Codes And Methods Improvements for VVER comprehensive safety assessment

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WP5 - Task 5.1

D5.1 - Description of the core reference test cases – Part 1

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Summary

In the framework of the H2020 CAMIVVER project, Work Package 5 (WP5) analyzes and provides coupled core neutronics-thermal-hydraulics best estimate calculations for VVER and PWR reactors. These results will serve as a starting point for future industrial level discussions of tools and methodologies to be adopted, as well as, advantages and disadvantages of the best-estimate coupled calculations in view of stricter safety regulations [1].

For the correct progress of the WP5, three main tasks were established in the project proposal [1]. Task 5.1 consists in the definition of the VVER and PWR reduced size core reference test cases with their corresponding initial and boundary conditions. Task 5.2 evaluates the aforementioned transient scenarios with coupled neutronics and closed channel thermal-hydraulics tools (APOLLO3®, SERPENT/SubChanFlow, PARCS/TRACE). By making use of the cases defined in Task 5.1 and the results to be obtained in Task 5.2, efforts are to be made in Task 5.3 for the development of a 3D neutronics-thermal-hydraulics reference calculation based on APOLLO3®/CATHARE3 coupling.

WP5 is tightly connected to the activities of WP4. Deliverable 4.3 [2] from WP4 provides most of the cores and fuel assemblies geometrical and material descriptions, as well as, nominal operating conditions. However, for the purposes of WP5, some of the data has been updated.

This document corresponds to Task 5.1 and its aim is to provide the VVER and PWR test cases, specifying its geometry, materials, thermophysical properties, transient scenarios (initial/ boundary conditions), and output parameters to be observed. These transient scenarios will be later simulated and intercompared with the multi-physics tools of the partners in Tasks 5.2 and 5.3.

In this deliverable, one transient scenario is provided for each minicore case to be analysed. These are a 32 Fuel Assemblies PWR minicore provided by Framatome and a 7 Fuel Assemblies Khmelnitsky-2 based VVER minicore. Moreover, additional data on a possible second scenario is provided and two additional core configurations (one PWR and one VVER) are provided in the Appendix.

Approval

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1 Introduction

In the framework of the H2020 CAMIVVER project, Work Package 5 (WP5) analyzes and provides coupled core neutronics-thermal-hydraulics best estimate calculations for VVER and PWR reactors. These results will serve as a starting point for future industrial level discussion of tools and methodologies to be adopted, as well as, advantages and disadvantages of the best-estimate coupled calculations in view of better answering to safety regulations [1].

For the correct progress of the WP5, three main tasks were established in the project proposal [1]. Task 5.1 consists in the definition of the VVER and PWR reduced size core reference test cases with their corresponding initial and boundary conditions. Task 5.2 evaluates the aforementioned transient scenarios with coupled neutronics and closed channel thermal-hydraulics tools (APOLLO3®, SERPENT/SubChanFlow, PARCS/TRACE). By making use of the cases defined in Task 5.1 and the results to be obtained in Task 5.2, efforts are to be made in Task 5.3 for the development of a 3D neutronics-thermal-hydraulics reference calculation based on APOLLO3®/CATHARE3 coupling.

WP5 is tightly connected to the activities of WP4. Deliverable 4.3 [2] from WP4 provides most of the cores and fuel assemblies geometrical and material descriptions, as well as, nominal operating conditions. However, for the purposes of WP5, some of the data has been updated.

As previously stated, Deliverable 4.3 [2] provides the benchmark specifications for the basis of this work. However, it provides more information than needed for this report. For the sake of clarity, the data used from D4.3 for the purpose of WP5 is summarized here, though, some information must be retrieved from D4.3 when referred to it.

Sections 2 and 3 gather the main information for the VVER and PWR small core study cases for WP5. In addition, thermophysical data for the coupled calculations can be found here. In Section 4.1 the initial coupled steady-state conditions are set and in Section 4.2 the transient scenarios to be studied are formulated. Finally, Section 5 defines the output parameters of the simulations to be compared between the partners.

In addition, Appendix A provides possible additional core configurations to be analysed, namely the Kozloduy-6 based minicore and KAIST based minicore cases.

Some of the data in this Deliverable is not definitive (e.g. reflectors, transient parameters, outputs) as some changes may arise during the simulation phase.

2 Description of the 7 FAs VVER minicore

Two VVER small core benchmarks were proposed in Deliverable 4.3 [2]. In this document we will refer to the Khmelnytsky-2 based benchmark specifications from D4.3, which is based on [3][4][5][6][7]. This core contains seven (7) Fuel Assemblies (FAs) of two types, denominated as 30AV5 and 390GO. A summarized description of the geometry and materials relevant to WP5 is shown in Section 2.1, but the reader is encouraged to refer to D4.3 [2] for detailed material isotopic composition.

2.1 Core description

2.1.1 Pin Cells

The hexagonal unit, fuel, guide tube with absorbers and central tube pin cells are shown in Figure 1-Figure 4 respectively. Geometrical and material specifications are shown in Table 1-Table 4 for each cell. Details on the material isotopic compositions can be obtained from D4.3 [2].

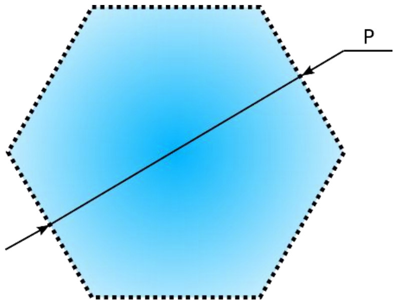

Figure 1 Hexagonal Unit Cell[1] (based on [2][7])

Table 1 Hexagonal Cell Pitch [2][5][7]

Hexagonal Unit Cell	
Unit Cell Pitch (P) [cm]	1.275

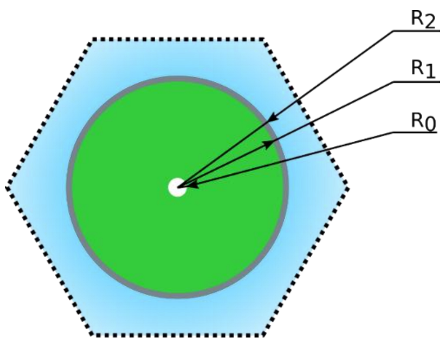

Figure 2 Fuel Pin Cell (based on [2][5][7])

Table 2 Fuel Pin Cell Geometry and Materials [2][5][7]

Fuel Pin Cell	
Central void radius (R_0) [cm]	0.0750
Fuel pellet radius (R_1) [cm]	0.3785
Cladding outer radius (R_2) [cm]	0.4550
Fuel pellet material	UO_2(3.0%, 3.6%, 4.0% ^{235}U) UO_2(2.4%, 3.3% ^{235}U) and 5.0% Gd_2O_3
Cladding material	Alloy E110
Void material	Void / He

[1] All images in this report were made with Inkscape [8]

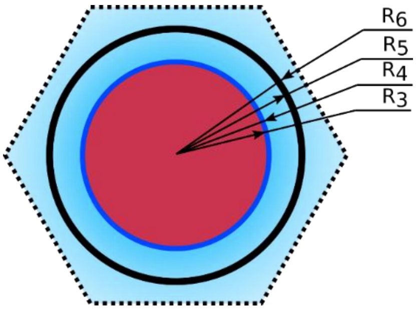

Figure 3 Guide Tube with Absorber (based on [2][7])

Table 3 Guide Tube and Absorber Geometry and Materials [2][5][7]

Guide Tube and Control Rod Cell	
Absorber radius (R_3) [cm]	0.350
Cladding outer radius (R_4) [cm]	0.410
Guide Tube inner radius (R_5) [cm]	0.545
Guide Tube outer radius (R_6) [cm]	0.630
Absorber material	B_4C or Dy_2O_3 TiO_2
Cladding material	Steel
Guide Tube material	Alloy E635

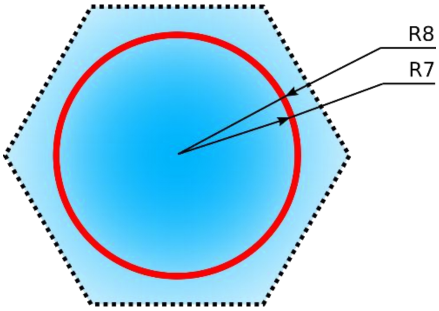

Figure 4 Central Tube Cell (based on [2][7])

Table 4 Central Tube Geometry and Materials [2][5][7]

Central Tube Cell	
Inner radius (R_7) [cm]	0.55
Outer radius (R_8) [cm]	0.65
Material	Alloy E635

In D4.3 [2], the composition for Alloy E110 is provided. However, as specified in it, the gap between the fuel pellet and the cladding will not be modelled. Therefore, the cladding thickness is increased to fill this gap, i.e. it is assumed that the cladding begins where the fuel pellet ends. As a consequence, the cladding thickness is increased and, to conserve the mass, the Alloy E110 is smeared in the volume. The new isotopic composition can be found in Table 5. This composition only applies to the fuel cladding, any other components (e.g. spacer grids) uses the composition reported in D4.3 [2].

Table 5 Alloy E110 Smeared Isotopic Composition for Fuel Cladding (ρ = 5.83237 g/cm^3)

Isotope	Atomic Density [10^{24} at/cm^3]
Zr-90	1.989312E-02
Zr-91	4.290439E-03
Zr-92	6.486708E-03
Zr-94	6.433606E-03
Zr-96	1.014852E-03
Nb-93	3.780509E-04
Hf-174	9.692532E-09
Hf-176	3.150172E-07
Hf-177	1.107631E-06
Hf-178	1.615392E-06
Hf-179	8.019970E-07
Hf-180	2.054158E-06

2.1.2 Fuel Assemblies

Among the several types of Fuel Assemblies specified in D4.3 [2], two of them will be used in this Work Package:

- Type 30AV5 (see Figure 5) with UO_2 (3.0% ^{235}U) Fuel Pins, and UO_2 (2.4% ^{235}U) Fuel Pins with 5.0% Gd_2O_3 Burnable Absorber Pins
- Type 390GO (see Figure 6): with UO_2 (4.0% ^{235}U) and UO_2 (3.6% ^{235}U) Fuel Pins, and UO_2 (2.4% ^{235}U) and 5.0% Gd_2O_3 Burnable Absorber Pins.

Both FA types have Alloy E635 stiffening plates in their corners (see D4.3 for the specifications). The FA lattice pitch is 23.6 cm with a reduced active height of 150 cm instead of 353 cm as reported in D4.3. This is, to have a height to diameter ratio closer to the actual VVER-100.

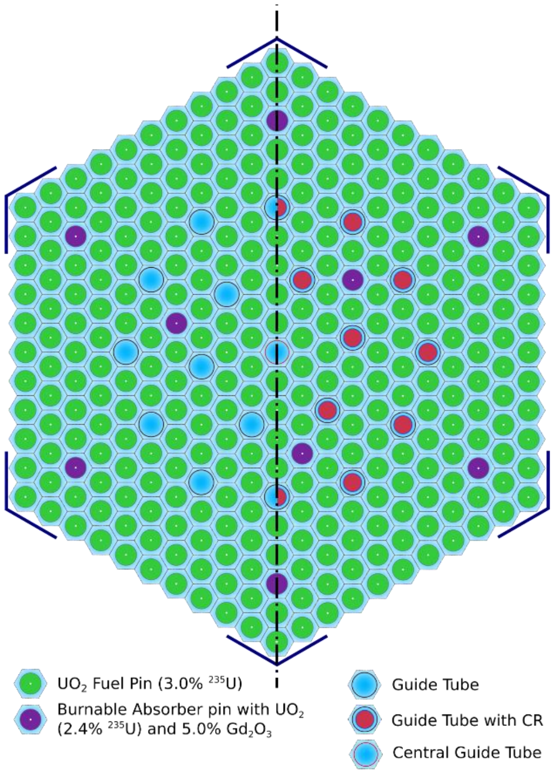

Figure 5 Fuel Assembly 30AV5 without (left) and with (right) Control Rods (CRs) (based on [2][5][7])

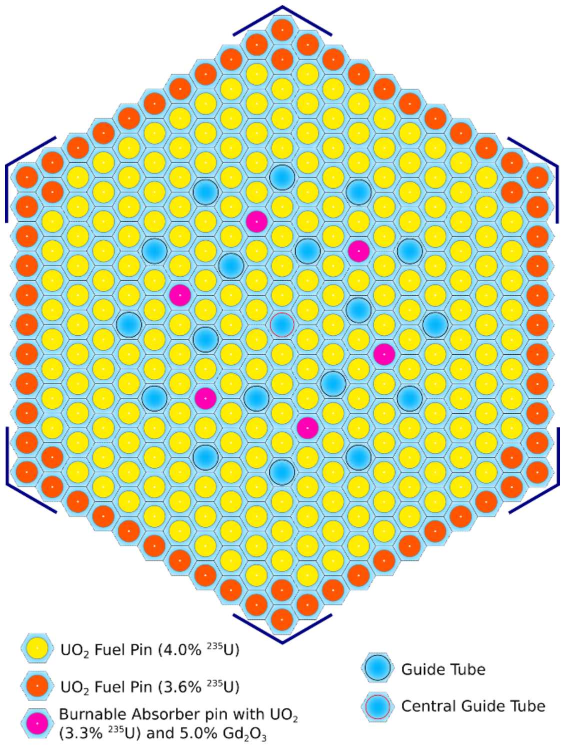

Figure 6 Fuel Assembly 390GO without Control Rods (CRs) (based on [2][5][7])

2.1.2.a Spacer Grids

The spacer grids are not explicitly model in D4.3 [2]. However, it suggests, as in ref. [7], to model the spacer grids as an extra thickness of Alloy E110 added to the fuel cladding.

Considering the specifications given in D4.3 [2] and assuming the original (not smeared) Alloy E110 density (6.4516 g/cm^3), this corresponds to a layer starting from the external radius of the cladding (R_2) to a radius of 0.50051187 cm (R_{SG}) as shown in Figure 7.

In [7], there are fourteen (14) spacer grids axially equally distributed in each FA. However, one of them is in the upper plenum outside the active height and the domain outside the active height is modelled as a smeared homogenous layer of the components. Therefore, thirteen (13) spacer grids in the active height are considered for the original active height of 353 cm. For the 150 cm reduced height the number of spacer grids is reduced to five (5). Their dimensions are given in D4.3 [2]. It should be noticed that the bottom of the first spacer grid starts at 25.5 cm from the bottom of the active height [7].

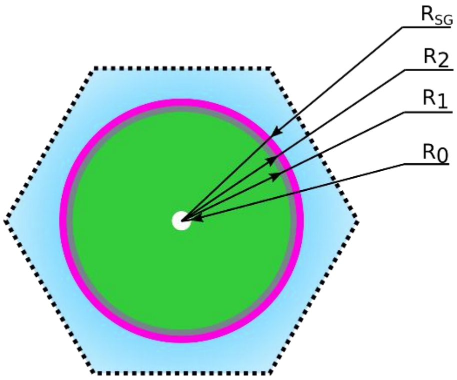

Figure 7 Fuel Pin Cell with Spacer Grid Extra Thickness (based on [2][7])

2.1.3 Core

The VVER minicore layout can be observed in Figure 8. It has seven (7) FAs: one (1) central 30AV5 type FA with the control rods partially inserted surrounded by six (6) 390GO type FAs.

Differently from D4.3, the radial reflector has been modified: the minicore is now surrounded by a layer of borated water with the same dimensions as the FAs (same pitch) and the height of the active core plus the axial reflectors. This radial reflector may suffer modifications in Tasks 5.2 and 5.3.

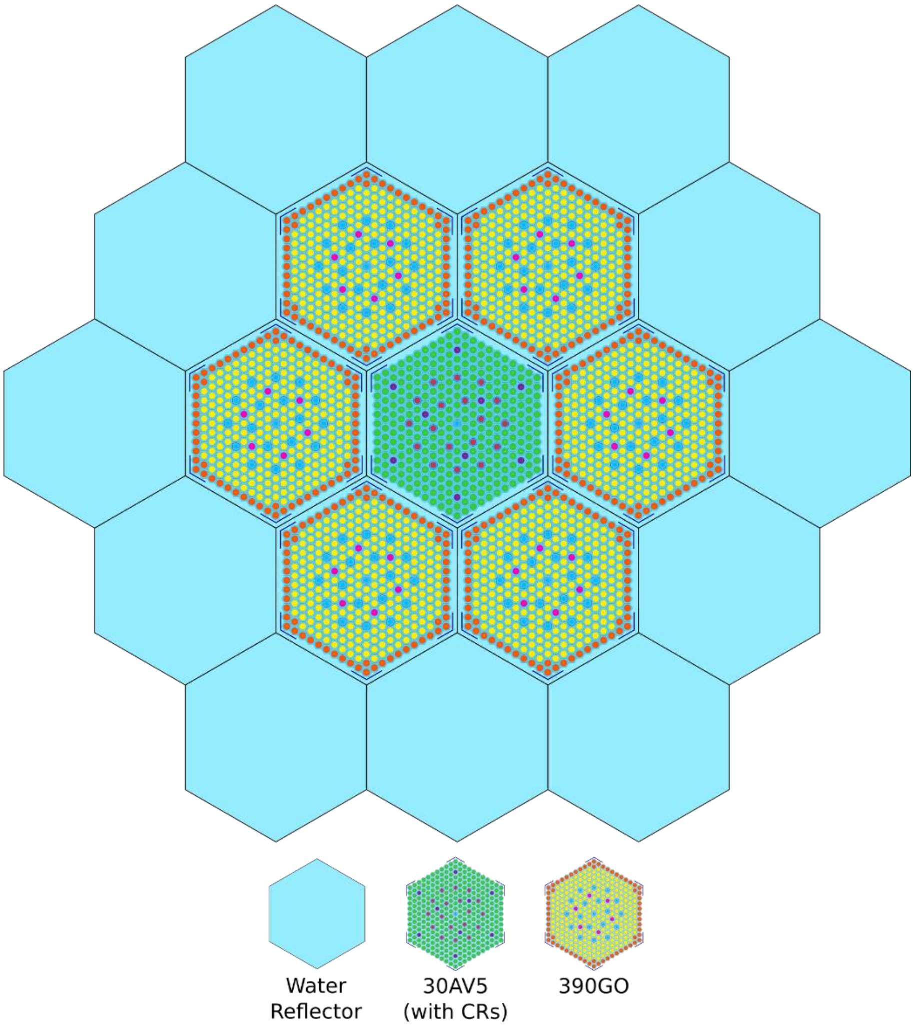

Figure 8 VVER Minicore Layout (based on [2][4][5][6])

The top and bottom axial reflectors are separated into homogenous layers of materials and they are described by different mixtures of moderator, steel, Alloy E635 and/or Helium [2]. In Figure 9, a schematic of the axial reflectors layers can be observed. The thickness of each layer is specified in Table 6 [2] and the material composition is given in D4.3 [2].

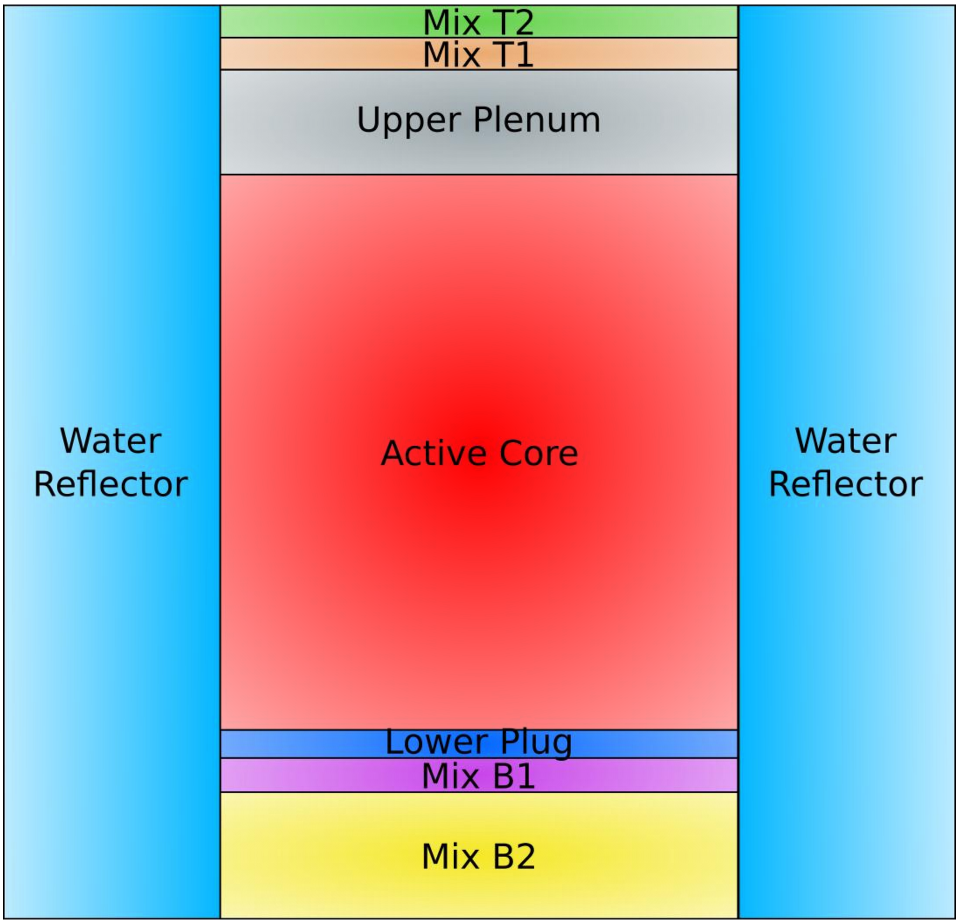

Figure 9 VVER minicore radial, top and bottom reflectors (based on [2]).

Table 6 VVER minicore axial dimensions [2]

Layer	**Thickness [cm]**
Mix T2	5.3
Mix T1	4.5
Upper Plenum	22.2
Active Core	353
Lower Plug	2.3
Mix B1	1.7
Mix B2	25

2.2 Thermophysical Properties

For the correct description of the coupled calculations to be performed in this Work Package, the thermophysical properties data are provided in Table 7-Table 10: thermal conductivity (k) and specific heat (C_p) of the fuel and cladding. These values were obtained from [5][9] which are based on benchmark [10] for UO_2 fuel[2] and Alloy E110 cladding for Kozloduy-6 from WP3 and they apply to all types of FAs simulated. We assume the same properties values in this report. For the sake of comparison between codes, linear interpolation is expected between the points on the table[3].

Table 7 Fuel thermophysical properties [5][9][10]

Parameter				**Value**			
T [K]	300	500	700	900	1100	1300	1500
k [W/mK]	8.15	6.7	5.4	4.4	3.75	3.25	2.8
Cp [J/kg K]	270	287	302	310	314	319	320

Table 8 Fuel thermophysical properties [5][9][10] (cont.)

Parameter				**Value**			
T [K]	1700	1900	2100	2300	2500	2700	2900
k [W/mK]	2.50	2.40	2.42	2.44	2.5	2.65	3.0
Cp [J/kg K]	328	340	364	390	426	470	520

Table 9 Cladding thermophysical properties [5][9][10]

Parameter					**Value**			
T [K]	293.15	373.15	473.15	573.15	673.15	773.15	873.15	973.15
k [W/m K]	17.2	18	19.3	20.1	20.5	20.9	21.8	22.9
C_p [J/kg K]		280	301	322	343	368	398	448

Table 10 Cladding thermophysical properties [5][9][10] (cont.)

Parameter					**Value**			
T [K]	1073.15	1173.15	1273.15	1373.15	1473.15	1573.15	1673.15	1773.15
k [W/m K]			27.8	29.0	30.1	31.2	32.3	33.4
C_p [J/kg K]	420	380	290					

No thermal expansion is considered; therefore, the fuel density is assumed to remain constant throughout all simulations (as specified in [2]). A constant fuel-clad gap conductivity of 104 W/m2K will be used for simplicity [5]. The IAPWS-97 formulation will be used for water properties [11].

[2] For fuel pins with burnable poisons, the same thermophysical data as for UO_2 will be used.

[3] If the temperature is below the lowest one, then, the value corresponding to the minimum temperature applies. If the temperature is over the highest one, then, the value corresponding to the maximum temperature applies.

3 Description of 32 FAs PWR minicore

In addition to the VVER benchmarks, two PWR small cores were proposed in D4.3 [2]. In this document, we will refer to the 32 FAs PWR minicore specifications, which is based on [12] for core layout, with geometry and material details in D4.3 [2]. This core contains thirty-two (32) Fuel Assemblies (FAs) of the same type. A summarized description of the geometry and materials relevant to WP5 is shown in Section 3.1, but the reader is encouraged to refer to D4.3 for material isotopic composition.

3.1 Core description

3.1.1 Pin Cells

The square unit, fuel, guide tube with absorbers and central tube pin cells are shown in Figure 10-Figure 13 respectively. Geometry and material specifications are shown in Table 11-Table 14 for each cell. Details on the material isotopic compositions can be retrieved from D4.3 [2].

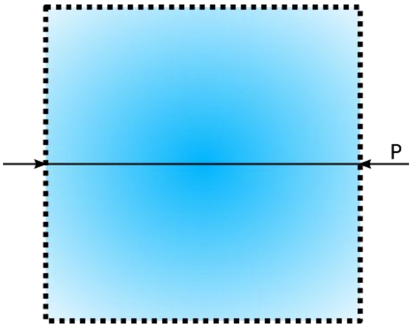

Figure 10 Square Unit Cell (based on [2])

Table 11 Square Cell Pitch [2]

Square Unit Cell	
Unit Cell Pitch (P) [cm]	1.260

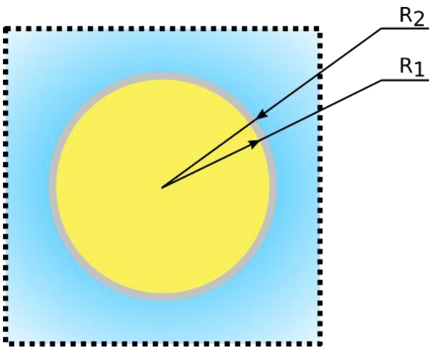

Figure 11 Fuel Pin Cell (based on [2])

Table 12 Fuel Pin Cell Geometry and Materials [2]

Fuel Pin Cell	
Fuel pellet radius (R_1) [cm]	0.4096
Cladding outer radius (R_2) [cm]	0.4750
Fuel pellet material	UO_2 (3.7% ^{235}U)
Cladding material	Zircaloy

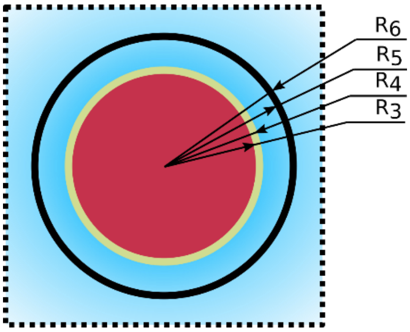

Figure 12 Guide Tube with Absorber (based on [2])

Table 13 Guide Tube and Absorber Geometry and Materials [2]

Guide Tube and Control Rod	
Absorber radius (R_3) [cm]	0.435
Cladding outer radius (R_4) [cm]	0.486
Guide Tube inner radius (R_5) [cm]	0.570
Guide Tube outer radius (R_6) [cm]	0.610
Absorber material	AIC
Cladding material	Zircaloy
Guide Tube material	Zircaloy

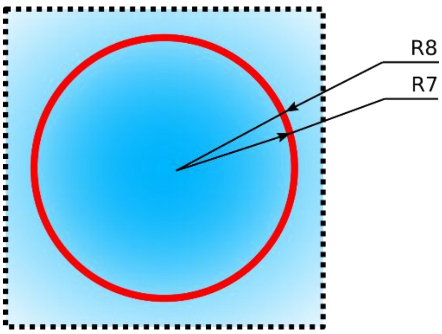

Figure 13 Central Tube Cell (based on [2])

Table 14 Central Tube Geometry and Materials [2]

Central Tube	
Inner radius (R_7) [cm]	0.570
Outer radius (R_8) [cm]	0.610
Material	Zircaloy

In D4.3 [2], the composition for Zircaloy is provided. As for the VVER minicore, the gap between the fuel pellet and the cladding will not be modelled, neither the gap between the absorber and its cladding. Therefore, the cladding thickness is increased to fill this gap, i.e. it is assumed that the cladding begins where the fuel/absorber pellet ends. Consequently, the cladding thickness is increased and, to conserve the mass, the Zircaloy is smeared in the volume. The new isotopic composition can be found in Table 15. This composition only applies to the fuel and absorber claddings, any other components (e.g. guide tubes) uses the composition reported in D4.3 [2].

Table 15 Zircaloy Smeared Isotopic Composition for Fuel Cladding (ρ = 5.666143 g/cm^3) and Absorber Cladding (ρ = 5.960678 g/cm^3)

Isotope	Atomic Density [10^{24} at/cm^3]		Isotope	Atomic Density [10^{24} at/cm^3]	
	Fuel Cladding	Absorber Cladding		Fuel Cladding	Absorber Cladding
Fe-54	1.785644E-05	1.878465E-05	**Sn-112**	4.433220E-06	4.663666E-06
Fe-56	2.803078E-04	2.948786E-04	**Sn-114**	3.016411E-06	3.173209E-06
Fe-57	6.489467E-06	6.826800E-06	**Sn-115**	1.553904E-06	1.634679E-06
Fe-58	8.615079E-07	9.062905E-07	**Sn-116**	6.645259E-05	6.990690E-05
Zr-90	1.884265E-02	1.982212E-02	**Sn-117**	3.510008E-05	3.692464E-05
Zr-91	4.109124E-03	4.322722E-03	**Sn-118**	1.106930E-04	1.164470E-04
Zr-92	6.280884E-03	6.607374E-03	**Sn-119**	3.925915E-05	4.129991E-05
Zr-94	6.365119E-03	6.695989E-03	**Sn-120**	1.489008E-04	1.566409E-04
Zr-96	1.025449E-03	1.078753E-03	**Sn-122**	2.116058E-05	2.226054E-05
			Sn-124	2.646221E-05	2.783775E-05

3.1.2 Fuel Assemblies

Only one type of Fuel Assembly is modelled for the 32 FAs PWR minicore. It is shown with and without rods in Figure 14 and Figure 15 respectively. The FA lattice pitch is 21.504 cm with an active height of 130 cm.

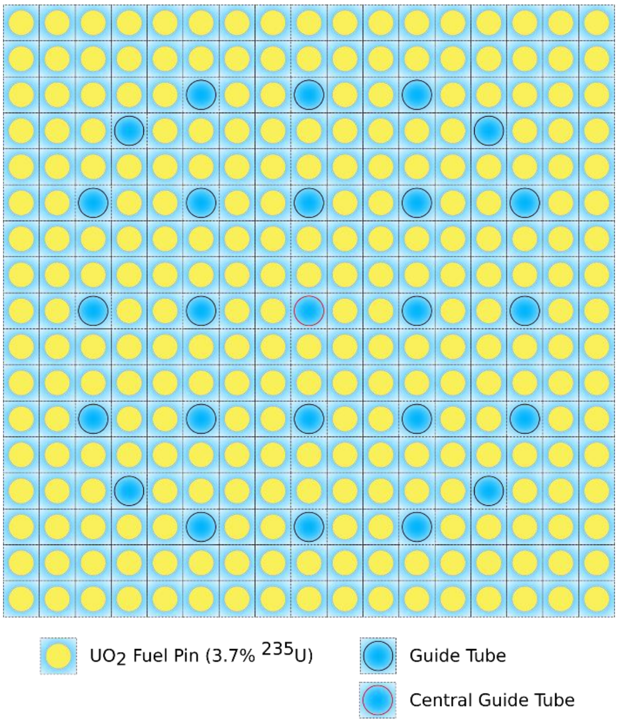

Figure 14 UO_2 Fuel Assembly (3.7% ^{235}U) without Control Rods (CRs) inserted (based on [2])

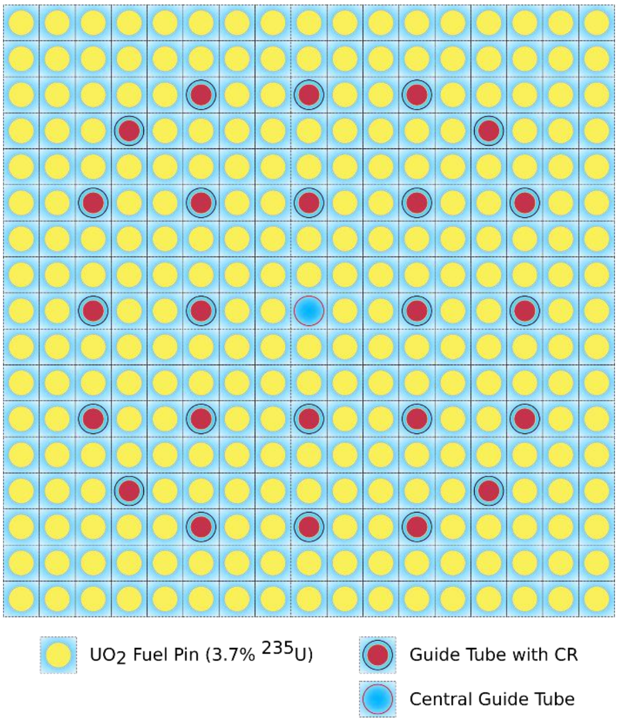

Figure 15 UO_2 Fuel Assembly (3.7% ^{235}U) with Control Rods (CRs) inserted (based on [2])

3.1.3 Core

The PWR minicore layout can be observed in Figure 16. It is composed of a six (6) by six (6) array of FAs without the corner ones, thus giving thirty-two (32) FAs. There are four (4) Control Rods (CRs) positions in the core [13].

The radial reflector contains four (4) layers of different mixtures of materials specified in D4.3 [2]. The radii of the layers are shown in Table 16. This radial reflector may suffer modifications in Tasks 5.2 and 5.3.

Table 16 Radial Reflector Layers Dimensions [2]

Layer	Radius [cm]
L_1 rad	78.9
L_2 rad	79.8
L_3 rad	86.6
L_4 rad	106.6

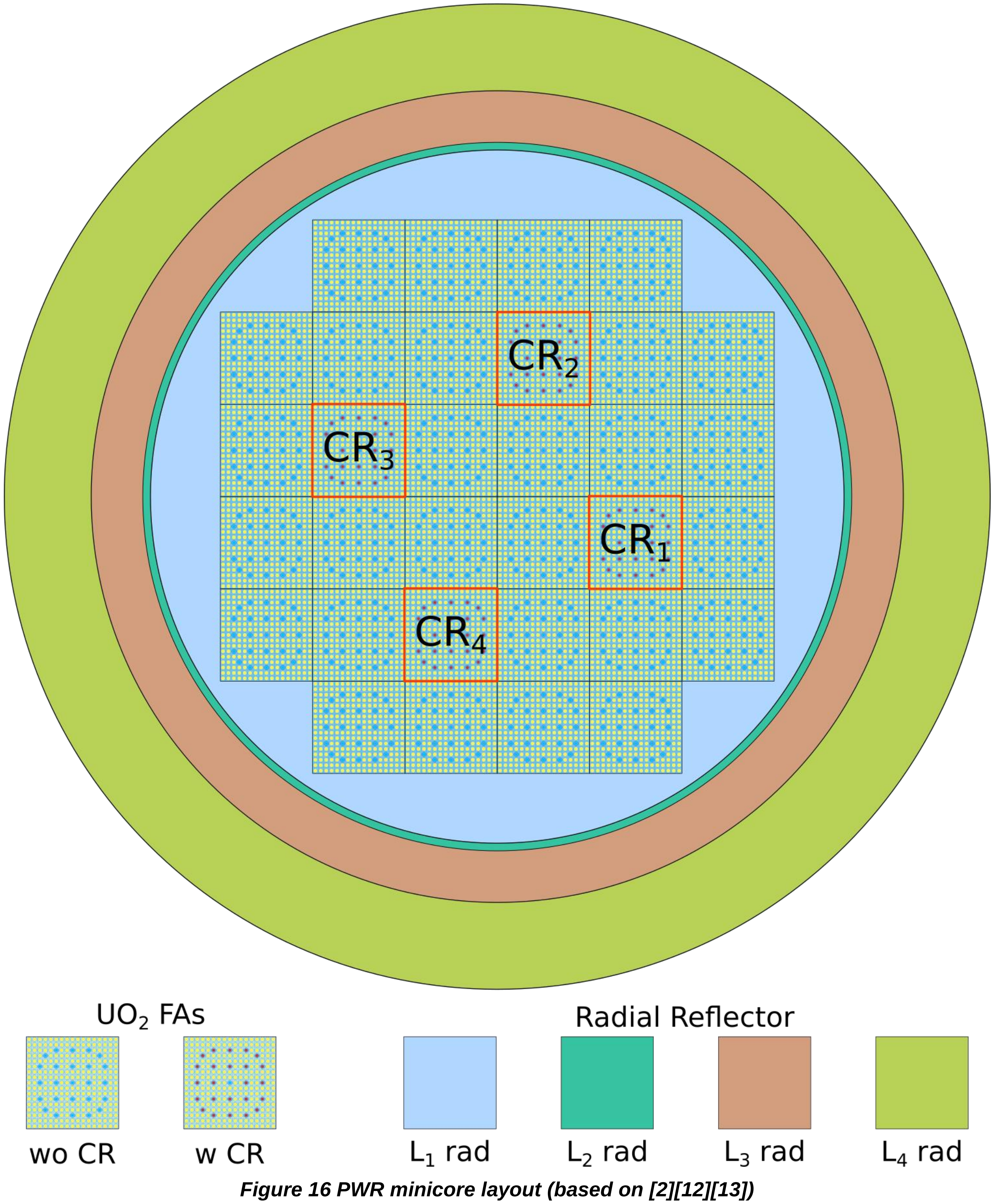

Figure 16 PWR minicore layout (based on [2][12][13])

Top and bottom axial reflectors are separated into homogenous layers of materials made of different mixtures of moderator, steel SS-304, Zircaloy and/or Helium [2]. In Figure 17, a schematic of the axial reflectors layers can be observed. The thickness of each layer is specified in Table 17 [2] and the material composition is given in D4.3 [2].

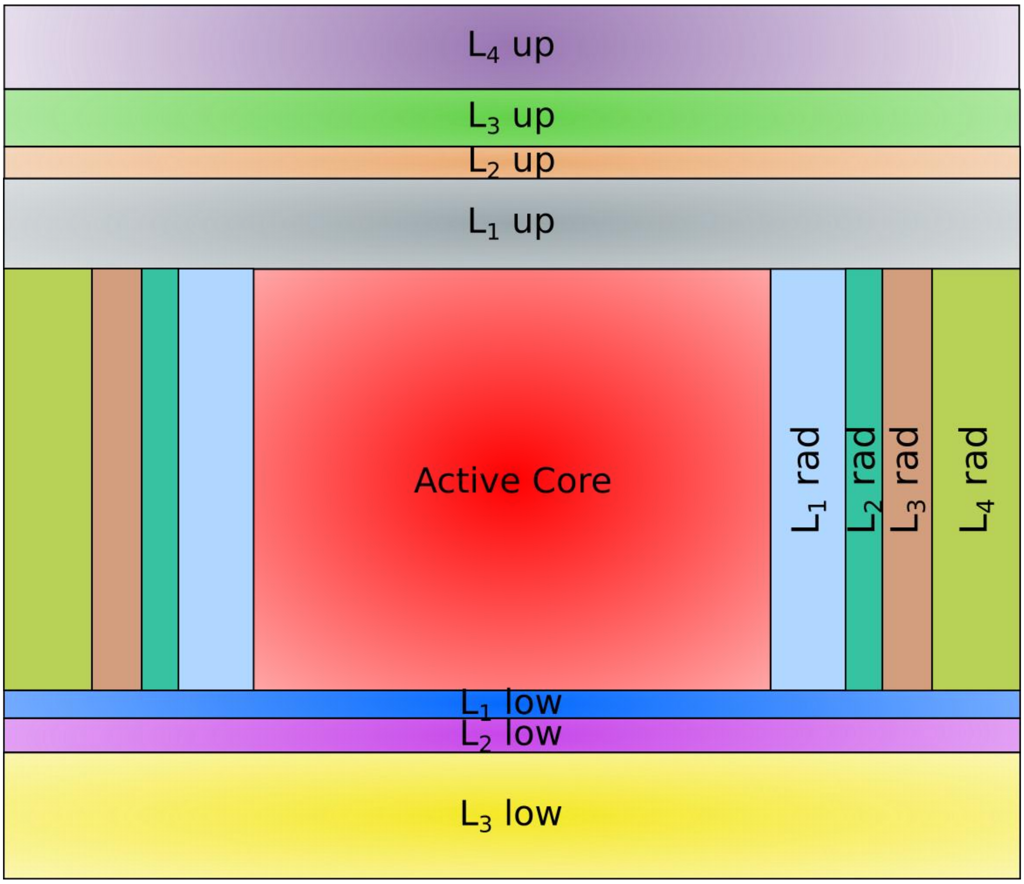

Figure 17 PWR minicore radial, top and bottom reflectors (based on [2][13])

Table 17 VVER minicore axial dimensions [2]

Layer	**Thickness [cm]**
L_4 up	20.0
L_3 up	15.6
L_2 up	3.7
L_1 up	16.5
Active Core	130.0
L_1 low	5.9
L_2 low	9.2
L_3 low	40.0

3.2 Thermophysical Properties

The thermophysical properties data (thermal conductivity (k) and specific heat ($C_{p)}$ of the fuel and its cladding) is provided in Table 18-Table 21. These values were obtained from correlations provided in the benchmark [14] for UO_2 fuel and Zircaloy cladding for a PWR core transient, as used in previous KIT publication [15]. The thermophysical data has been tabulated from the correlations to match with Table 6-Table 9 temperature ranges and to avoid discretization differences among the partners due to internal managing of the data by the codes. For the sake of comparison between codes, linear interpolation is expected between the points on the table[4].

Table 18 Fuel thermophysical properties (Adapted from [14])

Parameter	**Value**						
T [K]	300	500	700	900	1100	1300	1500
k [W/mK]	10.5	6.1	4.5	3.7	3.1	2.8	2.6
Cp [J/kg K]	234	262	280	289	292	294	296

Table 19 Fuel thermophysical properties (Adapted from [14]) (cont.)

Parameter	**Value**						
T [K]	1700	1900	2100	2300	2500	2700	2900
k [W/mK]	2.4	2.2	2.1	2.0	1.9	1.9	1.8
Cp [J/kg K]	302	316	339	375	428	500	594

Table 20 Cladding thermophysical properties (Adapted from [14])

Parameter	**Value**							
T [K]	293.15	373.15	473.15	573.15	673.15	773.15	873.15	973.15
k [W/m K]	12.6	13.7	15.0	16.2	17.3	18.5	19.8	21.2
C_p [J/kg K]	286	295	307	318	330	341	353	364

Table 21 Cladding thermophysical properties (Adapted from [14]) (cont.)

Parameter	**Value**							
T [K]	1073.15	1173.15	1273.15	1373.15	1473.15	1573.15	1673.15	1773.15
k [W/m K]	22.7	24.5	26.4	28.7	31.4	34.4	37.8	41.7
C_p [J/kg K]	376	387	399	410	422	433	445	456

No thermal expansion is considered; therefore, the fuel density is assumed to remain constant throughout all simulations (as specified in [2]). A constant fuel-clad constant gap conductivity of 104 W/m2K will be used for simplicity [5][14]. The IAPWS-97 formulation will be used for water properties [11].

[4] If the temperature is below the lowest one, then, the value corresponding to the minimum temperature applies. If the temperature is over the highest one, then, the value corresponding to the maximum temperature applies.

4 Transient Scenarios

Transient calculations are split into two steps. First, a steady-state calculation at Hot Full Power (HFP) that will serve as the initial condition. Secondly, the transient scenario with its corresponding boundary conditions and time evolution.

4.1 Initial conditions

As stated, the initial condition of the transient scenario will be a neutronics-thermal-hydraulics coupled steady-state calculation at the nominal conditions detailed in Table 22. Nominal conditions for the VVER minicore are specified in [6]. The total power and mass flow have been scaled from full core nominal conditions [2][6][7][16] to seven (7) FAs of reduced active height. Framatome provided nominal PWR minicore conditions in [13]. The values set in Table 22 are based on realistic full core conditions.

Table 22 Hot Full Power (HFP) Initial Conditions for VVER and PWR minicores [6][13]

Parameter	**VVER minicore**	**PWR minicore**
Total Power [MWth]	55	100
Total Mass Flow [kg/s]	784.5	1417.4
Inlet Water Temperature (T_{nom}) [K]	562.15	573.15
Outlet Pressure [MPa]	15.7	15.5
Control Rods Positions	Partially Inserted	CR_1 Fully Inserted
Boron	Critical Search	Critical Search
Irradiation	Fresh FAs	Fresh FAs

With the closed-channels codes, the coupled domain is restricted to the active height. Reflector properties (see D4.3 [2]) remain constant during the steady-state and transient calculations.

A boron critical search will be done in this step. Thus, the initial conditions consist in the coupled solution fields set to criticality by adjusting the boron concentration in the moderator.

4.2 Transient conditions

Two scenarios are proposed for the transient simulations of WP5: a rod ejection event [5][13] (Scenario I) and, an optional, sudden change of the thermal-hydraulics boundary conditions [5] (Scenario II). These conditions are applicable to the PWR and VVER minicore cases. Unless stated the contrary, all parameters (except for the total power) remains constant all through the transient evolution. The thermal power is considered generated uniformly over the fuel pellet radius.

4.2.1 Scenario I

The chosen transient scenario to study consists in a Reactivity Insertion Accident (RIA): starting from HFP conditions from Section 4.1 and the system critical with boron, the control rod is ejected in 0.1 seconds and the other boundary conditions are kept constant. It is moved at a constant velocity to the corresponding position. Then, the system evolution is simulated up to 2 seconds. The aim of this transient scenario is to have a high enough reactivity to analyse a fast transient, but low enough to stay as close as possible in monophasic conditions at all times.

For the 32 FAs PWR minicore the CR_1 starts from a fully inserted position and it is fully extracted in 0.1 seconds. For the VVER minicore, the central CR is partially inserted. The initial position is such that when extracted it will cause a reactivity insertion of 1.2$.

4.2.2 Scenario II

One of the objectives of the CAMIVVER project is the analysis of a Main Steam Line Break (MSLB) [1] as discussed in other WPs. For this reason, an alternative transient scenario from ref. [7] based on ref. [3] is proposed. Boron critical HFP conditions without CRs is the initial condition. Then, the inlet coolant temperature is decreased from its nominal value (T_{nom}) by 10K (i.e., ΔT = -10 K) and remains like this during the whole transient. The system evolution is then studied for 20 seconds. As stated before, this scenario is proposed as an alternative to the rod ejection event and will be treated as an optional case, subjected to partners and codes features availabilities.

5 Output Parameters

For comparing the partners' codes, certain parameters are considered as compulsory outputs [5]:

1. Initial boron concentration, i.e., the boron concentration obtained from the critical search at HFP conditions with and without CRs.
2. VVER minicore CR initial position.
3. Evolution over time of the total system power and dynamic reactivity. Several reactivity definitions are possible depending on the weighting function used to calculate it. For the sake of simplicity and comparison[5], the time dependent neutron balance approach will be used [17][18]. The dynamic reactivity (ρ) can be calculated as:

$$\boldsymbol{k_{eff}(t)} = \frac{\boldsymbol{gain}}{\boldsymbol{loss}} = \frac{\boldsymbol{N(t)}}{\boldsymbol{C(t)+F(t)+L(t)-S(t)}} \quad (1) \qquad \boldsymbol{\rho(t) = 1 - \frac{1}{k_{eff}(t)}} \quad (2)$$

   Where k_{eff} is the time dependent neutron balance multiplication factor (neutrons gain-loss ratio), N, C, F, L and S are the integrated[6] fission neutron production, capture, fission, leakage and scattering production (*nxn* reactions) rates respectively.

4. Evolution over time of average, maximum and minimum values for fuel and coolant temperature as well as coolant density.
5. Evolution over time of Fuel Assemblies axially integrated peaking factors given by Equation 3.

$$\boldsymbol{f_{FA} = \frac{P_{FA}^{MAX}}{P_{FA}^{AVE}}} \quad (3) \qquad \boldsymbol{P_{FA}^{AVE} = \frac{\int_{FA} P(\vec{r})dV}{V_{FA}}} \quad (4)$$

   Where P_{FA}^{MAX} and P_{FA}^{AVE} are the maximum and average volumetric power values, respectively, of a given FA[7]. The integration in Equation 2 is carried out over the FA volume in the active height and V_{FA} is the volume of the FA in the active height.

6. (Optional) Evolution over time of the axially integrated pin-power factors given by Equation 5.

$$\boldsymbol{f_{pin} = \frac{P_{pin}^{MAX}}{P_{pin}^{AVE}}} \quad (5) \qquad \boldsymbol{P_{pin}^{AVE} = \frac{\int_{pin} P(\vec{r})dV}{V_{pin}}} \quad (6)$$

   Where P_{pin}^{MAX} and P_{pin}^{AVE} are the maximum and average volumetric power values, respectively, of a given pin[8] in a given FA. The integration in Equation 4 is carried out over the pin fuel volume in the active height and V_{pin} is the volume of the pin fuel in the active height.

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[5] This approach can be considered as an unweighted calculation (or weighted with an unit-value function). This is to avoid additional calculation of the adjoint function. Eventually, other alternatives can be explored such as the inverse point kinetics method from [18].

[6] Integral over space, energy and direction (not time).

[7] FA positions to be compared will be determined during the simulation phase.

[8] FA and pin positions to be compared will be determined during the simulation phase.

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A Additional core configurations

This appendix provides possible additional core configurations to be analysed in WP5:

- **Kozloduy-6 based small core [2][5].** This core configuration based on the Kozloduy-6 VVER-1000 [4] is more aligned with other WPs. D3.2 [9] provides specifications for the Kozloduy NPP and D4.3 [2] specifies further geometrical and material details. However, the VVER minicore proposed in Section 2 was chosen as the reference case because of its more complex FA loading including burnable poisons [5]. Nonetheless, the Kozloduy case may be analysed as well for the sake of consistency between the WPs.
- **52 FA PWR small core [19].** This PWR small core is based on the KAIST 1A benchmark [20]. It was proposed in D4.3 [2] and in more detail in [19]. In this case, this core configuration presents a more heterogeneous core loading. However, the amount of FAs to be simulated will demand more computational resources and it may be impractical at the moment of comparing results among the partners, since several reruns of the cases might be necessary in case of modelling errors. The simpler 32 FA PWR minicore will be analysed first and, optionally, the KAIST core will be calculated based on the results previously obtained.

The aforementioned core configurations are not mandatory, they are left as optional study cases that may be added on top of the main study cases from Sections 2 and 3.

A.1 Optional VVER Study Case: Kozloduy-6 based minicore

The aforementioned Kozloduy-6 based small core is described in [5] and further detailed in D4.3 [2]. A summarized description of the geometry and materials relevant to WP5 is shown in Section A.1.1, but the reader is encouraged to refer to D4.3 [2] for detailed material isotopic composition. Similar to the reference case from Section 2, the core contains seven (7) FAs. The type of FA still needs to be determined but three possible types are presented in Section A.1.1b.

A.1.1 Core description

A.1.1.a Pin Cells

The hexagonal unit, fuel, guide tube with absorbers and central tube pin cells are shown in Figure 18-Figure 21 respectively. Geometry and material specifications are shown in Table 23-Table 26 for each cell. Details on the material isotopic compositions can be obtained from D4.3 [2].

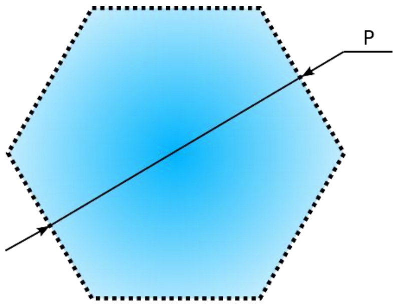

Figure 18 Hexagonal Unit Cell (based on [2])

Table 23 Hexagonal Cell Pitch [2][9]

Hexagonal Unit Cell	
Unit Cell Pitch (P) [cm]	1.275

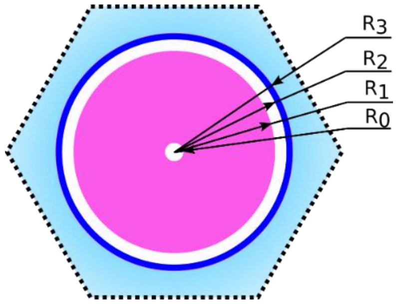

Figure 19 Fuel Pin Cell (based on [2][4][5])

Table 24 Fuel Pin Cell Geometry and Materials [2][9]

Fuel Pin Cell	
Central void radius (R_0) [cm]	0.070 (or 2.35 said in D4.3)
Fuel pellet radius (R_1) [cm]	0.378
Cladding inner radius (R_2) [cm]	0.386
Cladding outer radius (R_3) [cm]	0.455
Fuel pellet material	UO_2 (2.0%, 3.0%, 3.3%, 3.6%, 4.4% ^{235}U)
Cladding material	Alloy E110
Void material	Void / He

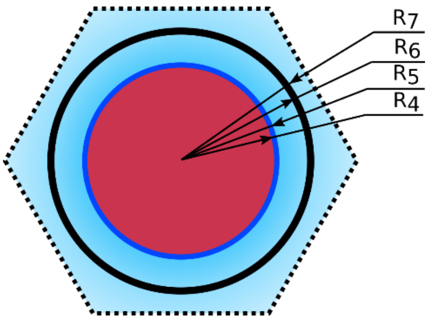

Figure 20 Guide Tube with Absorber (based on [2][7])

Table 25 Guide Tube and Absorber Geometry and Materials [2][9]

Guide Tube and Control Rod Cell	
Absorber radius (R_4) [cm]	0.350
Cladding outer radius (R_5) [cm]	0.410
Guide Tube inner radius (R_6) [cm]	0.550
Guide Tube outer radius (R_7) [cm]	0.630
Absorber material	B_4C
Cladding material	Steel 06X18H10T
Guide Tube material	Steel 08X18H10T

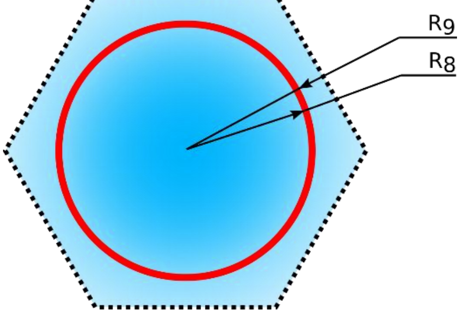

Figure 21 Central Tube Cell (based on [2][7])

Table 26 Central Tube Geometry and Materials [2][9]

Central Tube Cell	
Inner radius (R_8) [cm]	0.480
Outer radius (R_9) [cm]	0.560
Material	Alloy E110

As well as in the other minicores, the gap between the fuel pellet and its cladding is not modelled. Therefore, the gap is smeared in the cladding and the material density and isotopic composition decreases. The isotopic composition of the smeared material is not provided here and it has to be calculated from D4.3 specifications.

A.1.1.b Fuel Assemblies

There are three (3) types of FAs specified in D4.3 [2]:

- Homogeneous FA (Figure 22) with UO_2 (2.0%, 3.0%, 3.3% or 4.4% ^{235}U) Fuel Pins
- Heterogeneous profiled FA (see Figure 23): with UO_2 (3.0% ^{235}U) and UO_2 (3.3% ^{235}U) Fuel Pins
- Heterogeneous profiled FA (see Figure 24): with UO_2 (3.6% ^{235}U) and UO_2 (4.4% ^{235}U) Fuel Pins

These FAs do not have stiffening plates but it has spacer grids equal to the reference case (see D4.3 [2]). The FA lattice pitch is 23.6 cm with an active height of 353 cm. The active height may be modified as the reference case.

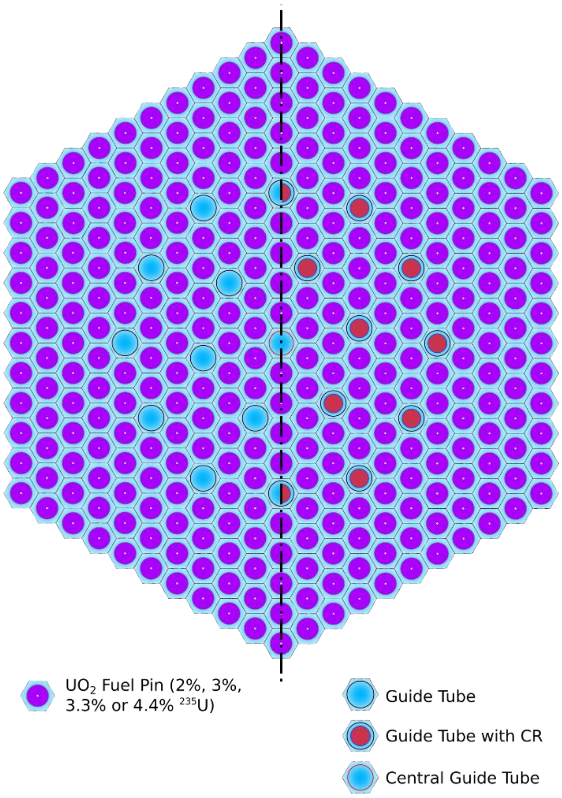

Figure 22 UOX Fuel Assembly without (left) and with (right) Control Rods (CRs) (based on [2])

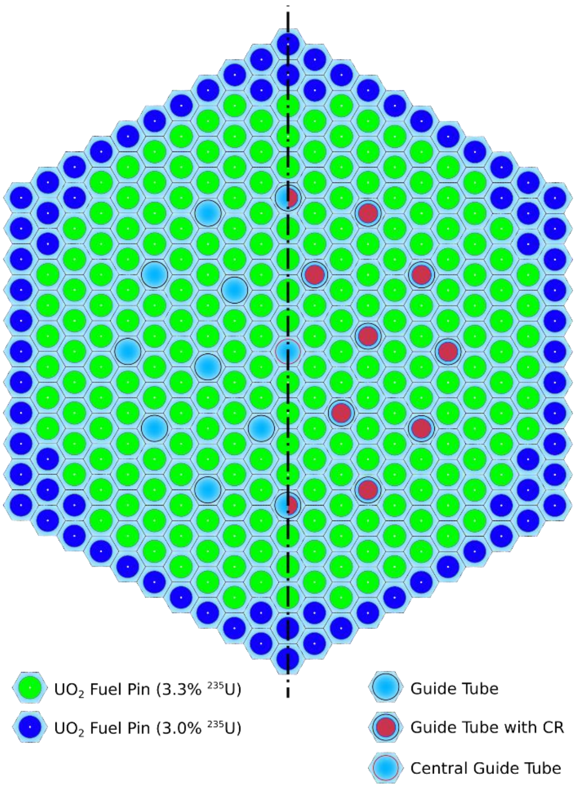

Figure 23 UOX Fuel Assembly without (left) and with (right) Control Rods (CRs) (based on [2][9])

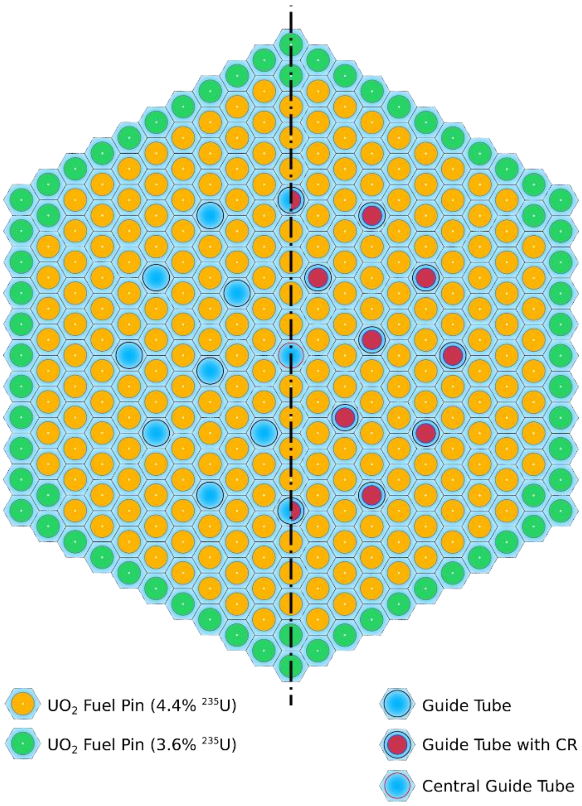

Figure 24 MOX Fuel Assembly without Control Rods (CRs) (based on [2][9])

A.1.1.c Core

The VVER minicore layout can be observed in Figure 25 [2][5]. Similar to the reference case, this core consists in seven (7) FAs with a central CR. The FAs are yet to be chosen from the types described in the previous section.

The radial reflector [2][5] consists in four (4) homogeneous layers composed of water and steel, water, steel, and water respectively. The height of the radial reflector is equivalent to the active core plus the axial reflectors. This reflector will need to be adapted in a similar way to the reference case reflector (Section 2.1.3) to satisfy some code constraints from the partner codes. In addition, material composition and geometry needs to be further discussed among the partners in case this core used.

The same top and bottom axial reflectors as the one used for the reference case (Figure 9 and Table 6) is considered for this minicore.

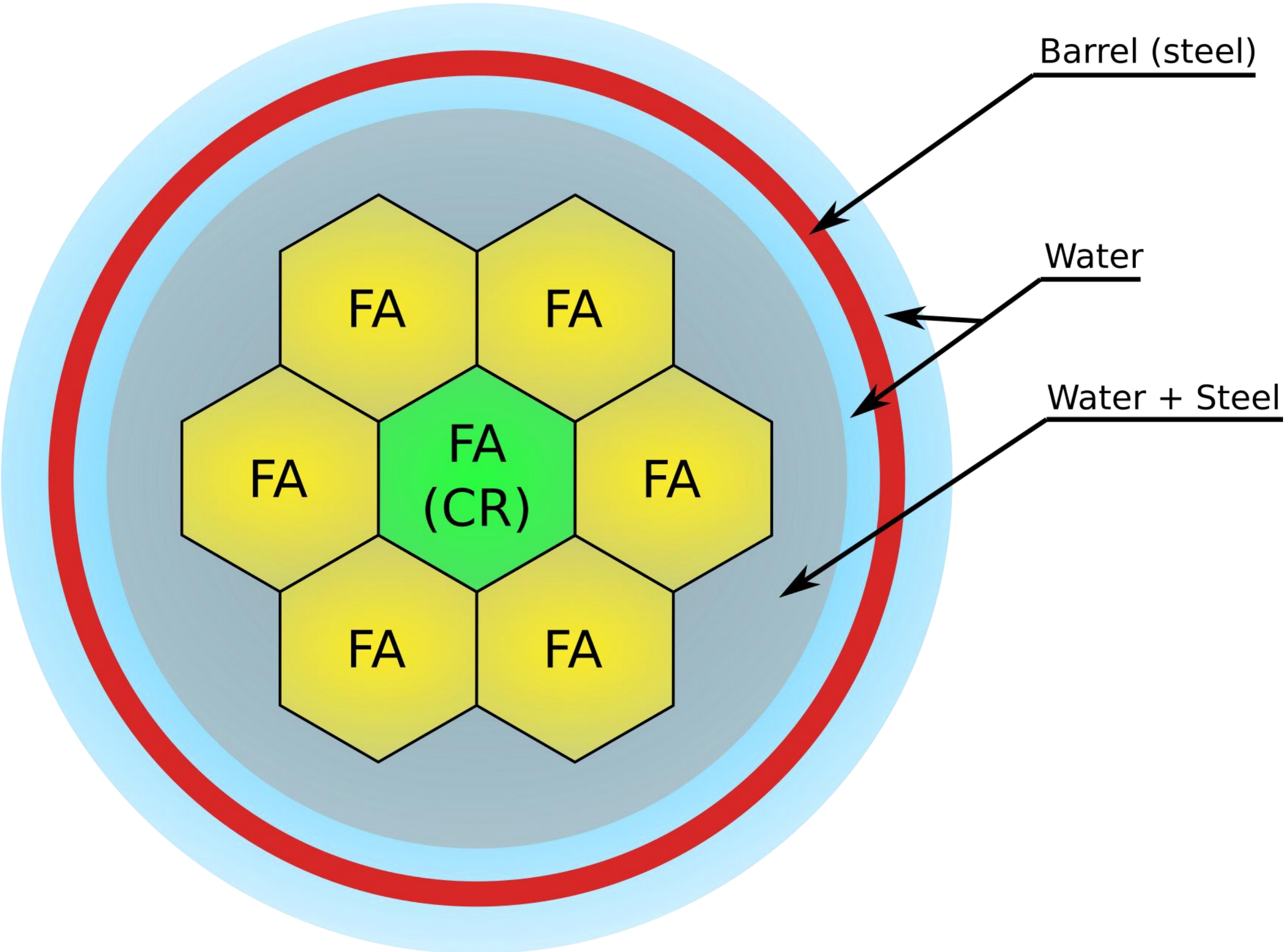

Figure 25 Kozloduy-6 based VVER minicore layout [2][5]

A.1.2 Thermophysical Properties

The thermophysical properties described in Section 2.2 can be used for this case as well, since they are based on Kozloduy-6 information given in D3.2 [9].

A.1.3 Transient Scenarios

A.1.3.a Initial Conditions

As in the reference cases, the initial condition of the transient scenario can be a neutronics-thermal-hydraulics coupled steady-state calculation at nominal conditions, as shown in Table 27. Nominal conditions for the VVER minicore are specified in [6]. The total power[9] and mass flow have been scaled from full core nominal conditions [2][6][10] to seven (7) FAs. The values set in Table 27 are based on realistic full core conditions.

Table 27 Hot Full Power (HFP) Initial Conditions for the Kozloduy-6 minicore [6]

Parameter	**Value**
Total Power [MWth]	128.8
Total Mass Flow [kg/s]	584.25
Inlet Water Temperature (T_{nom}) [K]	552.15
Outlet Pressure [MPa]	15.6
Control Rods Positions	Inserted
Boron	Critical Search
Irradiation	Fresh FAs

With the closed-channels codes, the coupled domain is restricted to the active height. Reflector properties remain constant during the steady-state and transient calculations.

A boron critical search will be done in this step. Thus, the initial conditions consist in the coupled solution fields set to criticality by adjusting the boron concentration in the moderator.

A.1.3.b Transient Conditions

The same or similar scenarios as for the reference cases (Section 4.2) can be used.

[9] The total power should be adjusted in case the active height is reduced.

A.2 Optional PWR Case: 52 FAs PWR small core

This optional PWR configuration based on the KAIST 1A benchmark [20] is described in D4.3 [2] and further detailed in [19]. The original benchmark is a 2D core loaded with fifty-two (52) PWR FAs of different types (UOX, MOX, FAs with burnable poisons). A summarized description of the geometry and materials relevant to WP5 is shown in Section A.2.1, but the reader is encouraged to refer to D4.3 [2] for material isotopic composition and [19] for the up to date geometry and nominal conditions. Further discussions among partners may bring modifications to this configuration before running the final version of the transient scenario.

A.2.1 Core description

A.2.1.a Pin Cells

The square unit, fuel and guide tube with absorber pin cells are shown in Figure 26-Figure 28 respectively. Geometry and material specifications are shown in Table 28-Table 30 for each cell. Details on the material isotopic compositions can be obtained from D4.3 [2][19].

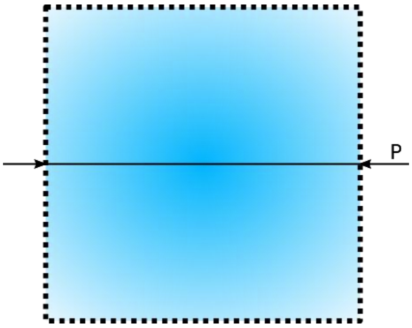

Figure 26 Square Unit Cell (based on [2][19])

Table 28 Square Cell Pitch [2][19]

Square Unit Cell	
Unit Cell Pitch (P) [cm]	1.260

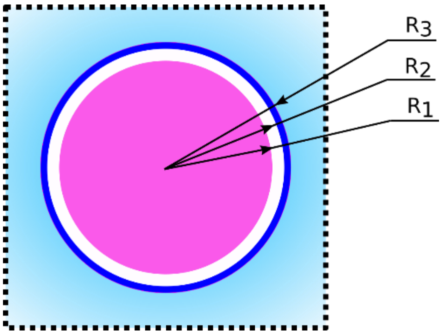

Figure 27 Fuel Pin Cell (based on [2][19])

Table 29 Fuel Pin Cell Geometry and Materials [2][19]

Fuel Pin Cell	
Fuel pellet radius (R_1) [cm]	0.4095
Cladding inner radius (R_2) [cm]	0.4180
Cladding outer radius (R_3) [cm]	0.4750
Fuel pellet material	UO_2(2.0%, 3.3% ^{235}U) MOX(4.3%, 7.0%, 8.7%) UO_2(0.711% ^{235}U) and 9.0% Gd_2O_3
Cladding material	Zircaloy

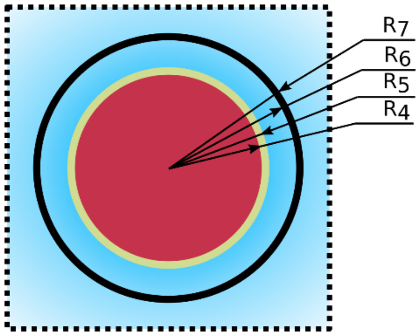

Figure 28 Guide Tube with Absorber (based on [2][19])

Table 30 Guide Tube and Absorber Geometry and Materials [2][19]

Guide Tube and Control Rod	
Absorber radius (R_4) [cm]	0.3823
Cladding outer radius (R_5) [cm]	0.4839
Guide Tube inner radius (R_6) [cm]	0.5715
Guide Tube outer radius (R_7) [cm]	0.6120
Absorber material	B_4C
Cladding material	Zircaloy
Guide Tube material	Zircaloy

As well as in the other minicores, the gap between the fuel pellet and its cladding is not modelled. Therefore, the gap is smeared in the cladding and the material density and isotopic composition decreases and has to be calculated from D4.3 [2] specifications.

A.2.1.b Fuel Assemblies

There are five (5) types of FAs specified in [19]:

- UOX-1: Homogeneous FA (Figure 29) with UO2 (2.0% ^{235}U) Fuel Pins
- UOX-2: Homogeneous FA (Figure 29) with UO_2 (3.3% ^{235}U) Fuel Pins
- UOX-2 (BA-16): Heterogeneous FA (see Figure 29): with UO_2 (3.3% ^{235}U) and UO_2 (0.711% ^{235}U) Fuel Pins with 9.0% Gd_2O_3 Burnable Absorber Pins
- MOX-1: MOX FA (Figure 30) with three plutonium content zones: 8.7%, 7.0% and 4.3%
- MOX-1 (BA-8): MOX FA (Figure 30) with three plutonium content zones: 8.7%, 7.0% and 4.3% and UO_2 (0.711% ^{235}U) Fuel Pins with 9.0% Gd_2O_3 Burnable Absorber Pins

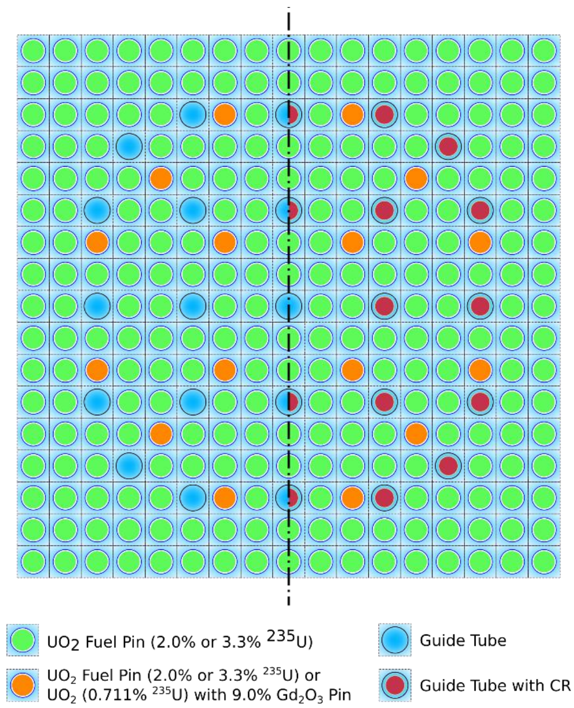

Figure 29 UOX Fuel Assembly without (left) and with (right) Control Rods (CRs) (based on [2][19])

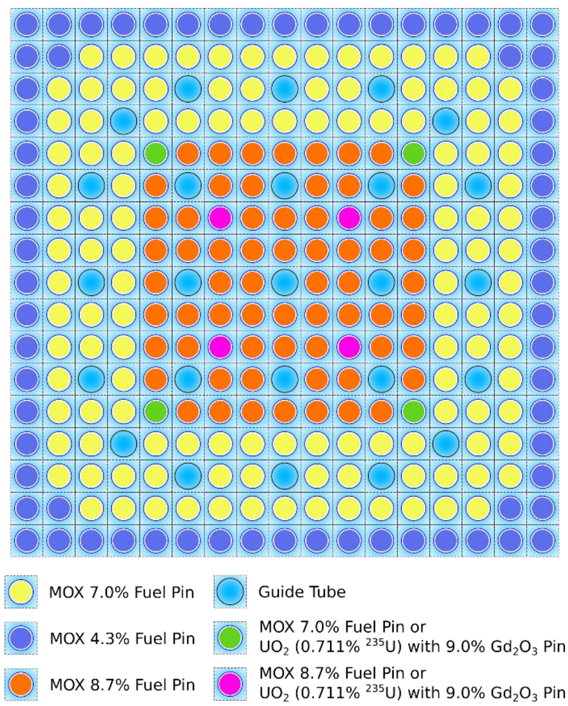

Figure 30 MOX Fuel Assembly without Control Rods (CRs) (based on [2][19])

The FA lattice pitch is 21.42 cm with an active height of 180 cm [19] (contrarily to the value of 365.76 cm indicated in D4.3 [2]).

A.2.1.c Core

A quarter of the 52 FAs PWR minicore layout can be observed in Figure 31. It is composed of an eight (8) by eight (8) array of FAs without three (3) FAs at the corner, thus giving fifty-two (52) FAs. There are four (4) Control Rods (CRs) positions per quarter, thus, sixteen (16) in the core [19].

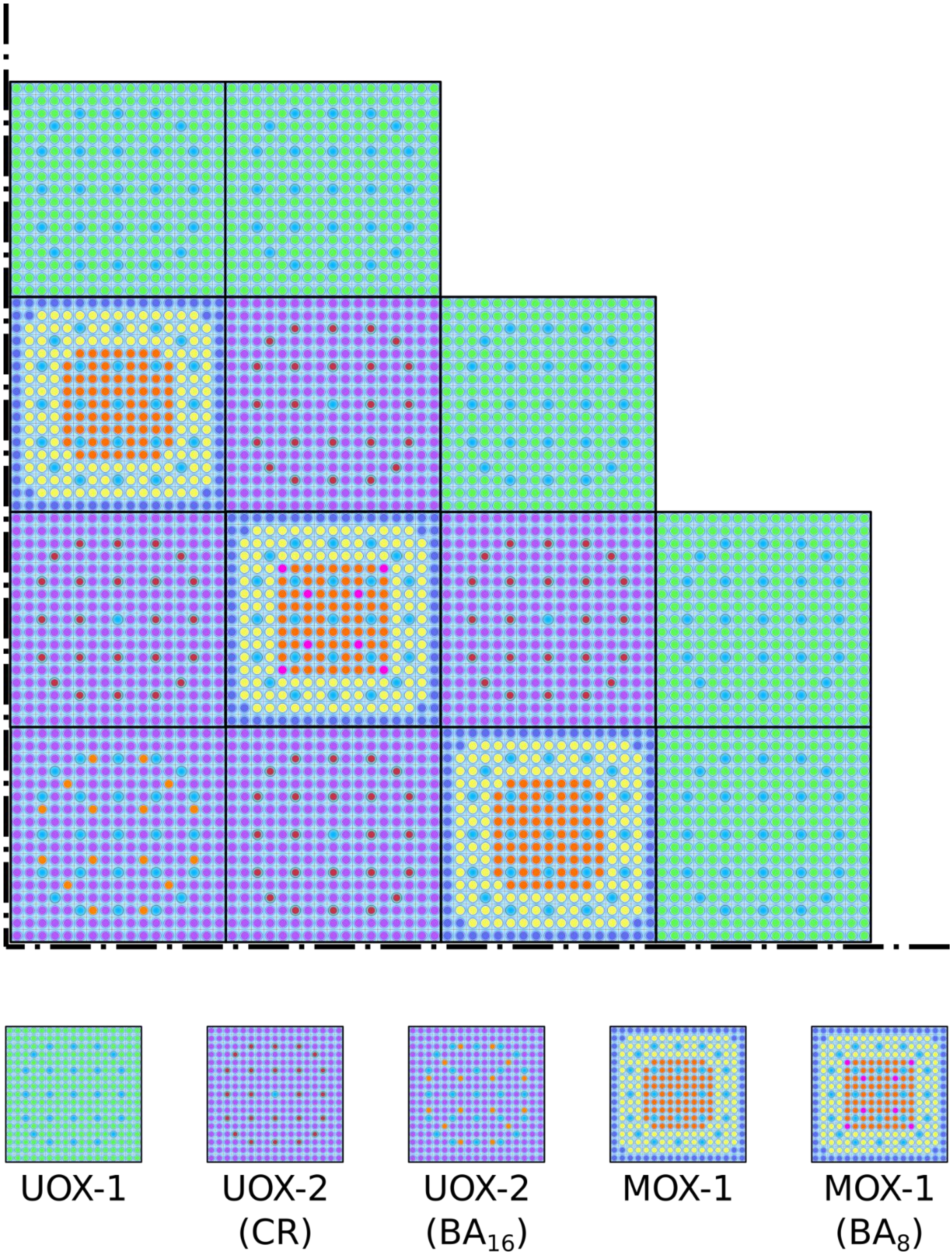

Figure 31 52 FAs PWR Minicore Layout (based on [2][19])

A.2.1.d Reflector

Partners and, in particular, the CEA are working in new options for the advanced modeling of the radial reflector in Task 4 of WP4. For WP5 needs, the radial reflector to be retained for the optional 52 FA core calculation needs to be discussed but in this first approximation the approach proposed for the 32 FAs minicore case may be applied here as well.The axial reflector may be consistent with the 32 FAs PWR minicore from Section 3.1.3.

A.2.2 Thermophysical properties

Thermophysical properties have to be determined for this case. As in Section 3.2, benchmark [14] provides properties for MOX as well making it a viable option.

A.2.3 Transient Scenarios

A.2.3.a Initial Conditions

As in the reference cases, the initial condition of the transient scenario can be a neutronic-thermal-hydraulics coupled steady-state calculation at nominal conditions, as shown in Table 31. Nominal conditions for the 52 FAs PWR minicore are specified in [19]. Total power is set to 15% of the nominal power of 900 MWth [19].

Table 31 Hot Full Power (HFP) Initial Conditions for the 52 FAs PWR minicore [19]

Parameter	Value
Total Power [MWth]	135
Total Mass Flow [kg/s]	4523.5
Inlet Water Temperature (T_{nom}) [K]	570
Outlet Pressure [MPa]	15.5
Control Rods Positions	See Figure 32
Boron	Critical Search
Irradiation	Fresh FAs

With the closed-channels codes, the coupled domain is restricted to the active height. Reflector properties remain constant during the steady-state and transient calculations.

A boron critical search will be done in this step. Thus, the initial conditions consist in the coupled solution fields set to criticality by adjusting the boron concentration in the moderator. Unless stated the contrary, all parameters (except for the total power) remains constant all through the transient evolution. The thermal power is considered generated uniformly over the fuel pellet radius.

A.2.3.b Transient Conditions

The same or similar scenarios as for the reference cases (Section 4.2) can be used in case this minicore is calculated.

For the RIA scenario the CR to be ejected is shown in Figure 33 [19]. The whole transient may be evaluated during the first 1.5s [19].

Additionally, a possible scenario consists in the automatic reactor shutdown by inserting all the initially non-inserted CR at 0.6s.

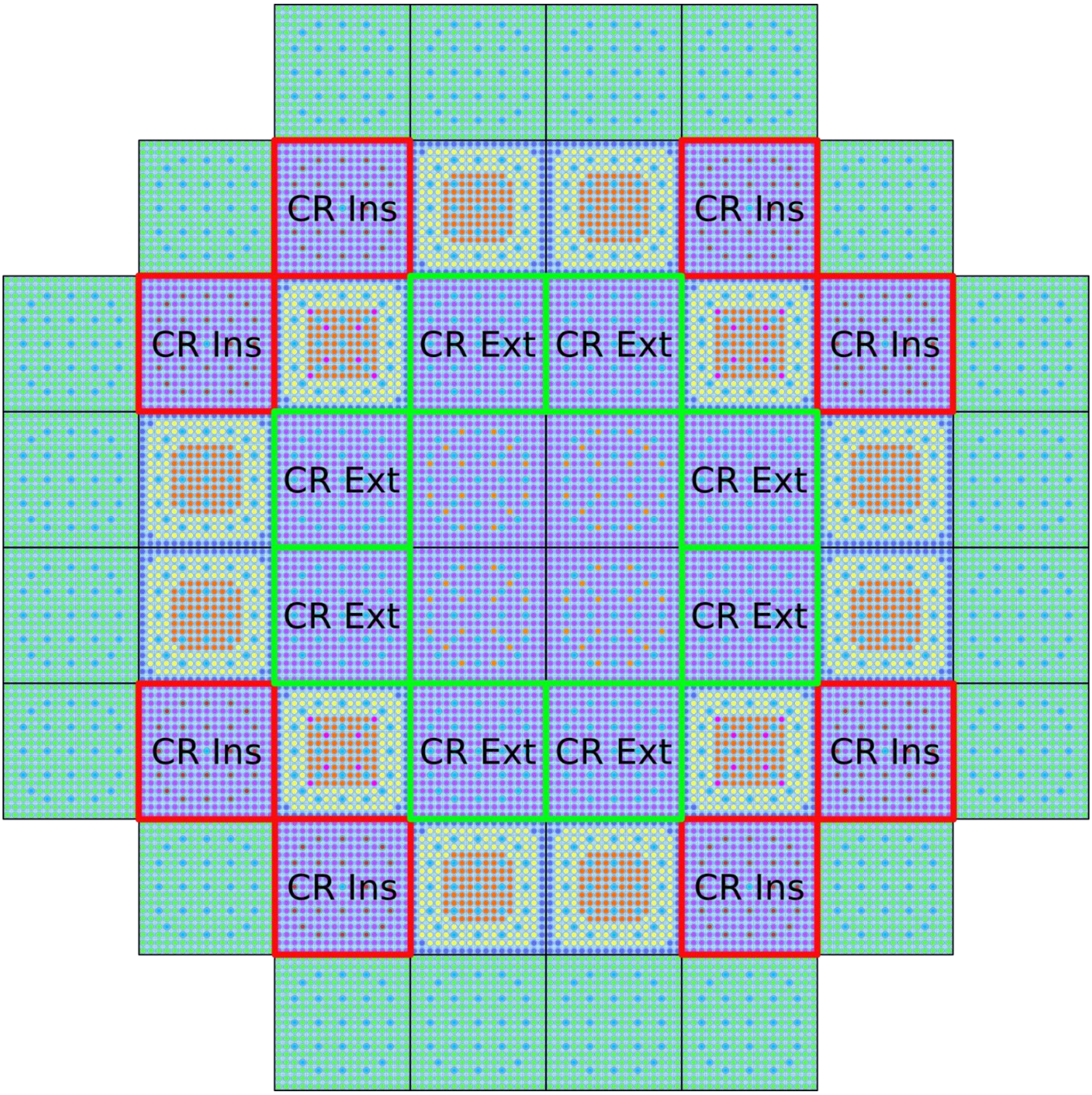

Figure 32 Nominal Core configuration. Inserted (Ins) and Extracted (Ext) CRs are indicated (based on [2][19])

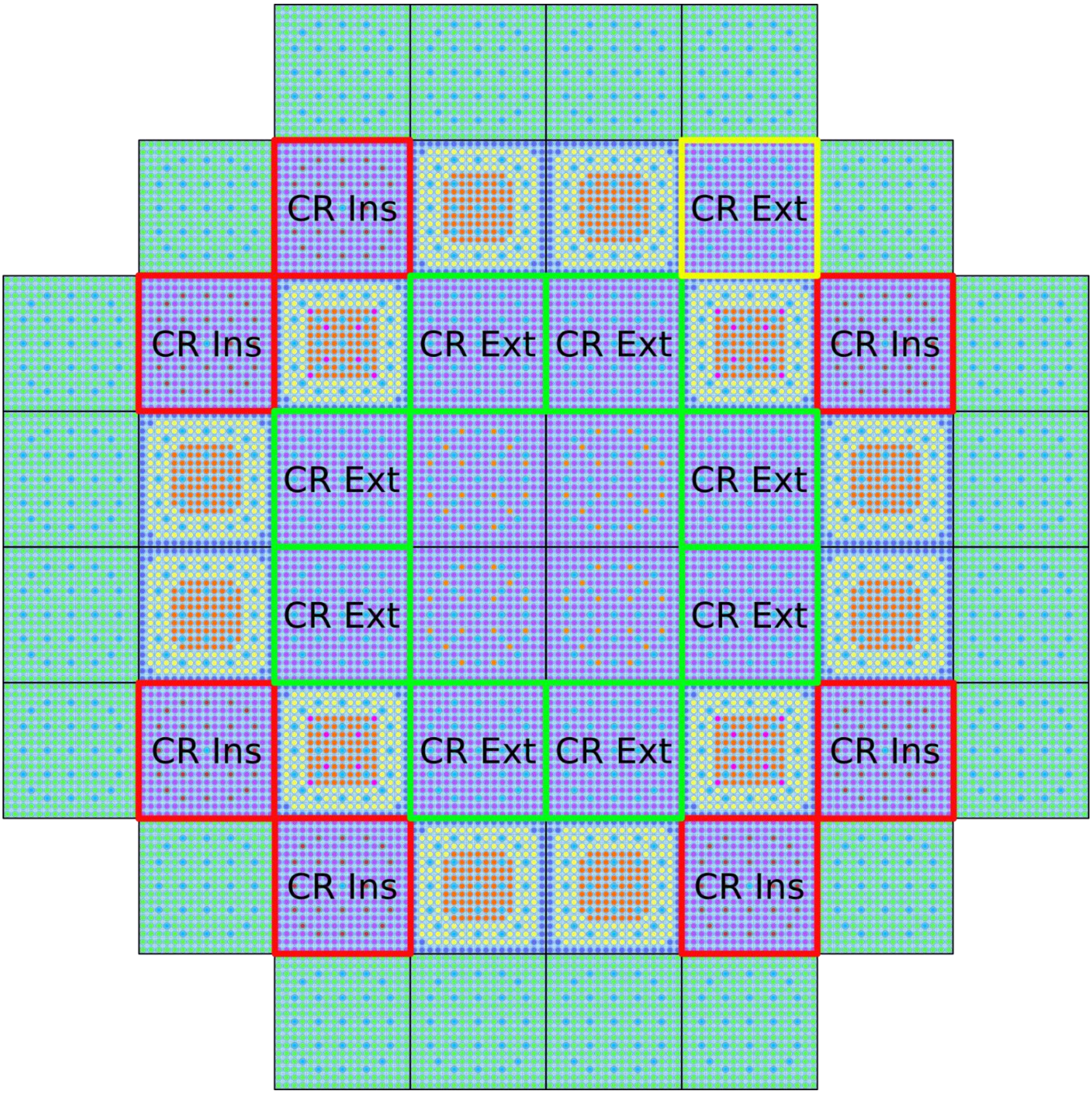

Figure 33 Nominal Core configuration. Inserted (Ins) and Extracted (Ext) CRs are indicated (based on [2][19])