-04
U238	2.19932e-02
O16	4.57138e-02

Table 40: Fuel composition data for UOX assembly

3.1.1. Reflector design

For preparing homogenized reflector libraries for the small core configurations, the simplified reflector model is described in the following parts. Temperature conditions in reflector parts are summarized in Table 41 Temperature values have not been tuned on the small core configuration but in a full scale reactor type. As for the other data, these values may evolve if needed.

Top reflector	[K]	592.75
Radial reflector	[K]	577.75, see Table 36
Bottom reflector	[K]	562.75

Table 41: Reflector temperature conditions [12]

3.1.1.1. Radial reflector

The radial reflector zone is shown in Figure 22. The compositions for the 4 layers are shown in Table 42.

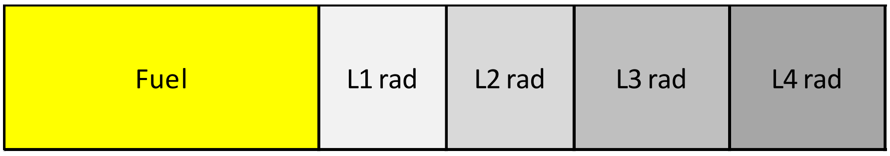


Figure 22. RADIAL REFLECTOR layout

Table 42. RADIAL REFLECTOR COMPOSITION

Layer	Material	Thickness [cm]	Composition	
			Material	%vol.
Fuel	UO2	65	UOX 3.7%	-
L1 rad	Reflector_L1_rad	13.9	Steel SS-304	39.2
			Moderator	60.8
L2 rad	Reflector_L2_rad	0.9	Moderator	100
L3 rad	Reflector_L3_rad	6.8	Steel SS-304	100
L4 rad	Reflector_L4_rad	20	Moderator	100

3.1.1.1. Axial reflectors

The lower reflector zone is shown in Figure 23. The compositions for the 3 layers are shown in Table 43.

Figure 23. Lower Reflector layout

Table 43. LOWER REFLECTOR COMPOSITION

Layer	Material	Thickness [cm]	Composition	
			Material	%vol.
Fuel	UO2	65	UOX 3.7%	-
L1 low	Reflector_L1_low	5.9	Zircaloy	6.72
			Steel SS-304	23.01
			Moderator	70.27
L2 low	Reflector_L2_low	9.2	Steel SS-304	34.83
			Moderator	65.17
L3 low	Reflector_L3_low	40	Moderator	100

The upper reflector zone is shown in Figure 24. The compositions for the 4 layers are shown in Table 44.

Figure 24. UPPER REFLECTOR layout

Table 44. UPPER REFLECTOR COMPOSITION

Layer	Material	Thickness [cm]	Composition	
			Material	%vol.
Fuel	UO2	65	UOX 3.7%	-
L1 up	Reflector_L1_up	16.5	He	26.57
			Zircaloy	11.51
			Steel SS-304	8.77
			Moderator	53.15
L2 up	Reflector_L2_up	3.7	Zircaloy	10.95
			Steel SS-304	2.75
			Moderator	86.30
L3 up	Reflector_L3_up	15.6	Steel SS-304	29.61
			Moderator	70.39
L4 up	Reflector_L4_up	20	Moderator	100

3.1.2. Material

3.1.2.1. Structural

Some of the atomic density has been calculated using the industrial version of APOLLO2 code.

Zircaloy [9] Density: 6.44 g/cm^3			
Elements	Wt%	Atomic density [10^{24} at/cm^3]	
Zr	97.91	Zr-90	2.14161e-02
		Zr-91	4.67033e-03
		Zr-92	7.13870e-03
		Zr-94	7.23444e-03
		Zr-96	1.16550e-03
Sn	1.59	Sn-112	5.03869e-06
		Sn-114	3.42838e-06
		Sn-115	1.76613e-06
		Sn-116	7.55284e-05
		Sn-117	3.98939e-05
		Sn-118	1.25811e-04
		Sn-119	4.46210e-05
		Sn-120	1.69237e-04
		Sn-122	2.40506e-05
		Sn-124	3.00763e-05
Fe	0.50	Fe-54	2.02952e-05
		Fe-56	3.18591e-04
		Fe-57	7.37577e-06
		Fe-58	9.79169e-07

Table 45 : Minicore – Zircaloy

Steel SS-304 [9] Density: 7.82 g/cm^3			
Elements	Wt%	Atomic density [10^{24} at/cm^3]	
Cr	19.152	Cr-50	7.53692e-04
		Cr-52	1.45342e-02
		Cr-53	1.64806e-03
		Cr-54	4.10237e-04
Mn	2.014	Mn-55	1.72641e-03
Ni	8.483	Ni-58	4.63357e-03
		Ni-60	1.78484e-03
		Ni-61	7.75859e-05
		Ni-62	2.47378e-04
		Ni-64	6.29999e-05
Fe	70.351	Fe-54	3.46748e-03
		Fe-56	5.44321e-02
		Fe-57	1.25707e-03
		Fe-58	1.67293e-04

Table 46 : Minicore – Steel SS-304

3.1.2.2. Absorber material

AIC [15]	
Elements	Atomic density [10^{24} at/cm^3]
Ag107	2.36159e-02
Ag109	2.19403e-02
Cd106	3.41523e-05
Cd108	2.43165e-05
Cd110	3.41250e-04
Cd111	3.49720e-04
Cd112	6.59276 e-04
Cd113	3.33873e-04
Cd114	7.84957e-04
Cd116	2.04641e-04
In113	3.44262e-04
In115	7.68050e-03

Table 47 : Minicore – AIC composition

3.1.2.3. Mixture

Moderator Density: 0.717 g/cm^3	
Elements	Atomic density [10^{24} at/cm^3]
B-10	4.76549e-06
B-11	1.91817e-05
H_2O	2.39611e-02

Table 48 : Minicore – Moderator – Boron concentration 600 ppm

3.2. The KAIST small core configuration

This configuration has been inspired by the well-known KAIST benchmark problem suite ([9][10]) for the core layout, differences remaining in the radial reflector description (see [11]). Data available in literature are included in the following part.

3.2.1. Nominal conditions

The nominal conditions are specified in Table 49. These conditions will be used during the depletion calculation. Information for branches calculations is provided in chapter 4.

Reactor power [MWth]	900
Linear power [W/cm]	179.24
Specific power [MW/MTHM][1]	32.7
Moderator temperature [K]	570
Moderator density [g/cm^3]	0.7295
Fuel temperature [K]	900
Cladding temperature [K]	630
Boron concentration [g/kg] [2]	4.575
Boron concentration [ppm]	800

Table 49: KAIST nominal conditions [9]

3.2.2. Fuel assembly design

Figures below describe 2D assembly geometry configurations. The assembly types that composed the KAIST core are:

- two homogeneous UOX assemblies (see Figure 25);
- one homogeneous UOX gadolinium assembly (UGD) (see Figure 25);
- one heterogeneous MOX assembly (see Figure 26);
- one homogeneous MOX assembly (see Figure 27).

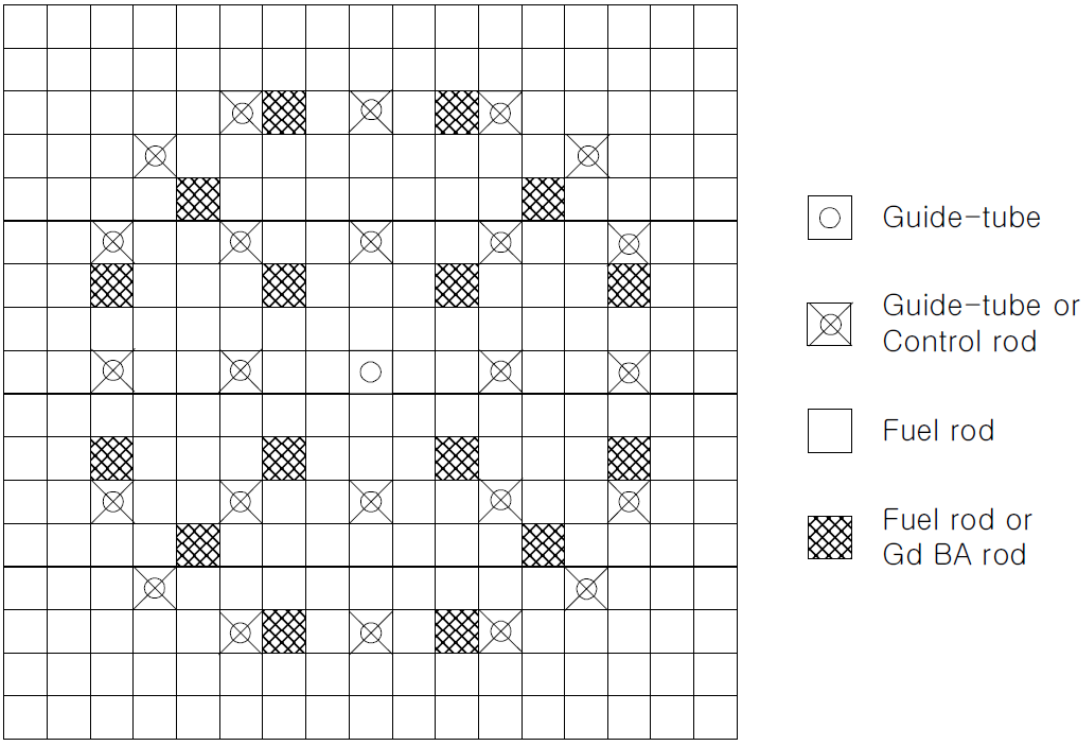


Figure 25: KAIST fuel assembly 2D assembly layout – UOX [9]

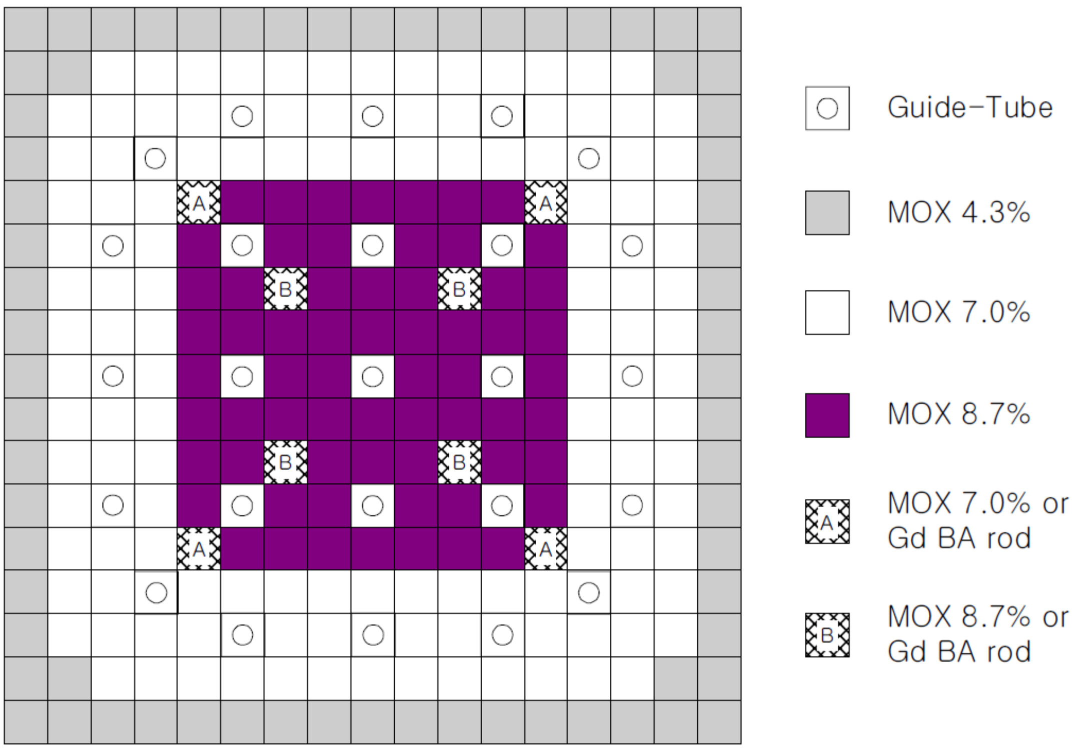


Figure 26: KAIST fuel assembly 2D assembly layout – MOX with zoning [9]

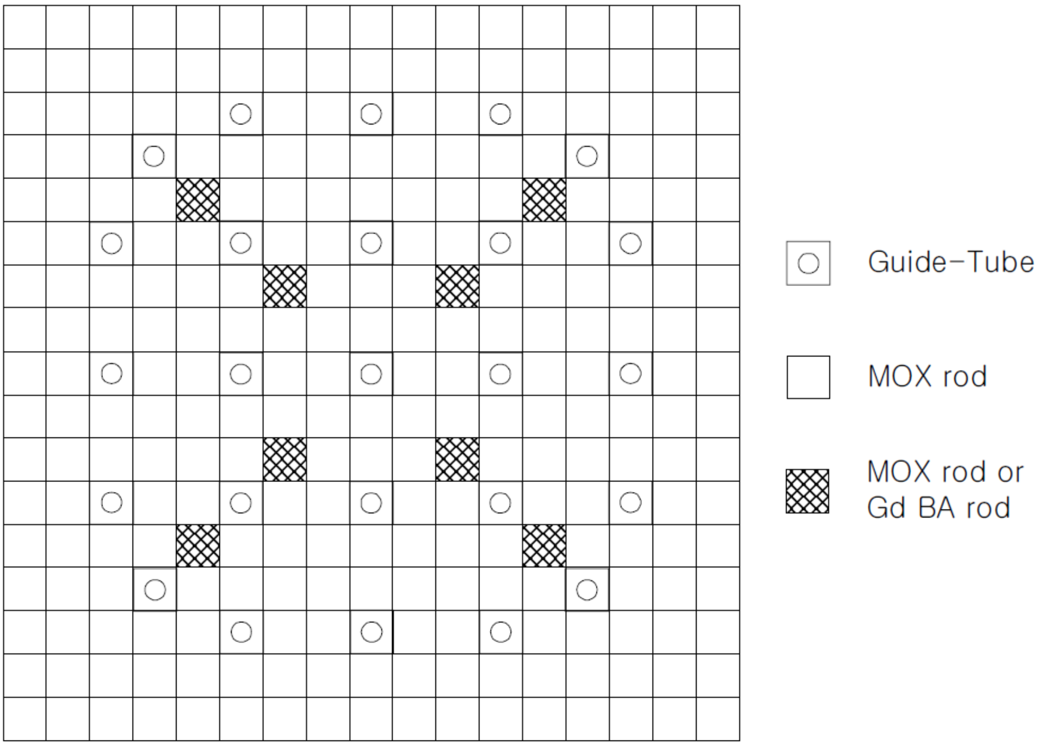


Figure 27: KAIST fuel assembly 2D assembly layout – MOX without zoning [10]

Geometrical data for 2D lattice description of assemblies are available in Table 50, Table 51 and Table 52. Material expansion is not considered in lattice calculation and so no expansion law will be provided in this document.

Figure 28 shows a detail of the fuel cell while Figure 29 shows control rod cell detail.

	KAIST
Number of fuel rods	264
Number of guide tubes	25
Assembly pitch [cm]	21.42
Assembly water blade [cm]	0
Active height [cm]	365.76

Table 50: KAIST assembly data

3.2.2.1. Cells description

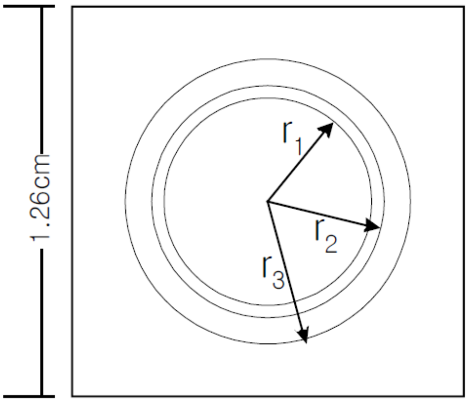


Figure 28: KAIST fuel cell [9]

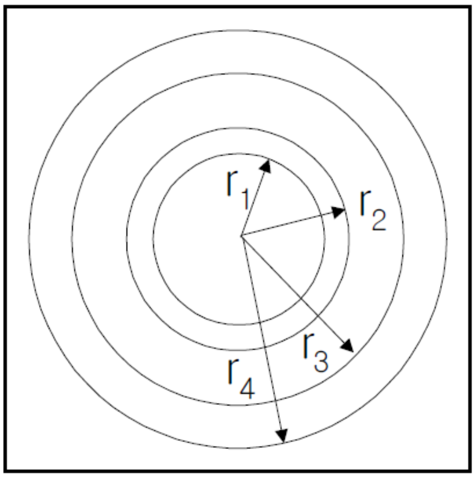


Figure 29: KAIST guide tube with control rod cell [9]

	KAIST
Unit cell pitch [cm]	1.26
Fuel pellet diameter [r1] [cm]	0.819
Fuel pellet material	UO_2, MOX or $UO_2 + Gd_2O_3$
Cladding inner diameter [r2] [cm]	0.836
Cladding outer diameter [r3] [cm]	0.95
Cladding material	Zircaloy
Gap material	He

Table 51: KAIST fuel cell data – Figure 28 [9]

	KAIST
Guide tube inner diameter [r3] [cm]	1.143
Guide tube outer diameter [r4] [cm]	1.224
Guide tube material	Zircaloy
Absorber number	24, fill in the guide tubes except central one
Absorber (control rods) pellet diameter [r1] [cm]	0.7646
Absorber material	B_4C
Absorber cladding outer diameter [r2] [cm]	0.9678
Cladding material	Zircaloy

Table 52: KAIST guide tube data – Figure 29 [9]

NB: It has been decided to smear the gap in the clad. The consequences are the modification on the clad inner diameter (equal to fuel pellet diameter) and the decrease of clad material density.

3.2.3. Fuel composition

NB: Atomic density has been calculated using the industrial version of APOLLO2 code.

	Fuel with enrichment 2.0 w/o	Fuel with enrichment 3.3 w/o
Fuel density [g/cm^3]	10.4	10.4
	Fuel composition [w/o]	
U235	2.0	3.3
U238	98.0	96.7
U234	0.0	0.0
	Fuel composition [10^{24} at/cm^3]	
U235	4.69778e-04	7.75118e-04
U238	2.27284e-02	2.24264e-02
O16	4.63963e-02	4.64031e-02

Table 53: Fuel composition data for UOX assembly [9]

	Burnable absorber with 0.711 w/o ^{235}U and 9.0% Gd_2O_3	
	[10^{24} at/cm^3]	w/o
U235	1.47010e-04	0.711
U238	2.02693e-02	99.289
U234		0.0
O16	4.53469e-02	
Gd152	6.01667e-06	0.1932
Gd154	6.55817e-05	2.0555
Gd155	4.45234e-04	14.5809
Gd156	6.15806e-04	20.4259
Gd157	4.70804e-04	15.6674
Gd158	7.47270e-04	24.9061
Gd160	6.57622e-04	22.1710
Fuel density [g/cm^3]	10.06	

Table 54: Fuel composition data for UO_2 + Gd_2O_3 [9]

MOX	Fuel with enrichment 4.3% Pu		Fuel with enrichment 7.0% Pu		Fuel with enrichment 8.7% Pu	
	w/o	[10^{24} at/cm^3]	w/o	[10^{24} at/cm^3]	w/o	[10^{24} at/cm^3]
U235	0.225	5.05805e-05	0.225	4.91545e-05	0.225	4.82566e-05
U238		2.21463e-02		2.15220e-02		2.11288e-02
U234	0.0		0.0		0.0	
O16		4.63750e-02		4.63676e-02		4.63629e-02
Pu238	1.83	1.82511e-05	1.83	2.97118e-05	1.83	3.69280e-05
Pu239	57.93	5.75331e-04	57.93	9.36607e-04	57.93	1.16408e-03
Pu240	22.50	2.22526e-04	22.50	3.62259e-04	22.50	4.50243e-04
Pu241	11.06	1.08928e-04	11.06	1.77329e-04	11.06	2.20398e-04
Pu242	5.60	5.49256e-05	5.60	8.94157e-05	5.60	1.11132e-04
Am241	1.08	1.06368e-05	1.08	1.73161e-05	1.08	2.15217e-05
Fuel density [g/cm^3]	10.4		10.4		10.4	

Table 55: Fuel composition data for MOX [9][10]

3.2.4. Reflector design

In this section, the radial reflector models for the KAIST core configuration are presented. Two variations have been proposed by CEA [11] as basis for the Task 4.4 activities on 2D small core modelling. These configurations are under consolidation and are briefly recalled here. More information are available in [11]. Radial reflector temperature will be set at the nominal moderator temperature, defined in Table 49.

For the 3D model to be investigated in WP5, the axial reflectors will be consistent with the one used for the 32 small core configuration described in 3.1.

3.2.4.1. Radial reflector

The original KAIST core and radial reflector configuration is shown in Figure 30.

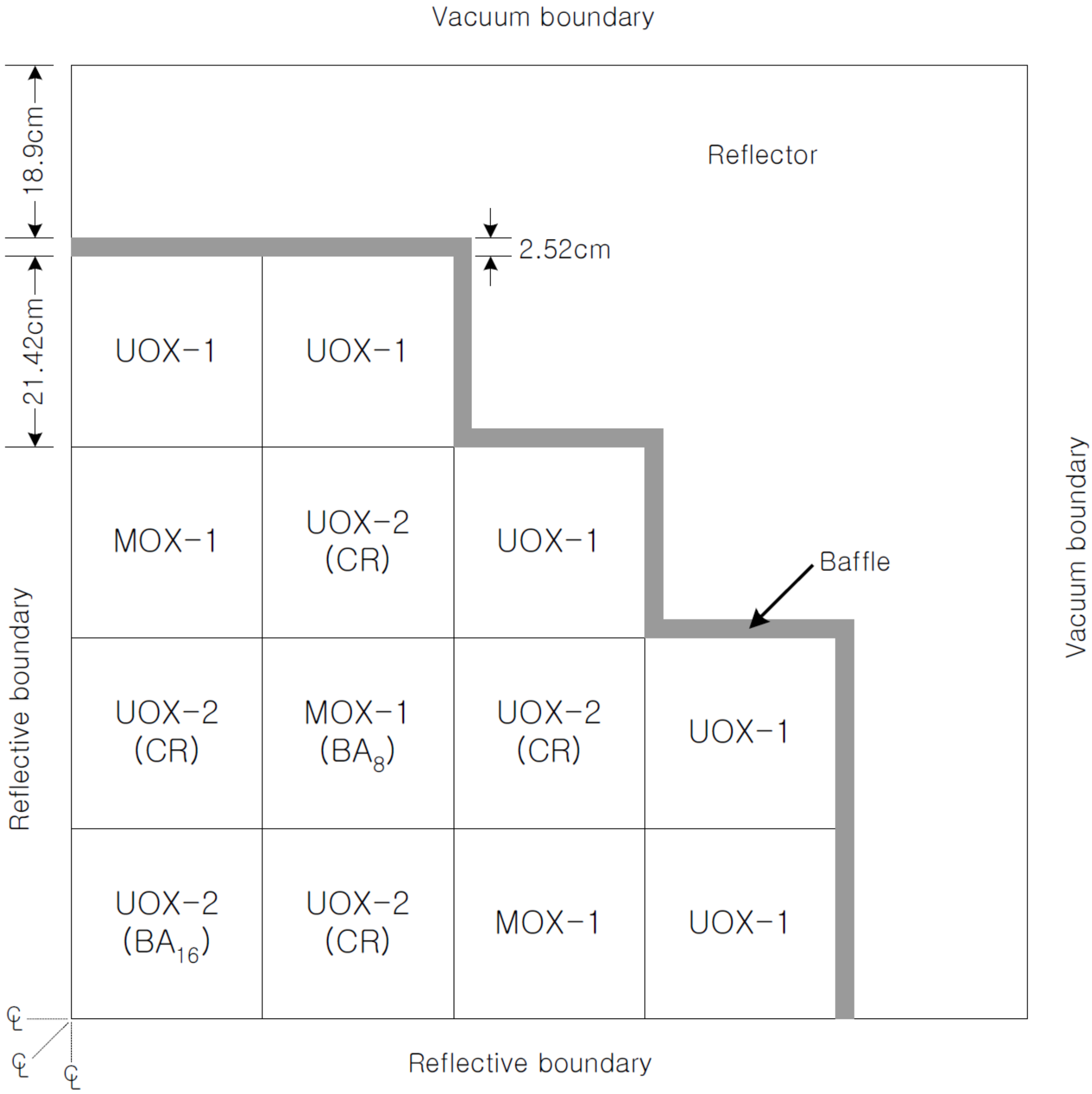


Figure 30: KAIST 2D core and radial reflector configuration [9]

KAIST radial reflector is composed with a stainless steel baffle enclosing the core and water at 570 K with same composition as moderator with 800 ppm of soluble boron concentration (see Figure 30).

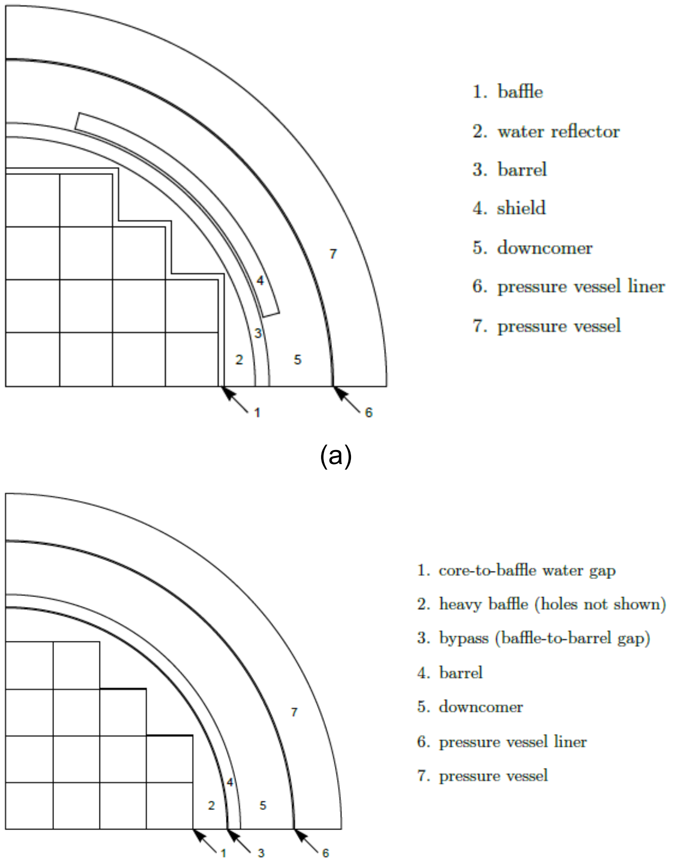
Layer	Material	Thickness [cm]
Baffle	Steel SS-304	2.52
Water_1 (Reflector in Figure 30)	Moderator	18.9
Vacuum	Vacuum	Boundary condition

Table 56: KAIST radial reflector data

3.2.4.2. Heavy reflector

As indicated in [11], the core configuration with 52 assemblies is small enough to perform fast direct whole-reactor calculations without spatial homogenization and to investigate the homogenization options of the traditional two-step calculation schemes, especially the methodology for reflector homogenization and therefore it looks quite attractive for investigating cases with heavy reflector.

CEA as part of Task 4.4 activities is proposing two configurations inspired by the BEAVRS benchmark [11] for the reactor vessel and its internals. The preliminary layout is shown in Figure 31 but detailed information will not be provided here (configurations under finalization). They will be shared with the partners as Task 4.4 contribution.



(b)

Figure 31 : Reflector configurations proposed by CEA:
(a) core layout with the light water reflector,
(b) core layout with the heavy reflector [11]

3.2.5. Material

3.2.5.1. Structural

NB: Atomic density has been calculated using the industrial version of APOLLO2 code.

Zircaloy [9] Density: 6.44 g/cm^3			
Elements	Wt%	Atomic density [10^{24} at/cm^3]	
Zr	97.91	Zr-90	2.141609e-02
		Zr-91	4.670333e-03
		Zr-92	7.138699e-03
		Zr-94	7.234437e-03
		Zr-96	1.165502e-03
Sn	1.59	Sn-112	5.069569e-06
		Sn-114	3.356515e-06
		Sn-115	1.770990e-06
		Sn-116	7.560289e-05
		Sn-117	3.987761e-05
		Sn-118	1.258372e-04
		Sn-119	4.454846e-05
		Sn-120	1.693040e-04
		Sn-122	2.402771e-05
		Sn-124	3.005942e-05
Fe	0.50	Fe-54	2.029518e-05
		Fe-56	3.185910e-04
		Fe-57	7.357656e-06
		Fe-58	9.791691e-07

Table 57 : KAIST – Zircaloy

Steel SS-304 [9] Density: 7.82 g/cm^3			
Elements	Wt%	Atomic density [10^{24} at/cm^3]	
Cr	19.152	Cr-50	7.53692e-04
		Cr-52	1.45342e-02
		Cr-53	1.64806e-03
		Cr-54	4.10237e-04
Mn	2.014	Mn-55	1.72641e-03
Ni	8.483	Ni-58	4.63357e-03
		Ni-60	1.78484e-03
		Ni-61	7.75859e-05
		Ni-62	2.47378e-04
		Ni-64	6.29999e-05
Fe	70.351	Fe-54	3.46748e-03
		Fe-56	5.44321e-02
		Fe-57	1.25707e-03
		Fe-58	1.67293e-04

Table 58 : KAIST – Steel SS-304

3.2.5.2. Absorber material

NB: Atomic density has been calculated using the industrial version of APOLLO2 code.

B_4C [9] Density: 1.84 g/cm^3		
Elements	Wt%	Atomic density [10^{24} at/cm^3]
B-10	14.43	1.596434e-02
B-11	63.84	6.425851e-02
C	21.73	2.006354e-02

Table 59 : KAIST – B4C

3.2.5.3. Mixture

Moderator Density: 0.7295 g/cm^3 Temperature: 570 K	
Elements	Atomic density [10^{24} at/cm^3]
B-10	6.46924e-06
B-11	2.60395e-05
H_2O	2.43856e-02

Table 60 : KAIST – Moderator – boron concentration 800 ppm

3.3. Other PWR assembly cases

The MOX fuel assembly adopted in the KAIST core is quite complex. In order to have an indication of the good behaviour of the prototype for standard MOX configuration and additional assembly case may be included. The specifications may be provided during the project.

4. Working Horse calculation methods

The multi-parametric neutron data libraries generator prototype is developed in order to generate two kinds of libraries: neutron library for fuel assembly and for reflector zones. The specifications will be detailed in Deliverable 4.1. These libraries are filled with the results of the Boltzmann transport equation solved by the deterministic multi-group spectral code APOLLO3®. The following sections described the different tentative calculation type and options for starting the analysis. These “working horse” data may be subjected to an evolution following the discussions foreseen and within Task 4.1 and 4.3.

4.1. Fuel depletion

First step in the neutron library generation process is to calculate fuel’s isotopic depletion during irradiation. This depletion is carried out by a series of multi-group flux calculations at different steps (commonly burn-up steps) at nominal conditions.

For PWR assemblies with square lattice, the traditional deterministic lattice code APOLLO2 will be used to verify the evolution in the prototype. Some of the options used for depletion calculation are summarized in Table 61.

For VVER, the validation of the depletion process in the prototype will be done through a code-to-code comparison against SERPENT’s result using the same configuration. APOLLO3®’s depletion calculation options are the same as the one presented in Table 61 with leakage fixed to zero in order to compare APOLLO3® and SERPENT’s results as critical B2 option will not be available. Another APOLLO3®’s evolution must be launched with critical B2 when generating libraries.

	VVER	PWR
Evaluated nuclear data reaction library	JEFF3.1.1	
Depletion chain	CEAV2005_V3[5]	
Leakage	No leakage / Critical B2	No leakage / Critical B2
Burn-up range[6] [GW.d/T]	0 - 70	0 - 60

Table 61: Depletion calculation options

4.2. Feedback calculation parameters

After the depletion performed in nominal condition, fuel isotopic composition is fixed for each burn-up steps and feedback is calculated in such a way that the libraries are available in different reactor conditions. These parametric calculations are deployed in order to cover the evolution of the following values: burn-up, boron concentration, fuel temperature, moderator density and xenon level. The variation range for each parameter is shown in Table 62 and Table 63. If not differently indicated, these data are considered as starting point, but they could be modified in accordance to WP5 needs and suggestions. For VVER, the ranges are also provided in D3.1.

To cover calculation with moderator steam phase, moderator temperature axis also need to be considered but additional information about data range should be provided by WP5.

[5] This chains contains fission products and decay data are extracted from JEFF311 evaluation.

[6] For APOLLO2, possible burn-up points are : 0, 0.01, 0.02, 0.03, 0.04, 0.05, 0.075, 0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4, 0.45, 0.5, 0.75, 1.0, 1.5, 2.0, 2.5, 3.5, 4.0, 4.5, 5.0, 6.0, 7.0, 8.0, 9.0, 10.0, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 32, 34, 36, 38, 40, 42, 44, 46, 48, 50, 52, 54, 56, 58, 60, 62, 64, 66, 68, 70 in [GW.d/T].

Burn-up[7]	[GW.d/T]	0 - 70
Boron concentration	[ppm]	0 - 2933.33
Boron concentration	[g/kg]	0 - 16.77
Fuel temperature	[K]	300 - 3100
Moderator Density	[g.cm^{-3}]	0.1 - 1.0
Moderator Temperature	[K]	
Xenon level	w/o	equilibrium

Table 62: VVER feedback calculation parameters for deterministic codes [5]

Burn-up	[GW.d/T]	0 - 60
Boron concentration	[ppm]	0 - 2000
Boron concentration	[g/kg]	0 - 11.44
Fuel temperature	[K]	293.15 - 2273.15
Moderator Density	[g.cm^{-3}]	0.4 - 1.0
Moderator Temperature	[K]	
Xenon level	w/o	equilibrium

Table 63: PWR feedback calculation parameters for deterministic codes

4.3. Energy and Space Collapsing

Lattice calculation's results must be stored in the MPO according to a specific space and energy collapsing. The collapsing energy mesh is provided by WP5 analyses. Some possible collapsed energy meshes are summarized in Table 64. Multi-groups (> 2) and depends on the WP requirements. They will be confirmed in another document.

Requirements for	Space condensation	Energy condensation	Energy cut
WP5	Homogeneous Assembly	2 groups	0.625 eV
WP5	Pin by pin	4, 8 groups	To be defined later

Table 64: Output condensation structure

[7] Benchmarks proposed in WP5 are set at 0 MW.d/T which means MPO provided by Task 4.2 to WP5 don't need feedback according to burn-up parameter. Eventually WP7 would require MPO at different burn-up points. If so, a specific feedback mesh will be proposed for this parameter according to the transient calculated.

4.4. Depletion comparison

The depletion comparison will be performed on four different burn-up point (0, 0.150, 20 and 60 GW.d/T) toward simplification of the physical interpretation of the results. The observation data compared in depletion calculation are described in section 5.1.

4.5. Comparison state-point against stochastics codes

Stochastic calculations are much more time consuming than deterministic ones and a restricted parameters space must be considered when comparing APOLLO3® and SERPENT/TRIPOLI-4 feedback. Furthermore, fuel temperature and moderator density are coupled to match realistic conditions. Table 65 summarizes the parameters selected to perform these comparisons. In conclusion, each case will require at least eight stochastic calculations to be compared with APOLLO3® results.

Irradiation	[GW.d/T]	0		
Fuel temperature	[K]	300	nominal	2000
Moderator Density	[g.cm^{-3}]	1.0	nominal	0.4
Xenon	w/o	equilibrium		
Bore concentration	[ppm]	0	nominal	

Table 65: State-point parameters for deterministic/stochastic comparison

To compare APOLLO2 and APOLLO3® results and to generate neutron libraries, parametric calculations will be performed with critical leakage model (critical B2). The exhaustive list of observation data in these branches calculation are described in section 5.1.

Then, to compare results from deterministic codes and stochastic codes, parametric calculations will be performed without leakage model (B2 fixed to zero). The observation data compared in these branches calculation are described in section 5.3.

4.6. Reflector

Since there is no neutron creation in the reflector, reflector calculation required to define a nurturing zone close to the reflector. This nurturing zone is composed from an assembly at 150 MW.d/T with homogenized isotopic composition.

5. Expected results

Validation and verification of the prototype's development will be performed against five VVER assemblies, three PWR assemblies and three rods type as shown in following Table 66 and Table 67. Reflector calculation in 1D model is taken in the radial reflector configuration of Kozloduy-6's minicore described in 2.4.1.1.

Sections 5.1, 5.2 and 5.3 detail the datasets compared between APOLLO3® results and other codes.

Grid smearing feature is checked with assembly 13AU (VVER), in addition to the configuration described in Table 66. This test only required the comparison between APOLLO3® and SERPENT results on nominal conditions at burn-up 0 MW.d/T. The dataset is described in section 5.3.

The "Library" line on the following tables shows for which assemblies an MPO must be generated and provided to other Work Packages.

	Khmelnitsky-2								**Kozloduy-6**					
	13AU	22AU	439GT	398GO	30AV5	390GO	430GO	39AWU	UOX 2%	UOX 3%	UOX 3.3%	UOX 4.4%	Profiled FA 3.3/3.0	Profiled FA 4.4/3.6
Fuel Type	UOX	UOX	UGD	UGD	UGD	UGD	UGD	UGD	UOX	UOX	UOX	UOX	UGD	UGD
Rod						Dy_2O_3 TiO_2							B_4C	
AP3 depletion	Table 61				Table 61	Table 61						Table 61	Table 61	
AP3 feedback	Table 62				Table 62	Table 62						Table 62	Table 62	
AP2 depletion														
AP2 feedback														
SERPENT depletion	Table 61				Table 61	Table 61						Table 61	Table 61	
SERPENT feedback	Table 65				Table 65	Table 65						Table 65	Table 65	
TRIPOLI4 feedback	Table 65				Table 65	Table 65						Table 65	Table 65	
Library	WP5				WP5	WP5						WP5	WP5	

Table 66: VVER test cases for verification and validation

	minicore	**KAIST**					**Other PWR**
	UOX 3.7%	UOX 2.0%	UOX 3.3%	UGD	MOX heterogeneous	MOX homogeneous	MOX
Fuel Type	UOX	UOX	UOX	UGD	MOX	MOX	MOX
Rod	AIC						
AP3 depletion	Table 61		Table 61	Table 61	Table 61	Table 61	
AP3 feedback	Table 62		Table 62	Table 62	Table 62	Table 62	
AP2 depletion	Table 61			Table 61	Table 61		
AP2 feedback	Table 62			Table 62	Table 62		
SERPENT depletion	Table 61			Table 61	Table 61		
SERPENT feedback	Table 65			Table 65	Table 65		
TRIPOLI4 feedback	Table 65			Table 65	Table 65		
Library	WP5		WP5	WP5	WP5	WP5	

Table 67: PWR test cases for verification and validation

5.1. Depletion results

The results of the depletion process with deterministic and stochastic codes are compared on specific dataset towards verification and validation of the depletion feature. Dataset selected to be observed are presented in Table 68.

Dataset	Difference Mode
Infinite multiplication factor	pcm
Normalized 2D map of fission rate	Relative
Compositions of relevant isotopes at selected pins	Relative

Table 68: Dataset for depletion comparison

5.2. State-point: APOLLO3® vs APOLLO2

Deterministic codes generate several dataset expected for core calculation. The comparison between an industrial established code APOLLO2 and APOLLO3® on a large dataset is relevant to verify and demonstrate prototype's efficiency. The exhaustive list of selected parameter for the comparison is available Table 69, if necessary this list can be shorten during the calculation and comparison process.

Dataset	Difference Mode
Assembly flux discontinuity factors on external surfaces of the whole fuel assembly	Relative
Geometrical buckling B2	Relative
Assembly flux discontinuity factors on external corners of the whole fuel assembly	Relative
Infinite multiplication factor	pcm
Multi-group flux homogenized on the full assembly	Relative
Value of absorption assembly-homogenized macro XS for energy group g	Relative
Value of fission spectrum for energy group g	Relative
Value of diffusion assembly-homogenized macro XS for energy group g and anisotropy order a	Relative
Value of total delivered energy XS for energy group g	Relative
Value of fission assembly-homogenized macro XS for energy group g	Relative
Value of leakage coefficient * B2	Relative
Value of (n,2n) assembly-homogenized macro XS for energy group g	Relative
Value of fission XS * number of neutron per fission	Relative
Value of scattering assembly-homogenized macro XS for initial energy group g, final group h and anisotropy order a	Relative
Value of total assembly-homogenized macro XS for energy group g	Relative
Particle number density of all isotopes	Relative

Dataset	Difference Mode
Normalized 2D map of absorption rate	Relative
Normalization factor for pin absorption rate	Relative
Normalized 2D map of fission rate	Relative
Normalization factor for pin fission rate	Relative
Normalized 2D map of pin burn-up	Relative
Normalization factor for pin burn-up	Relative
Normalization factor for pin flux	Relative
Normalized 2D map of pin deposited power	Relative
Normalization factor for pin delivered power	Relative
Effective average delayed neutron fraction for precursor group L	Relative
Average delayed neutron energy spectrum for precursor group L and for one output energy macro-group k	Relative
Average inverse velocity of delayed neutrons for one output energy macro-group k	Relative
Decay constant for precursor group L	Relative
Average neutron generation time	Relative
Decay constants for all isotopes and all decay channels available in the primary library	Relative
Fission yield matrix for all explicit fissile isotopes, fission products and fission yield macro-groups	Relative

Table 69: Dataset for APOLLO2/APOLLO3® comparison

5.3. State-point: APOLLO3® vs TRIPOLI-4/SERPENT

APOLLO3® prototype's validation is realized by comparison with stochastic references. The difficulties in interpreting the differences between deterministic and stochastic results force us to reduce the range of observable data. The dataset selected to be compared are available Table 70.

Dataset	Difference Mode
Infinite multiplication factor	pcm
Multi-group flux homogenized on the full assembly	Relative
Normalized 2D[8] map of fission rate	Relative
Normalized 2D[9] map of absorption rate	Relative

Table 70: Dataset for deterministic/stochastic comparison

[8] For 3D calculations in task 4.4, 3D normalized map of fission rates.

[9] For 3D calculations in task 4.4, 3D normalized map of absorption rates.

6. References

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[3] NURISP – Specification and results of the VVER lattice benchmark using APOLLO2, TRIPOLI4 and COBAYA3 pin-by-pin. G. Todorova, N. Zheleva, N. Petrov, N.P. Kolev and JJ. Herrero.

[4] VVER-1000 coolant transient benchmark – Phase 1 (V1000CT-1). Volume I: Finale Specifications – B. Ivanov, K. Ivanov, P. Groudev, M. Pavlova, V. Hadjiev.

[5] D3.2 – The CAMIVVER Definition report with specification for NPP VVER 1000 reactor with respect to selected transient – A. Stefanova, N. Zaharieva, P. Vryashkova, P. Groudev. Draft Version.

[6] Corrections and additions to the proposal of a benchmark for core burnup calculations for a VVER-1000 reactor – T. Lötsch, V. Khalimonchuk, A. Kuchin.

[7] X2 VVER-1000 benchmark revision: Fresh HZP core state and the reference Monte Carlo solution. Y. Bilodid, E. Fridman, T. Lötsch. [Excel file material_composition.xlsl (X2 benchmark specification dataset – Y. Bilodid – URL: http://doi.org/10.14278/rodare.200]

[8] MEMO: Preliminary agreement for Task 5.1: Definition of VVER and PWR test cases for transient calculations – D. Ferraro (KIT)

[9] Benchmark Problem 1A: MOX Fuel-Loaded Small PWR Core (MOX Fuel with Zoning) – Nam Zin Cho. http://nurapt.kaist.ac.kr/benchmark

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[12] The CAMIVVER project: Assembly and reflector description for PWR minicore - Task 5.3 Benchmark - Framatome document D02-DTIPD-F-20-0580 A

[13] CAMIVVER - The CAMIVVER project - WP5 task 5.3 - PWR test case to be employed in coupled neutronic and thermal hydraulic analysis - Framatome document D02-DTIPD-F-20-0582 A

[14] C. Patricot et al., Upgraded of APOLLO3® internal thermohydraulic feedback model with THEDI and application to a control rod ejection accident, M&C 2019 - Cyril PATRICOT, Roland LENAIN, and Dominic CARON

[15] VERA Core PhysicsBenchmark Progression Problem Specifications, CASL-U-2012-0131-004

7. Appendix

The following sections provide information for whole core description and specific diagram for reflector description can be found on deliverables D3.1 and D3.2 ([5]).

7.1. Kozloduy-6: Cycle 1

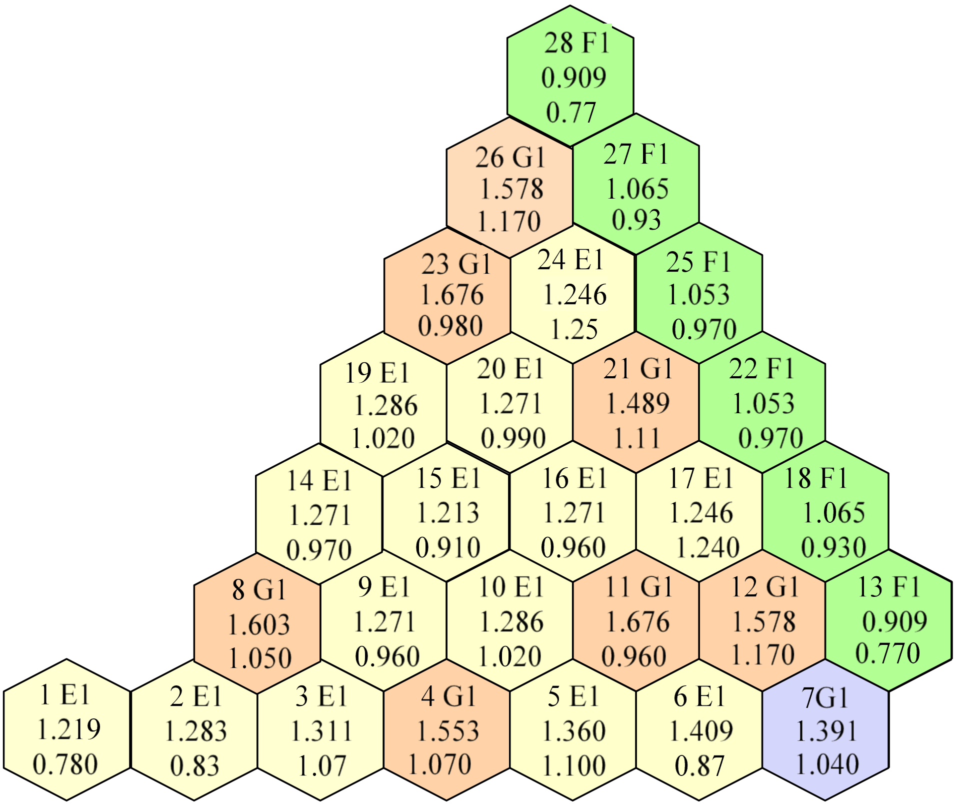


Figure 32: Core loading for cycle 1 – Kozloduy-6 [5]

FA with 2.0% enrichment

Profiled FA with 3.3% enrichment

FA with 3.0% enrichment

7.2. Kozloduy-6: Cycle 6

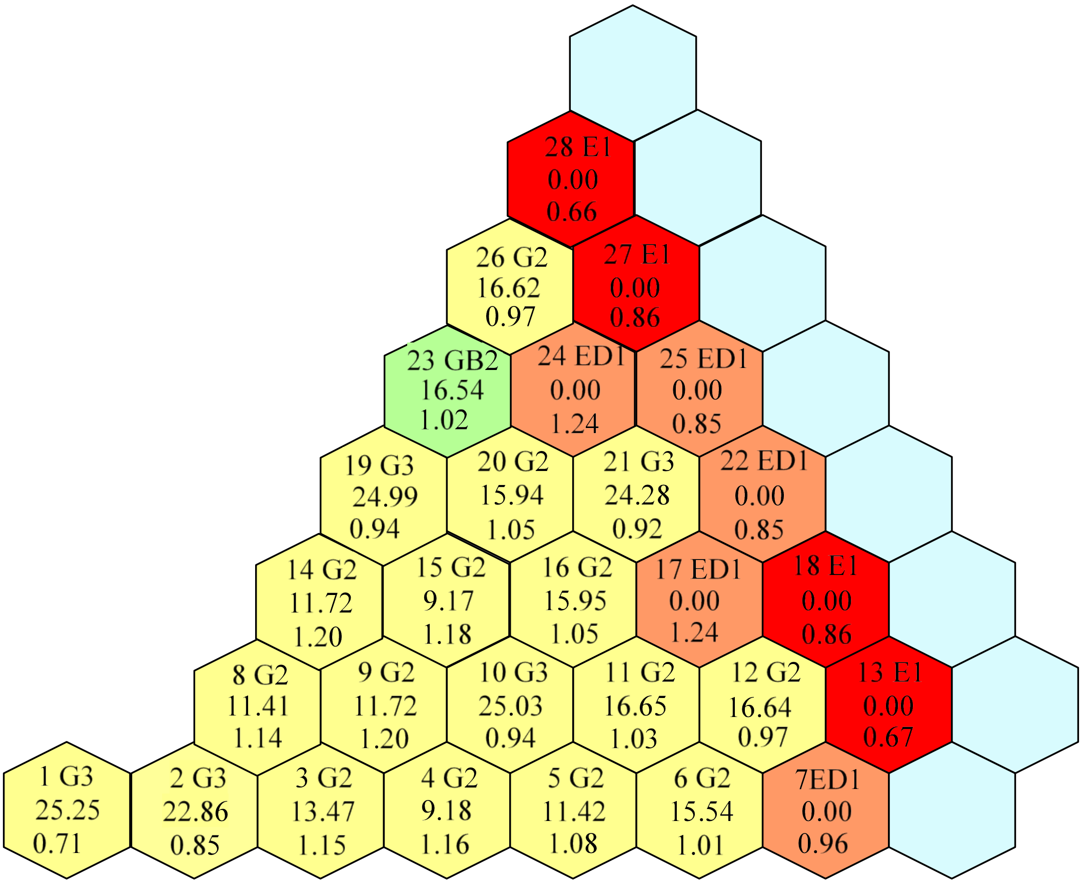
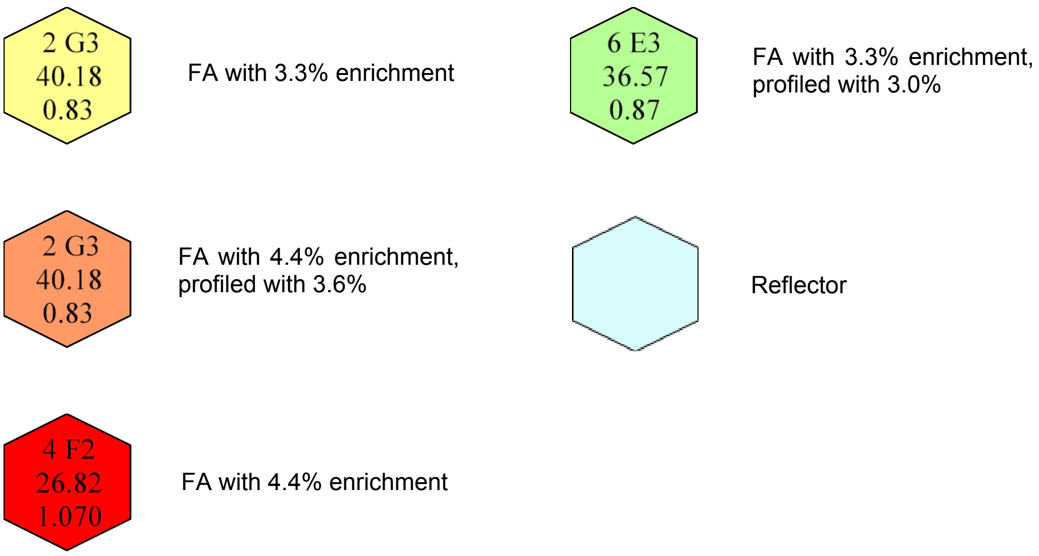


Figure 33: Core loading for cycle 6 – Kozloduy-6 [5]



7.3. Kozloduy-6: Cycle 8

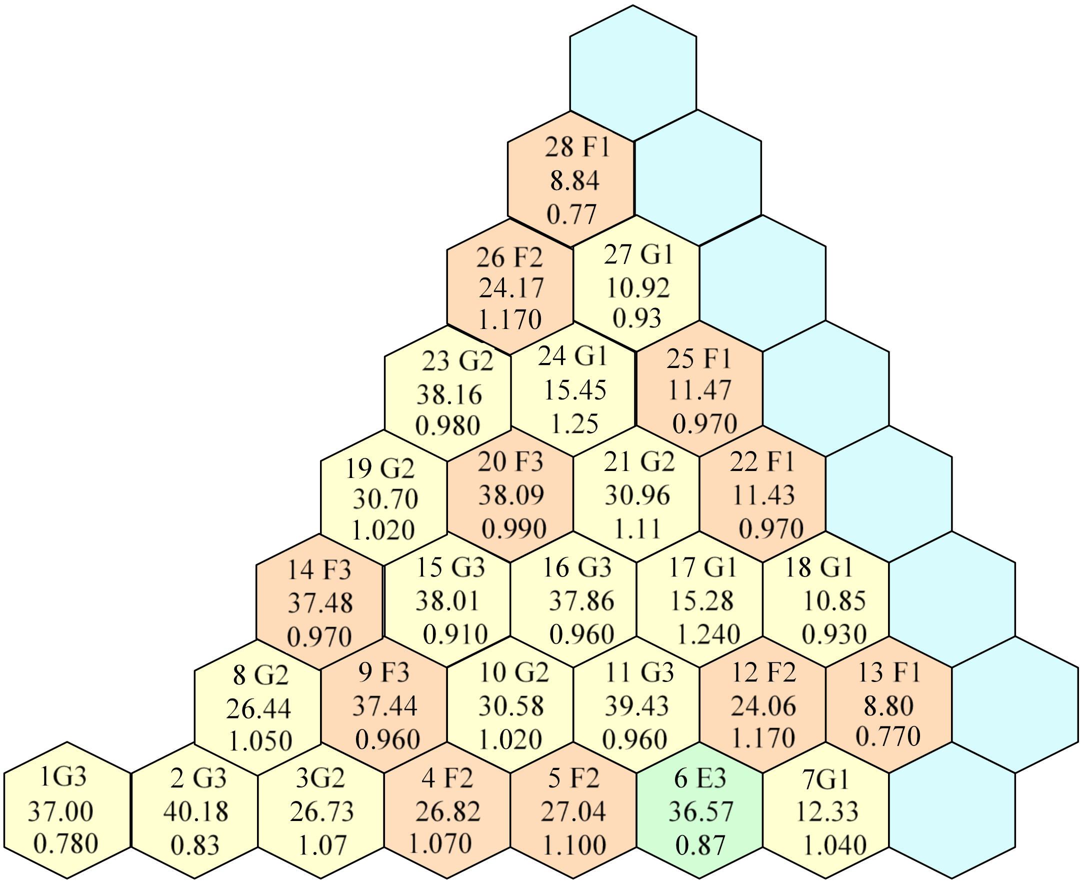
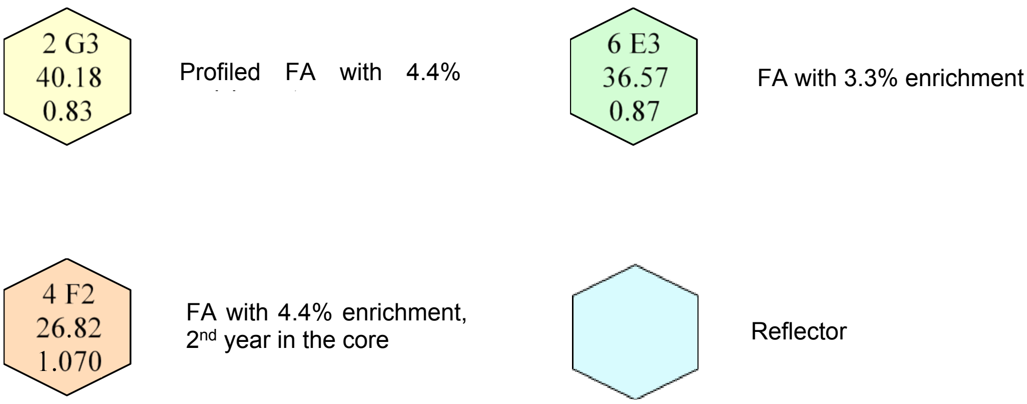


Figure 34: Core loading for cycle 8 – Kozloduy-6 [5]



7.4. Khmelnitsky-2: Cycle 1

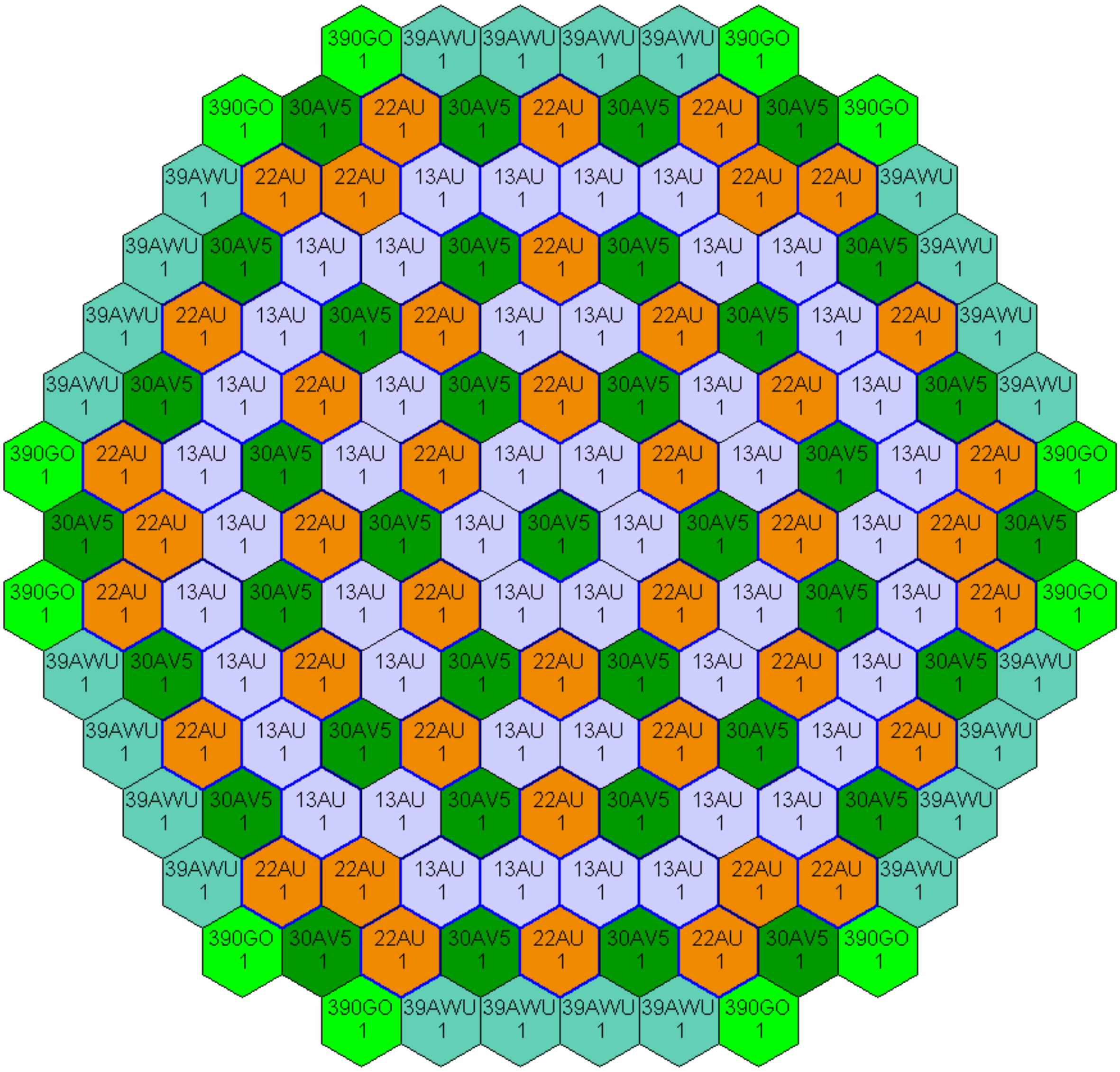


Figure 35: Core loading for cycle 1 – Khmelnistky-2 [6]

7.5. Khmelnitsky-2: Cycle 2

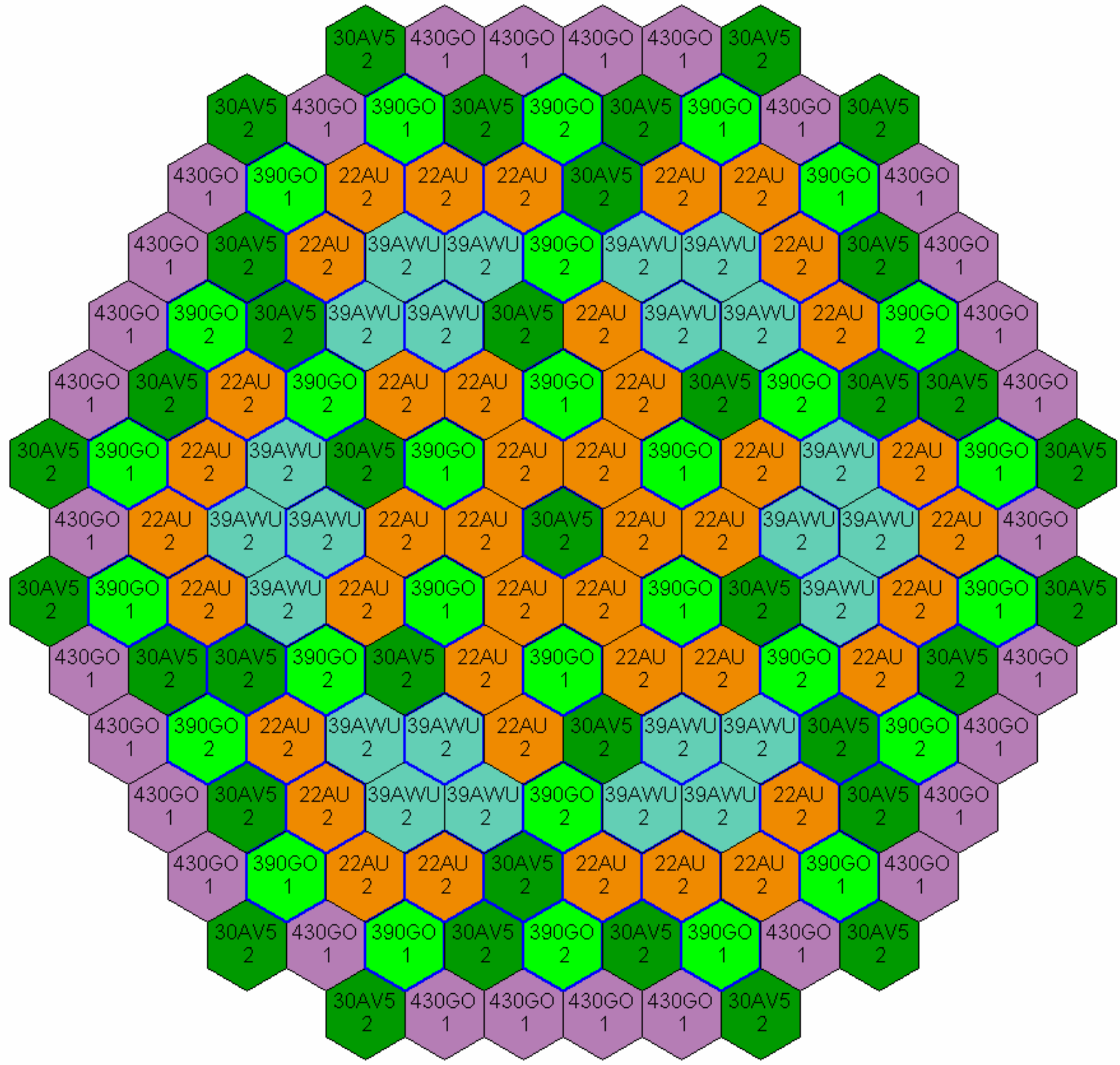


Figure 36: Core loading for cycle 2 – Khmelnistky-2 [6]