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Codes And Methods Improvements for VVER comprehensive safety assessment

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WP5 - Task 5.4

D5.4 – First step to a reference multi-physics approach: results of 3D neutronics and thermal-hydraulics coupling small core calculations

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Summary

The present document corresponds to Deliverable 5.4 "First step to a reference multi-physics approach: results of a 3D neutronics and thermal-hydraulic coupling small core calculations" of the CAMIVVER project. This document is the corner stone to establish the overall calculation platform and for driving the design and developpement of core codes. This document is a first step forward in the multiphysics coupling calculation approach based on steady-state and kinetic coupling prototype employing APOLLO3® and CATHARE3 codes. The Deliverable 5.4 proposed at the end of Task 5.3 activities, intends to describe advances in developing and application of the prototype to CAMIVVER WP5 small core benchmarks. The prototype is a multiphysics coupling between the APOLLO3® neutronic core code, up to now developed at CEA and mostly applied as a research computational tool, and the CATHARE3 thermal-hydraulic code, latest evolution of system thermal-hydraulic code CATHARE3. The CAMIVVER project enables some developments and validations of such a coupling for PWR and VVER applications. In this deliverable, achievements concerning the multiphysics neutronic and thermal-hydraulic calculations at core level are mostly treated but some information concerning application to a full VVER core APOLLO3® modeling and a first application of such a core to primary and secondary system thermal-hydraulic modeled with CATHARE3 will be shortly presented here. After a first introduction concerning context and needs identified at industrial level asking for advanced 3D multiphysics coupling for core calculations, the present report will focuses on the description of both codes (APOLLO3® and CATHARE3) and major principles of such a coupling. A short description of considered benchmarks (full details available in Deliverables D5.1 and D5.2) and comparison with other reference codes in the framework of WP5 activities (both related to task 5.2 and task 5.3) will be presented in second part of the report. Several acces of improvements have been identified and will be presented as well in a dedicated section.

Approval

Version	First Author	WP leader	Project Coordinator
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Acronyms

APEX	APollo EXchange file
API	Application Programming Interface
BOC	Begin Of Cycle (of a fuel assembly in a nuclear reactor)
BWR	Boiling Water Reactor
CAL_RS	CALculation back-end Requirements Specification
CEA	Commissariat à l'Énergie Atomique et aux énergies alternatives
CPU	Central Processing Unit
CZP	Cold Zero Power
DDM	Domain Decomposition Method
DOM	Discrete Ordinates Method
EDF	Électricité de France
EOC	End Of Cycle (of a fuel assembly in a nuclear reactor)
EPR	European Pressurised Reactor / Evolutionary Power Reactor
FEM	Finite Element Method
FHS	Filesystem Hierarchy Standard
FLOPS	Floating Point Operations per Second
FS	Fine Structure
GiB	Gibibyte - 2^{30} bytes
HDF	Hierarchical Data Format
HFP	Hot Full Power
HPC	High Performance Computing
HZP	Hot Zero Power
IC-CPM	Interface Current Collision Probability Method
ISO	International Organization for Standardization

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JHR	Jules Horowitz Reactor
KAIST	Korean Advanced Institute for Science and Technology
LWR	Light Water Reactor
MDL_RS	Multi-parameter Data Library Requirements Specification
MOC	Method Of Characteristics
MPI	Message Passing Interface
MPO	Multi Parametric Output
PBS	Portable Batch System
PWR	Pressurized Water Reactor
QoI	Quantity of Interest
RAM	Random Access Memory
RFC	Request For Comments
RMS	Root Mean Square
SFR	Sodium-cooled Fast Reactor
SHEM	Santamarina Hfaiedh Energy Mesh
SMR	Small Modular Reactor
Sn	Segment n
SPH	"SuPer-Homogénéisation"
SPn	Simplified Pn (Spherical Harmonics)
SYS_RS	System Requirements Specification
UC	Use Cases specification
UDM	User Data Model
VVER	Vodo-Vodyanoi Energetichesky Reaktor (water-water power reactor)
WP	Work Package

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1. Introduction

The H2020 CAMIVVER project Work Package 5 (WP5) is dedicated to advanced coupled neutronic and thermal-hydraulics core calculations for both PWRs and VVERs and to benchmarking activities with advanced codes.

In WP5, three main tasks were established in the project proposal [1] specially conceived to support multiphysics core calculations. Task 5.1 with its associated D5.1 [3] and D5.2 [4] 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 transient scenarios with VVER [5] geometries with different core neutronics and channel thermal-hydraulics tools (APOLLO3®/THEDI, SERPENT2/SUBCHANFLOW). 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 [1] for the development of a 3D neutronics-thermal-hydraulics reference calculation based on APOLLO3®/CATHARE3 coupling and to apply it to PWR and VVER cases.

The need of such calculations is justified at industrial level to have access to advanced calculation tools supporting the maintaining in operation of existing power plants towards Long Term Operation (LTO) and also the design of innovative solutions and concepts.

WP5 is tightly connected to the activities of WP4. Deliverable 4.3 [2] provides most of the cores, reflectors and fuel assemblies geometrical and material descriptions, as well as nominal operating conditions. However, for the purposes of WP5, some of the data (mainly boundary conditions) have been updated and specific recommendations have been introduced in dedicated deliverables that are summarized in D5.2 [1].

This document takes into account the recommendations issued from Task 5.1 providing the VVER and PWR test cases, specifying their geometries, materials, thermophysical properties, transient scenarios (initial/ boundary conditions), and output parameters to be extracted and compared. These transient scenarios have been simulated by participants with available multi-physics tools and results contribute to both Tasks 5.2 (mainly oriented to VVER minicore case) and 5.3 (mainly oriented to PWR minicore cases).

In Chapter §2 the current and future trends for multiphysics calculations will be presented.

In Chapter §3 the objectives of Task 5.3 are briefly presented with the definition of the PWR oriented test case. The main hypotheses associated to scenario definition and boundary conditions are summarized as well for steady-state and transient.

In Chapter §4 the new coupling prototype applying the codes APOLLO3® and CATHARE3 for steady-state and transient 3D multiphysics core calculations will be introduced. In Chapter §5 and in Chapter §6 the benchmark results for the PWR and the VVER cases are respectively presented, with comparisons among partners codes and tools focusing on best practices of multiphysics modeling, taking as reference an high fidelity coupling such as the SERPENT2/SUBCHANFLOW. In Chapter §7 complementary information is provided concerning other analyses realized on the PWR and VVER test cases with both configurations APOLLO3® stand-alone, APOLLO3® with its thermal-hydraulic module THEDI and the coupling APOLLO3®/CATHARE3 with applications going from small to full core cases.

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2. Context of multiphysics calculations

The European increasing need in decarbonated sources of electricity imposes a strong attention to Long Term Operation (LTO) strategies for both PWR and VVER type of reactors.

For such challenges it is of primary importance having access to several full 3D core neutronic codes and coupling tools in order to improve the prediction capabilities in reactor core analyses.

For the moment, specific applications have mainly focused on the neutronic modeling improvement (e.g., nuclear data, heterogeneity, numerical methods, etc.). Neutronics mainly contributes to physics phenomena involved in core analyses during evolution and kinetic transient, however the feedbacks coming from coupling with other physics are to be accounted as well.

More in general, current industrial codes and methods need to keep innovation as driving force in order to properly consider:

- New reactor designs (e.g., EPR, VVER, SMR, HTR, …);
- New requirements from Safety Authorities (ASN Guide n°28)[6];
- New cycle-oriented loading strategies (e.g., plutonium multi-recycling);
- New challenges of Long-Term Operation dedicated projects.

For the next decade, an industrial stake is to enhance the codes interoperability and the multi-scales analyses as a solution for improving the single and coupled physical phenomena investigation and resolution for different reactor designs including the innovative ones.

2.1. State-of-the-art on core physics design and safety analysis

The classical approach in reactor physics analysis, commonly known as “two-step calculation”, has been defined in D4.1 [6], namely the generation of a multi-parametric homogenized cross section library where a spatially detailed multigroup flux solution at fuel assembly level is used as reference flux to produce few-group homogenized cross sections to be provided as input to the 3D full-core calculation. This comprises the multi-physics coupling that produces the temperature and density distributions that in turn define the local values of the cross sections. The local-condition dependent cross sections are then taken from the multi-parameter library by interpolation.

As far as multiphysics feedbacks, these are often provided by simplified tools modeling core thermal-hydraulics and fuel rod temperature distribution in a dedicated control volume.

2.2. Major contributions of the CAMIVVER project

CAMIVVER brings to the international Community significant contributions to the evolution of the state-of-the-art for VVER and PWR safety analysis since it proposes a unique step-by-step integral approach for numerical benchmarks definition, starting from geometrical data, fuel composition, test cases definition and both steady-state and transient scenarios for adapted comparison of different modeling options always keeping in mind the lab-to-industry process.

Several discussions on multi-physics resolutions are available at international level. The activities carried out in WP5 have allowed making a step forward [8] by integrating industrial view and needs at the international level [1] combining at the same time new codes applications and experiences of the partners involved.

In addition, in the framework of the CAMIVVER project some calculation tools and scientific codes have been developed and improved by partners to enable benchmarks for both PWR and VVER configurations at lattice, core and full system level with the objective to open the discussion around best practices to be applied at industrial level for core multi-physics approach by neutronics and thermal-hydraulics coupled Best-Estimate simulations.

WP5 mainly focused on actions finalized to provide test cases representative of PWR and VVER configurations and boundary conditions to assess:

- performances of APOLLO3® core solvers using its internal multi-1D thermo-hydraulic library (THEDI) and comparing its results towards other state of the art codes [9] [12];
- multi-parametric neutron data libraries generated at WP4 for VVER and PWR different configurations and homogenizations.
- a newly proposed APOLLO3®/CATHARE3 coupling and benchmarking against existing 3D high fidelity models based on SERPENT/SCF coupling [9], [11].

The APOLLO3® code has been selected in the WP5 activity for testing the potentiality of its core solvers on treating hexagonal geometries (specific of VVER and other GEN IV concepts) [9] and identifying points of improvement for a possible industrialization on the long term.

To test and support comparisons with high-fidelity models a huge work has been done on the definition and the assessment of the reference test cases, with adapted boundary conditions and selected transients [10]. For reducing the expected calculation time and allowing sensitivity studies, parametric analyses and testing, several options for small core sizes-oriented calculations have been selected. This choice of simplified geometry is in line with studies on-going on PWR framework (i.e., OECD/NEA) where multi-physics approaches are tested on cluster of assemblies or small cores [13].

The type of configurations selected has allowed further testing against high-fidelity resolutions (e.g., SERPENT2/SCF couplings) developed in previous EU projects (e.g., H2020 McSAFE project). In case no experimental data are available, these higher order solutions may be used to check the prediction accuracy of low-order solutions based on diffusion and simplified transport approximations.

2.3. Present and current trends of multiphysics coupling

The already industrialized current approaches and trends on multiphysics coupling schemes in support to reactor safety analysis are described hereafter.

At industrial level, neutronics, thermal and thermal-hydraulics feedbacks [15] calculation adopted for reactor design and safety analysis are typically attained by code platforms composed by a neutronic code (nodal or finite elements based), using homogenized (with different schemes but often assembly-wise or a fraction of assembly) cross section data libraries delivered by an autonomous lattice module, coupled with mainly 1D thermal-hydraulics, heat transfer within the fuel rod and a fuel depletion solver, as described in [16]. The thermal-hydraulics module may solve the enthalpy balance for each FA modeled as a closed axial channel with imposed inlet mass flow; it hence provides a 3D mapping of parallel channels, each modeled in 1D or it enables the modeling of transverse flow redistribution among fuel assemblies, too. In Figure 1 a summary of the main applications is provided.

The system thermal-hydraulic influence is imposed by boundary conditions at core inlet and outlet physical domain enabling the possibility of considering primary and secondary circuit heterogeneities and their effects for instance on core inlet temperature and mass flow.

Current trends in research and development activities at industrial level concern the possibility of better representing any simplified, decoupling hypothesis at the interface among codes and models, improving the robustness of the overall steady-state or transient phenomena evaluation over the entire domain. The recent French Safety Authority N° 28 Guide [6] provides a coherent set of recommendations accompanying Scientific Computing Tools qualification for Safety Analysis applications.

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Having access to innovative integrated solutions with a smaller degree of approximations (e.g., 1 step, coupled core/systems investigations) needs the access to integral Verification and Validation tests and benchmarks with higher fidelity codes, in particular for coupled multiphysics phenomena simulation, see Figure 2.

Mid-term strategies are supporting tools and methods reducing the calculation mesh size specifically adapted to account for local behaviors, heterogeneities of relevant parameters but guaranteeing an acceptable performance concerning number of parallel CPUs involved and memory size dimensioning. At core level, a global trend exists towards next generation codes capable of gaining in accuracy on standard core configurations and of correctly modeling the heterogeneous LWR cores just by switching the modeling options, mostly in the following two areas [7]:

- full 3D pin-by-pin transport calculation at assembly/core level for reference calculations.
- calculations at core level in cell-based approach with diffusion and simplified transport flux solver (e.g., SPn) for standard industrial calculations.

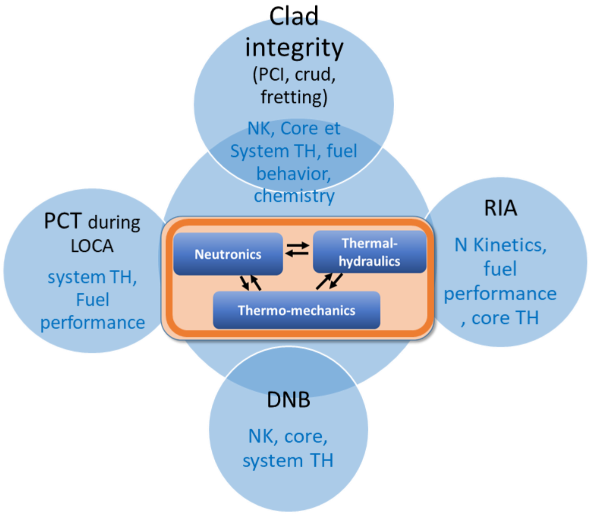

FIGURE 1: EXEMPLE OF A COUPLED CALCULATION SCHEME

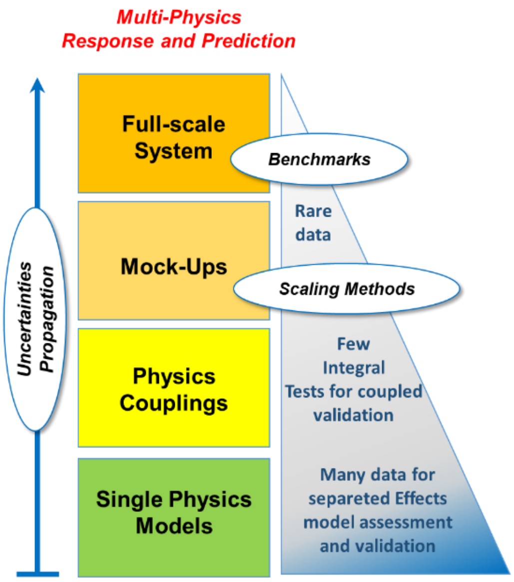

FIGURE 2: EXEMPLE OF PROGRESSIVE NEEDS IN V&V FOR QUALIFICATION

The CAMIVVER project is mainly oriented to contribute with innovative solutions on this scenario, proposing a state-of-the-art of the current approaches and a step forward in V&V of new modeling solutions, see Figure 3.

APOLLO3® offers a set of computational modules applicable to lattice and core simulations allowing to perform a classical two-step lattice/core neutronics scheme, but also direct transport calculations without homogenization and thermal feedbacks on small geometries (multi-clusters, mock-ups) [7].

In this sense, these new EU codes prepare discussions toward long term strategies for safety analysis that will be probably oriented to solutions providing answer at different scales, depending on the physical property under investigation and time scale. Any complex system may be reproduced by numerical tween where the resolution of core physics may be realized in the same calculation domain with an integrated multiphysics approach. Also at core level, in long term simulation strategies a step from the separation between core and spectral codes to a new paradigm in integrated neutronics calculation platforms is envisaged.

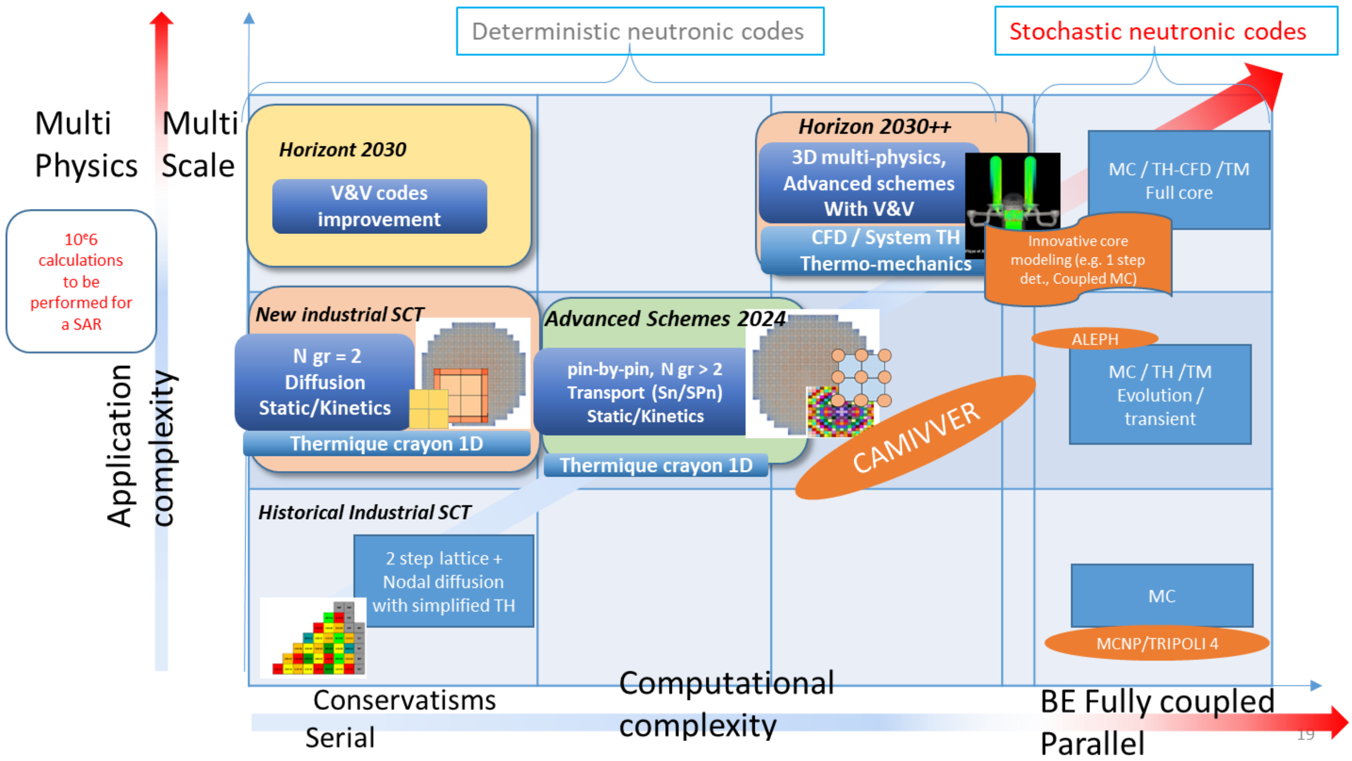

FIGURE 3: CURRENT TREND OF CODES V&V IMPROVEMENT

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3. WP5 task 5.3 main objectives

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 roadmaps 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 steady-state and transient scenarios with coupled neutronics and closed channel thermal-hydraulics tools (APOLLO3®/THEDI, SERPENT2/SUBCHANFLOW). By making use of the cases defined in Task 5.1 and the results to be obtained in Task 5.2, efforts have been 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 have been updated.

The document corresponding to Task 5.1 [3] aims at providing 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 simulated and intercompared with the multi-physics tools of the partners in Tasks 5.2 and 5.3.

In deliverable D5.1 [3], transient scenarios are provided for both the PWR and VVER test cases.

The development of the multiphysics coupling prototype based on APOLLO3® and CATHARE3, is a major objective to finalize the comparison between this former and a high accuracy coupling based on SERPENT2/ SUBCHANFLOW on a typical PWR type configuration.

The selected PWR exercise identified for comparisons is a 32 FAs minicore, which is initially based on [17] for core layout, with geometry and material isotopic composition and any other details newly specified in the framework of the CAMIVVER project in D4.3 [2].

3.1. Core description

Even if all information concerning the core description is provided in D4.3 [2], some details concerning the core description is provided also hereafter. The Cartesian fuel together with its guide tube with absorbers and central tube pin cells are shown in Figure 4 to Figure 7 [3]. Geometry and material specifications are provided here in Table 1 to Table 4.

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FIGURE 4: SQUARE UNIT CELL (BASED ON [2])

TABLE 1: SQUARE CELL PITCH [2]

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

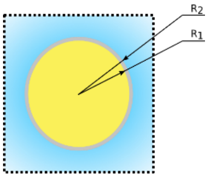

FIGURE 5: FUEL PIN CELL (BASED ON [2])

TABLE 2: 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

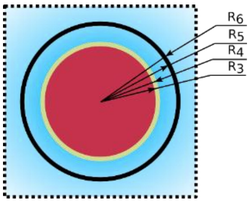

FIGURE 6: GUIDE TUBE WITH ABSORBER (BASED ON [2])

TABLE 3: 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

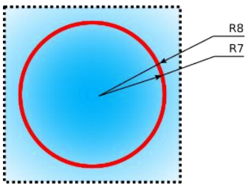

FIGURE 7: CENTRAL TUBE CELL (BASED ON [2])

TABLE 4: CENTRAL TUBE GEOMETRY AND MATERIALS [2]

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

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 within the volume. The new isotopic composition can be found in D5.1 [3]. This composition only applies to the fuel and absorber claddings and any other components (e.g., guide tubes) uses the composition reported in D4.3 [2].

Only one type of fuel assembly is modelled for the 32 FAs PWR minicore (see Figure 8 and Figure 9 for the rodded and unrodded cases respectively). The FA lattice pitch is 21.504 cm with an active height of 130 cm.

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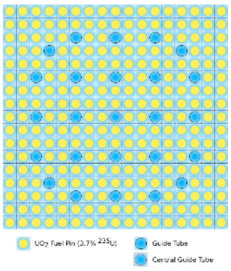

FIGURE 8: UO2 FUEL ASSEMBLY (3.7% 235U) WITHOUT CONTROL RODS (CRS) INSERTED (BASED ON [2])

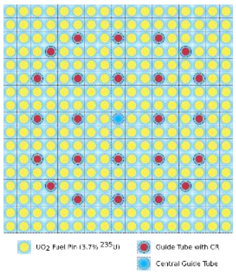

FIGURE 9: UO2 FUEL ASSEMBLY (3.7% 235U) WITH CONTROL RODS (CRS) INSERTED (BASED ON [2])

3.2. Core description

The PWR minicore layout can be observed in Figure 10. It is composed of a six (6) by six (6) arrays of FAs without the corner ones, thus giving thirty-two (32) FAs. There are four (4) Control Rods (CRs) positions in the core [3] with some information provided here.

Concerning the radial reflector, a first hypothesis has been provided in D4.3 [2]: four (4) layers of different mixtures of materials with radii of the layers provided in TABLE 16 of the same deliverable.

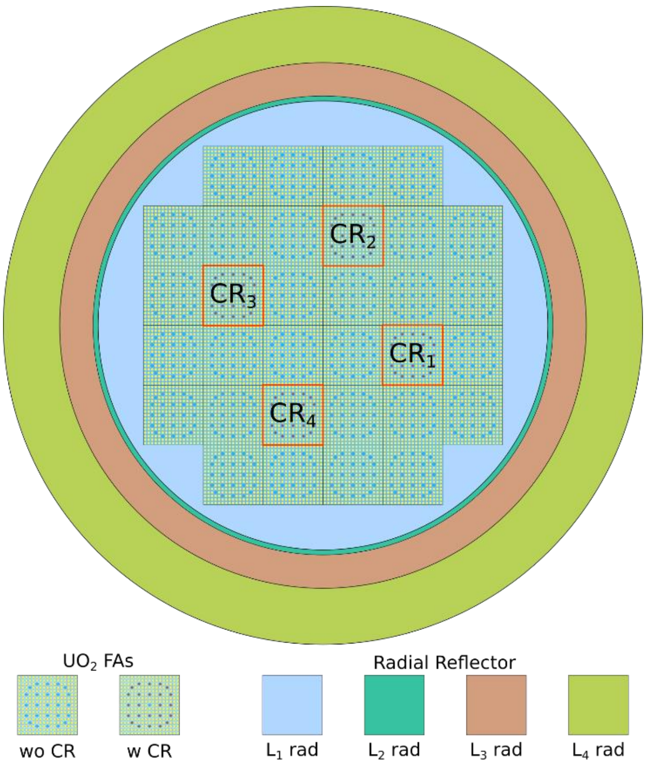

FIGURE 10: PWR MINICORE LAYOUT (BASED ON [3][17])

Top and bottom axial reflectors are separated into homogenous layers of materials and are described by different mixtures of moderator, steel SS-304, Zircaloy and/or Helium [2]. In Figure 11, a schematic of the axial reflector layers can be observed. The thickness of each layer is specified in TABLE 17 of D4.3 [2] and the material composition of the same deliverable.

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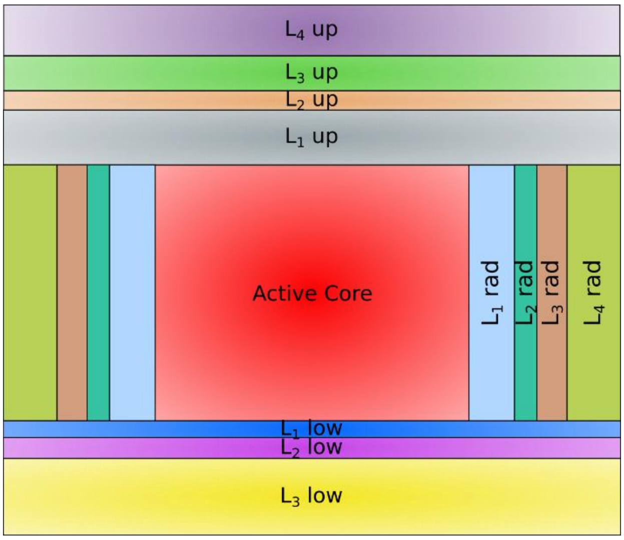

FIGURE 11: PWR MINICORE RADIAL, TOP AND BOTTOM REFLECTORS (BASED ON [3][18])

The thermophysical properties data (thermal conductivity (k) and specific heat (Cp) of the fuel and its cladding) is provided in Table 18 to Table 21 of deliverable D5.1 [3]. These values were obtained from correlations provided in the benchmark [18] for UO2 fuel and Zircaloy cladding for a PWR core transient, as used in previous KIT publication [19], [22].

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 10^4 W/m^{2}K will be used for simplicity [18]. The IAPWS-97 formulation will be used for water properties [21].

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3.3. Transient Scenario

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

3.3.1. Initial conditions

As stated, the initial condition of the transient scenario will be a neutronic-thermal-hydraulics coupled steady-state calculation at the nominal conditions detailed in Table 5. Nominal PWR minicore conditions have been provided in [3]. The values set in Table 5 are based on realistic full core conditions [23].

In order to confirm the initial hypothesis and to provide intermediate step-by-step comparisons, the initial steady-state before the transient has been attained by using high-fidelity Monte Carlo code before and communicated to partners, see Figure 12. At the end of the iteration among partners on the initial conditions, the values in Table 5 have been finally adopted.

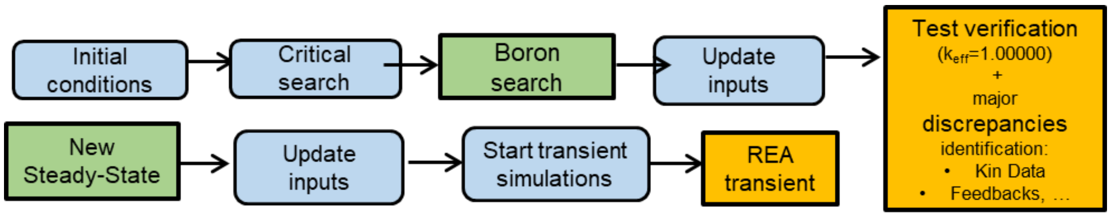

FIGURE 12: INITIAL STEADY-STATE DEFINITION APPROACH

TABLE 5 HOT FULL POWER (HFP) INITIAL CONDITIONS FOR PWR MINICORE [3], [23]

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

With the closed-channels codes, the calculation 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.

3.3.2. Transient conditions

Two scenarios have been proposed for the transient simulations of WP5: a rod ejection event [3] (Scenario I) and an optional, sudden change of the thermal-hydraulics boundary conditions (Scenario II). The project

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partners decided to focus on the scenario 1 to investigate it deeply in the limited project time available, before moving to scenario 2 studies that will be considered for a following phase.

The thermal power is considered generated uniformly over the fuel pellet radius.

The chosen transient scenario to be analyzed consists in a Reactivity Insertion Accident (RIA): starting from HFP conditions and the system critical with boron, the control rod is ejected in 0.1 seconds and the other boundary conditions are kept constant. The rod is moved at a constant velocity to the corresponding final position and the system evolution is simulated up to 2 seconds. The aim of this transient scenario is to have a high enough reactivity insertion to analyze a fast transient, but low enough to always stay in monophasic conditions.

For the 32 FA minicore the CR1 starts from a fully inserted position, and it is fully extracted in 0.1 seconds. The initial position is such that when extracted it will cause a reactivity insertion of ~1.1$.

3.4. Output Parameters

For comparing the partners' codes, certain parameters are considered as important outputs as it has been defined in reference [3].

Major quantities of interest are referred as follows:

1. Initial boron concentration, i.e., the boron concentration obtained from the critical search at HFP conditions with and without CRs. Indicated mainly by the reference solution proposed by SERPENT2/SUBCHANFLOW.
2. Evolution over time of the total system power and dynamic reactivity when available. Several reactivity definitions are possible depending on the weighting function used to calculate it. For the sake of simplicity and comparison[1], the time dependent neutron balance approach will be used [3]. The dynamic reactivity (ρ) can be calculated as:

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

Where k_{eff} is the time dependent neutron balance multiplication factor (neutrons gain-loss ratio), N, C, F, L and S are the integrated[2] fission neutron production, capture, fission, leakage and scattering production (*nxn* reactions) rates respectively.

Other quantities of interest may be added for further investigations.

[1] 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 [24].

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

4. APOLLO3®/CATHARE3 proof of concept of an advanced multiphysics coupling prototype

One of the CAMIVVER purpose is the development and validation of best estimate calculation tools for VVER and PWR reactors. The development of a first prototype of APOLLO3® core code and CATHARE3 core 3D multiphysics coupling with its first testing on a cartesian small PWR core is the result of several months and interactions among different R&D Projects, in collaboration with CEA developers of both the APOLLO3® and CATHARE3 codes.

The development of this coupling has been achieved in collaboration among French partners (mainly Framatome and CEA) and is one of the first feasibility assessments of 3D coupling between the thermal-hydraulic code CATHARE3 [25] with a neutronic core code, such as APOLLO3® [26], at core level.

Both codes are coupled through the C3PO Python coupling library [27].

The APOLLO3® code sources are shared with Framatome in the framework of the CAMIVVER project as presented in reference [9]. CATHARE3 was already provided to French partners and C3PO has an Open-source access [28].

The CATHARE3 3D functionalities used in the framework of the past three years of the CAMIVVER project mainly support cartesian geometry. On this basis the 32 FAs small core has been simulated with the 3D module to provide thermal-hydraulic feedbacks to the neutronic code APOLLO3®.

During the three years duration of the CAMIVVER Project, the work program was oriented firstly to the multiphysics coupling development and then to provide first tests on a simplified configuration, improving in the same time calculation procedures and tools for simulating a reactor core.

For VVER small and full core calculations, the POC APOLLO3®/CATHARE3 coupling prototype was extended to hexagonal FAs core geometry too. For this first tentative application, a simplified representation of hexagonal FAs through equivalent thermal-hydraulic and geometrical properties (surface area, hydraulic diameter, etc.), has been also realized in the framework of the project.

This has been judged to be sufficient for the purpose of providing thermal-hydraulic feedbacks to APOLLO3® neutronic core code, as complementary contribution in comparison with the APOLLO3®/THEDI option in Task 5.3, and for supporting the task 7.4. Some results will be proposed in next chapters.

The CATHARE3 code enables the simulation of both core and system thermal-hydraulics and a first feasibility analysis was also oriented to extend the calculation domain from the core to the vessel and then to the primary system with a multiscale approach. Thanks to the functionalities of the CATHARE3 code, enabling 3D junctions, the 3D core may be associated to vessel and primary circuit modeling. This activity has been identified as a possible contribution to task 7.4 [1], feeding the discussion about improvements in MSLB accident simulation. For this purpose, the full core Kozloduy NPP Unit 6 3D core modeling at steady-state calculations have been realized in collaboration between WP5 and WP7. The last part of the project is dedicated to the integration of such a core into a Kozloduy NPP Unit 6 full primary and secondary CATHARE3 model, based initially on the Task 7.2 MCP start-up test case. The same functionalities will be injected into a deck of first attempt modeling an MSLB scenario as asked in Task 7.4, mode details are provided in D7.4.

4.1. Coupling engine

In the framework of the CAMIVVER project the standard approach for code interfaces follows the ICoCo norm defined by CEA. This is the case for both the APOLLO3® and CATHARE3 codes. Any new code

API already compatible with ICoCo norm may be easily coupled to the others thanks to a derived class implemented at the interface between the code and the coupling engine C3PO.

In accordance with CEA, it was decided during the CAMIVVER WP5 kickoff meeting and later technical meetings to adopt C3PO as coupling engine. The C3PO main objectives are the following:

- Simplifying and standardizing coupling scripts writing;
- Simplifying MEDCoupling use;
- Providing advance coupling algorithms;
- Simplifying MPI use;
- Allowing to share, perpetuate and verify advances in coupling methodologies.
- Development started one year ago.
- Python only (no "installation").
- Prerequisites: numpy, MEDCoupling and (in option) mpi4py.

Methods available in the coupling engine are described below:

- setDataFile(filename), setMPIComm(mpicomm)
- Initialize(), terminate()
- presentTime(), computeTimeStep(), initTimeStep(dt), isStationary()
- solveTimeStep(), iterateTimeStep()
- validateTimeStep(), abortTimeStep()
- save(label, method), restore(label, method), forget(label, method)
- getInputFieldsNames(), getOutputFieldsNames()
- setInputMEDField(name, field), getOutputMEDField(name), getInputMEDFieldTemplate(name)
- getInputValuesNames(), getOutputValuesNames()
- setValue(name, value), getValue(name)

Figure 13 presents the information management offered by C3PO.

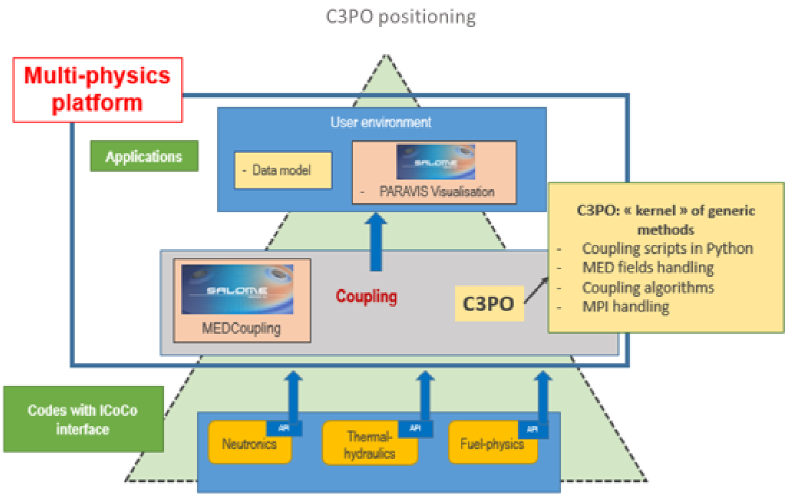

FIGURE 13: C3PO DATA MANAGEMENT [28]

4.2. PoC release and calculation environment

Recently the APOLLO3®/CATHARE3 coupling first prototype has been managed under GitLab platform for participative development purposes and it has been installed on the Framatome/EDF HPC computing cluster [29].

The components and different modules directly called and supervised by the C3PO coupling engine are the following:

- ICoCo [36]
- APOLLO3®-2.2 (following version 2.3 has been tested too on a limited number of cases and new versions should be easily compatible too) [9]
- CATHARE3 (dynamically driven by a specially conceived python API) [36].

Input options are provided by a short ASCII input deck, specifying the scenario data and the python preprocessor options for PWR or VVER geometries. Calculations are then possible in steady-state and transient.

A limited number of optional features and procedures for post-processing are available but further improvements will be necessary with developments oriented to consolidate and automatize the approaches.

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5. Benchmark results for 32 FAs PWR test case

In this Chapter a short description of the WP5 activities, the modeling and the major's results related to the 32 FAs PWR minicore are provided.

Partners have contributed to compare results for the 32 FAs small core test case with different approaches, according to their code platform.

Results obtained by KIT and Framatome [10] are proposed with special attention to preliminary analysis and step-by-step comparisons and discussions oriented to support improvement in modeling and verification practices.

The WP5 results obtained during the CAMIVVER project concern codes, tools and MPOs that have been obtained by successive versions of the NEMESI prototype still under development.

In this chapter any improvement and significant modifications of calculation tools, MPOs and modeling options are also presented.

Such results are oriented to analyze codes behavior in steady-state and transient calculations, providing comparisons among a high-fidelity coupling (SERPENT2/SUBCHANFLOW), the APOLLO3®/THEDI code and also the 3D Multiphysics coupling APOLLO3®/CATHARE3.

5.1. Modeling approaches

The first preliminary results [10] of the same 32 FAs small core (Figure 14) undergoing a REA transient are provided in the following sections. The last version of same results with updated MPOs and code versions are also detailed below with special attention to KIT and Framatome approaches. Advanced modeling of such small core with a pin-by-pin radial discretization has also been realized within the CAMIVVER project and is detailed in a dedicated section to complementary analyses.

A short summary of the 32 FAs PWR core benchmark is provided in the sections below underlying some additional details not yet available in D5.1 [3], see Table 7 and Table 8, such as:

- Control rod material definition: AIC
- Control rod position: all inserted at 130 cm from the top
- Boron concentration = 2791 ppm
- Control rod ejection time = 100 ms
- Kinetic data (see Table 10)
- Fresh fuel composition (BU= 0 GWd/tiHM)

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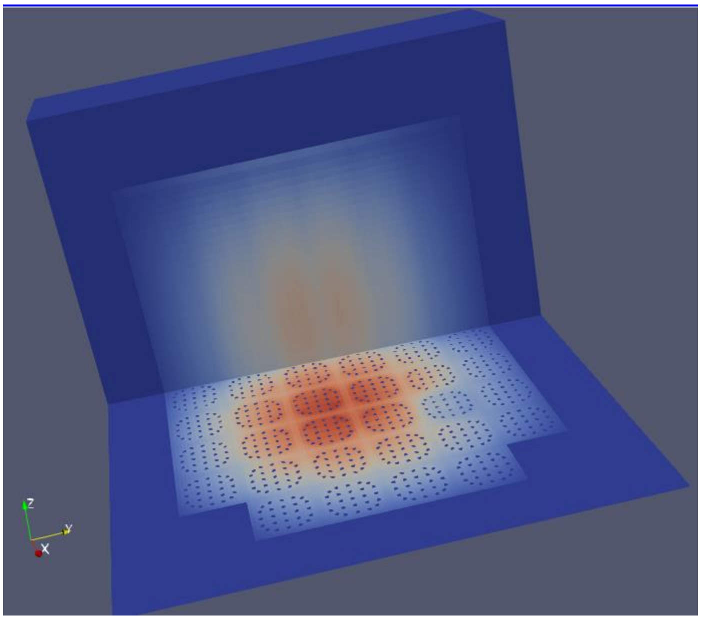

FIGURE 14: 32 FAS PWR MINI-CORE.

5.1.1. *The high-fidelity approach*

The coupling tool between the neutronic Monte Carlo code SERPENT2 [30] and the subchannel thermal-hydraulic code SUBCHANFLOW (SCF) [31] has been used as the high-fidelity solution for the rod ejection transient in the 32 FA PWR minicore. Extensive literature about the coupling tool can be referred to in [32], [33] and [34]. A description of the neutronics and TH models is presented in this section.

Figure 15 shows the model developed in SUBCHANFLOW for the 32FA PWR, which consists in a coolant-centered model. A total amount of 9248 rods (32FA x17x17) and 10368 channels (32FA x18x18), both rods and channels divided axially into 26 cells (5 cm per cell). A MedPreprocessor program developed at KIT allows the creation of the layout geometry for SCF (layout and connectivity files for rods and channels), the IFC[3] files needed by SERPENT2, and the mapping files that link pin-by-pin and channel-by-channel the two domains defined by each code.

[3] Universal multi-physics interface (IFC) is used in SERPENT2 to easily bring in temperature and density solutions from any external solvers. With the IFC, the solution fields (temperature/density) can be overlaid on top of the base geometry model [35].

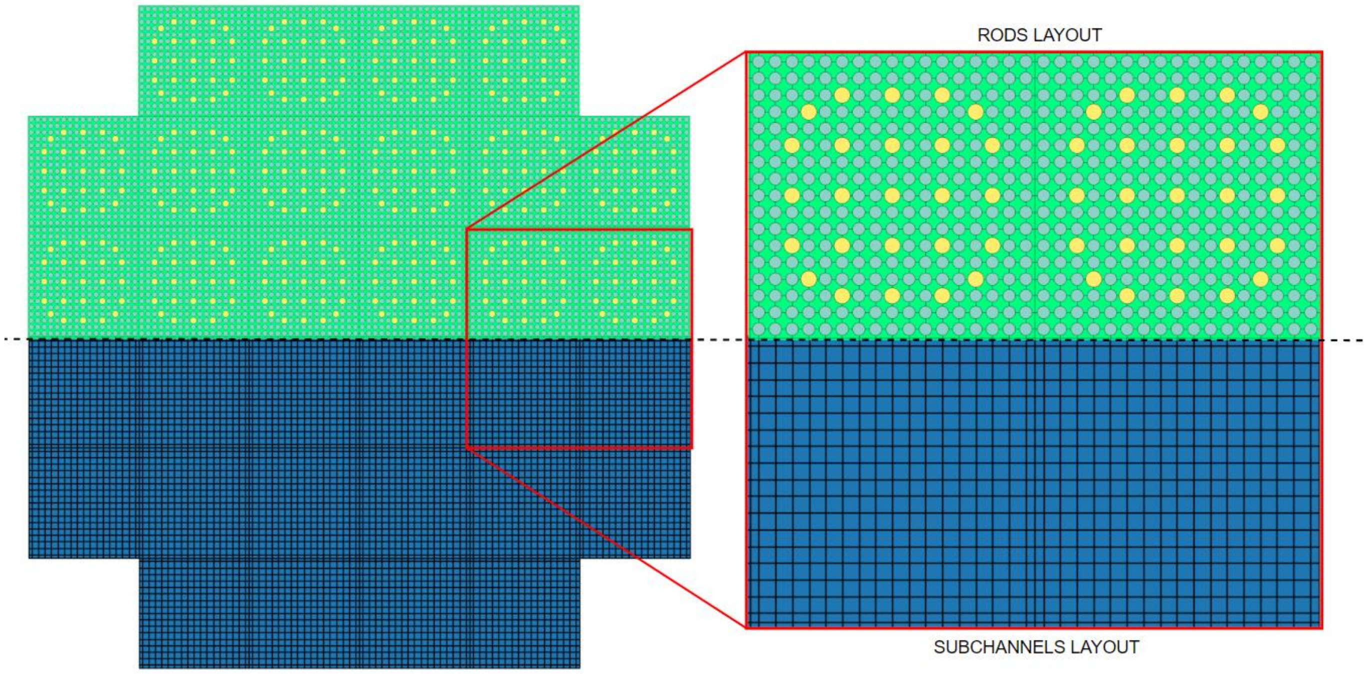

FIGURE 15: SUBCHANFLOW COOLANT CENTERED MODEL AT PIN/SUBCHANNEL LEVEL. 17X17 ROD AND 18X18 SUBCHANNEL LAYOUT PER FUEL ASSEMBLY IS CONSIDERED. UPPER AND LOWER PART SHOW THE ROD AND CHANNEL LAYOUT RESPECTIVELY

Figure 16 shows the full core model developed in SERPENT2 as specified in [3]. Figure 17 shows the fuel IFC file's header, where the feedback takes place in the ***uo2*** (fuel) material, and the discretization used is 6x6x26 (in the X, Y, and Z directions respectively) at core-level (3rd line), and 17x17x1 at assembly-level (4th line), the final mesh is a superposition between the two discretizations. Figure 21shows the coolant IFC file's header where the feedback occurs in the ***wat*** (coolant) material. The main difference with the fuel IFC file is the discretization at the assembly-level of (18x18x1) that has to match with the rods and channels layout defined for the coolant-centered model in SUBCHANFLOW. JEFF 3.1.1 nuclear data library is considered.

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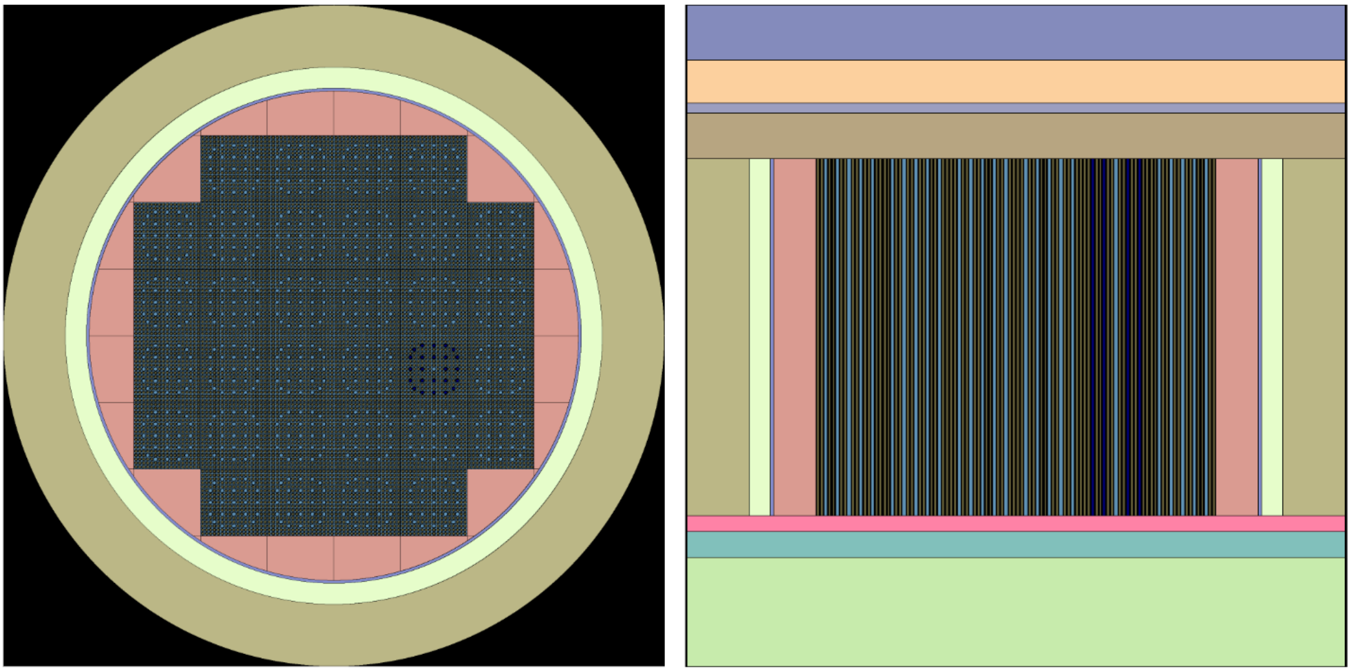

FIGURE 16: RADIAL AND AXIAL SERPENT2 MODEL DETAILS RESPECTIVELY FOR THE 32 PWR MINICORE

```
22 uo2 2 fuel.ifc.out
3
 12 1   6 -6.451200e+01  6.451200e+01   6 -6.451200e+01  6.451200e+01  26 -6.500000e+01  6.500000e+01
  5 1  17 -1.071000e+01  1.071000e+01  17 -1.071000e+01  1.071000e+01   1 -1.000000e+18  1.000000e+18
  0 1   1 -1.000000e+18  1.000000e+18   1 -1.000000e+18  1.000000e+18   1 -1.000000e+18  1.000000e+18
```

FIGURE 17: FUEL IFC FILE'S HEADER

```
22 water 0
3
 12 1   6 -6.451200e+01  6.451200e+01   6 -6.451200e+01  6.451200e+01  26 -6.500000e+01  6.500000e+01
  5 1  18 -1.134000e+01  1.134000e+01  18 -1.134000e+01  1.134000e+01   1 -1.000000e+18  1.000000e+18
  0 1   1 -1.000000e+18  1.000000e+18   1 -1.000000e+18  1.000000e+18   1 -1.000000e+18  1.000000e+18
```

FIGURE 18: COOLANT IFC FILE'S HEADER

Doppler temperature with a factor of 0.7[4] is considered for the fuel temperature feedback in SERPENT2. Each fuel pellet is radially subdivided into ten rings in SUBCHANFLOW to take into account the temperature profile inside each pellet, and two rings for the cladding. Constant thermophysical properties (e.g., thermal conductivity and specific heat) are considered for the fuel and cladding materials, as well as constant fuel-clad gap conductance, and no thermal expansion is considered as specified in [3].

Table 6 presents the main TH correlations used in the SUBCHANFLOW model.

[4] Doppler temperature is defined as: $T_{Doppler} = 0.3 \times T_{center} + 0.7 \times T_{outer}$, where T_{center} means temperature in the centreline and T_{outer} is the temperature in the outer surface of the fuel pellet.

TABLE 6. SUBCHANFLOW CORRELATIONS USED IN THE MODEL.

Correlation	Option Selected
Turbulent friction	Blasius
Heat transfer	Dittus Boelter
Critical heat flux	Westinghouse-3
Water properties	IAPWS-97

The first step in the SERPENT2/SUBCHANFLOW simulations consisted in the determination of the critical state. Taking the initial conditions defined in [3], with the control rod CR1 totally inserted, a critical boron search is performed in a steady-state calculation, after the critical boron concentration is found and updated in the inputs, a new steady-state is performed to generate the live and precursors neutron sources needed by SERPENT for the transient simulation. Two kinds of coupled simulations are performed; these are steady-state and transient simulations. For the steady-state simulations 1e7 histories divided in 1e3 cycles with 100 inactive cycles is selected in SERPENT. For the transient simulations 5e4 primary particles per batch and MPI is considered. As part of a sensitivity analysis, 10ms, 5ms and 1ms are used as time bins for the population control in SERPENT2 and time steps in SUBCHANFLOW.

5.1.2. *The APOLLO3®-based solutions*

The H2020 CAMIVVER project promotes the use of multi-disciplinary deterministic methodologies to describe the interaction between thermal-hydraulics and neutronics by a proof of concept of APOLLO3®/CATHARE3 coupling, see §4, that will be compared to other solutions. In the whole project two approaches for Multiphysics solutions have been adopted and tested by Framatome and are described as follows:

- APOLLO3®/THEDI core calculations used in order to improve knowledge around the new generation code APOLLO3® core solver, investigates the multi-1D thermal -hydraulic feedback model available with the code treating single- and two-phase conditions. The 3D neutron flux resolution used in the framework of the CAMIVVER Project is based on the finite element method (FEM) using 2 energy groups and the diffusion approximation.
- APOLLO3®/CATHARE3 coupling is the proposed proof of concept developed in CAMIVVER for investigating the 3D core capabilities of the CATHARE3 code, improving knowledge of new code features and providing feedbacks around its usage for Multiphysics couplings.

APOLLO3® is the new generation French deterministic code for lattice and core calculations, developed since 2007 at the CEA with support of EDF and Framatome [9].

A synthetic description of the solvers available for APOLLO3® lattice and core calculations is shown in Figure 19.

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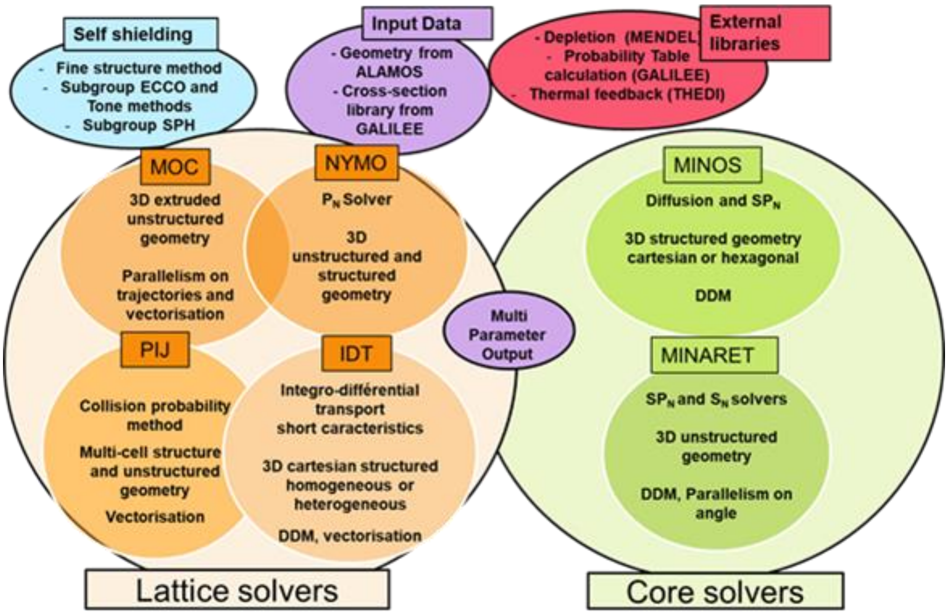

FIGURE 19: APOLLO3® SOLVER AVAILABLES.

For the activities carried out in Task 5.3, for core calculations the following options have been used:

- MINOS solver: SPN equation on Cartesian and Hexagonal 3D structured geometries using Raviart-Thomas space finite elements,
- Diffusion approximation adopted,
- 2 energy groups calculations
- Homogeneous assembly XS

In the framework of the APOLLO3® project, the thermal-hydraulic model (THEDI—THErmohydraulique DIphasique) for internal coupling has been developed and integrated since September 2018 [10]. THEDI is a multi-1D, two-phase flow solver able to treat Cartesian and hexagonal (as VVER) geometries. The THEDI thermo-hydraulic library is one-dimensional and solves a four-equation model composed of total mass conservation, vapor mass conservation, total motion equation and total internal energy conservation. The core is treated as separated 1D channel that contains several solid objects, such as fuel rods. THEDI computes the temperature distribution in each of them by solving a one-dimensional heat transfer diffusion equation. [17].

As already mentioned in §4, the proof-of-concept APOLLO3®/CATHARE3 is based on the C3PO engine [28]. This multiphysics tool was developed to improve the 3D capabilities of the CATHARE3 code in comparison to the multi-1D approach. C3PO is a Python coupling platform initially developed by CEA allowing to switch the use of different codes other than APOLLO3®, CATHARE3, etc. The C3PO application in CAMIVVER project aims to increase exchanges between partners to support and facilitate the improvement of the robustness of the PWR industrial couplings. C3PO enables the interchangeability of core neutronics and thermal-hydraulic codes favorizing the flexibility and the benchmarking basing code interfaces on the ICoCo norm.

For the 32 FAs case analyzed, the multi-parametric cross section libraries have been generated by using APOLLO3® encapsulated in the NEMESI prototype [7] that has been developed as part of the CAMIVVER

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project. The scheme adopted is based on the Method of Characteristics, MOC, and TDT-solver for flux resolution over a refined 2D assembly geometry.

The last year of the project has been used to test and to propose feedbacks to the tentative MPOs newly generated by NEMESI as indicated in Appendix 1 – MPOs tests during the project. Results are preliminary as the APOLLO3® encapsulated in the NEMESI prototype is still under development for faster improvement of its level of industrialization at the end of the CAMIVVER Project.

This effort toward industrialization and consolidation of physical results may be continued in the follow up of the project.

5.2. Results and discussions

In the following paragraphs the results generated by KIT and Framatome with the tools previously presented are first discussed as related to the steady state in order to fix the core operating conditions before the transient.

In §5.2.1 values and graphics obtained at the end of 2022 during an intermediate mid-term point dedicated to preliminary results comparison are discussed.

In §5.2.2 very last improvements and final discussions are presented.

5.2.1.Preliminary analyses of mid-term point comparisons

The steady-state core operating conditions before transient are in part described in §3.3.1 and major information are summarized in Table 7 below.

TABLE 7: 32 FAS CORE INITIAL OPERATING CONDITIONS BEFORE TRANSIENT

First results Steady-state	SERPENT2	APOLLO3®
Initial Power [MW]	100	100
Boron [ppm]	2791	2800
Xe/Sm	0	0
CR1 insertion [cm]	130	130
Pression Out [MPa]	15.5	15.5
Inlet Temperature [K]	573.15	573.15
mass flow [kg/s]	1417	1417

The core geometrical features and control rod locations, with the specification of the ejected one, are provided in Table 8.

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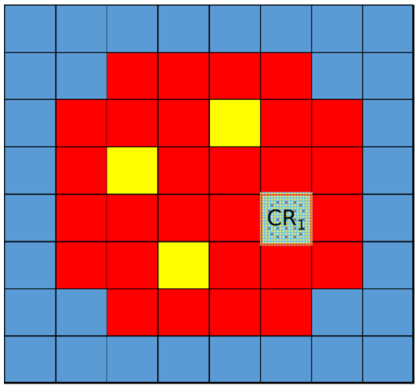
TABLE 8 : 32 FAS GEOMETRICAL DATA AND CR LOCATION

Geometrical data	
Total Flow area [m2]	0.79
Total core cross section area [m^2]	1.48
heated perimeter [m]	252.12
wetted perimeter [m]	282.79



According to the steady-state and the transient scenario specifications, the CRs are ejected at constant velocity of 0.1 seconds. At the beginning of the REA transient, since the CR worth is over 1$, the system quickly becomes super prompt critical and therefore the fission chain can be sustained only by prompt neutrons with generation times of a few µs. In this way, an extremely rapid exponential power increase is observed. The increase of the fuel temperature first and the decrease of the moderator density subsequently will counteract the reactivity increase with some delay due to the energy deposition mechanisms until it drops below 1$. At this point also the delayed neutron production will be needed to sustain the chain reaction and consequently the power will decrease until the delayed neutron generation is strong enough to sustain the fission chain again.

During the first part of the benchmarking exercise the comparison among CR worth enables the verification of such targeted reactivity insertion. If a non-negligible difference was detected in APOLLO3® based tools, in order to keep the comparison satisfactory even during transient, a penalization on the beta effective has been adopted in order to be as closed as possible to the targeted reactivity insertion as detailed below. The SERPENT2/SCF axially integrated pin-power map distributions normalized to the nominal powers at the steady-state prior to the transient and at power peak time are shown in Figure 20 for the 32 FAs PWR case, in which the power hot spots close to the ejected CRs can be highlighted. The maximum and average statistical uncertainties associated to the pin power calculations is below 8%.

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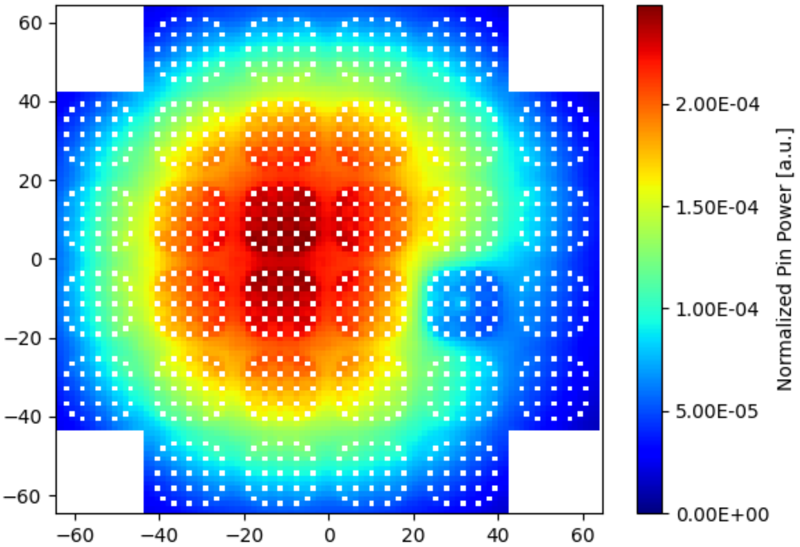
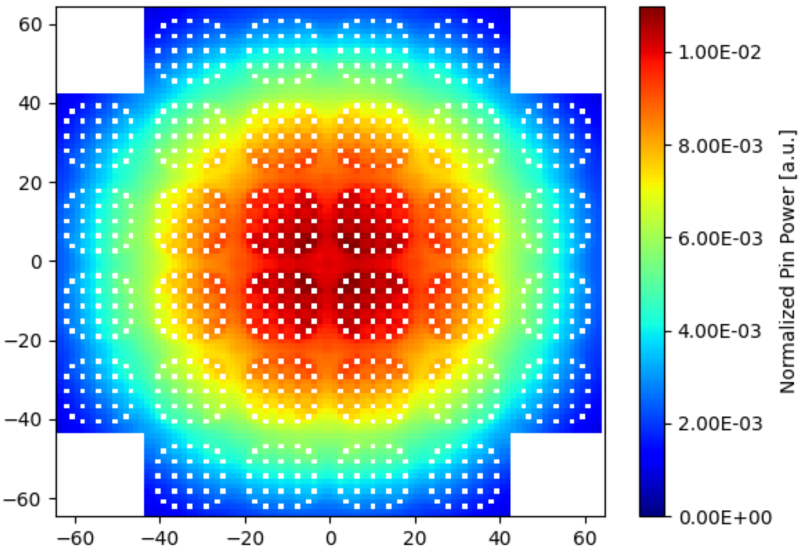


(a)



(b)

FIGURE 20: PWR MINI-CORE: SERPENT2/SCF AXIALLY INTEGRATED NORMALIZED PIN RADIAL POWER DISTRIBUTION FOR THE STATE BEFORE THE TRANSIENT (A) AND AT PEAK TIME (B)

The axial distributions of the center fuel temperature and coolant temperature at power peak times are also provided in Figure 21. This provides an example of the high-resolution capability of the SERPENT2/SCF tools which allows the prediction of reactor safety parameters at the local level.

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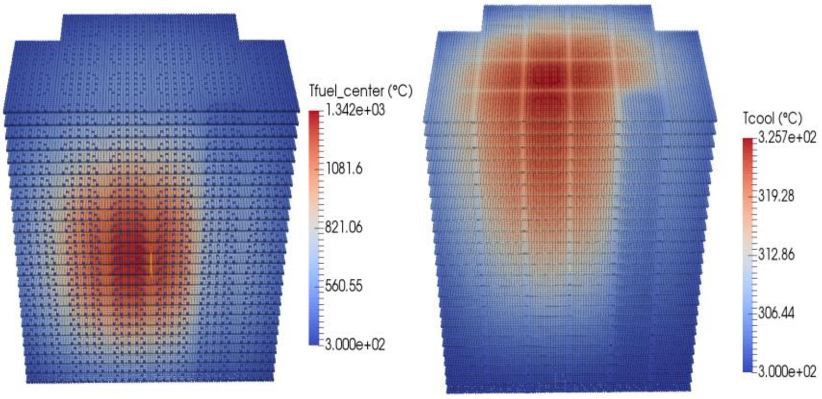

FIGURE 21: PWR MINI-CORE: SERPENT2/SCF CENTER FUEL TEMPERATURE (LEFT) AND COOLANT TEMPERATURE (RIGHT) DISTRIBUTION AT T=0.12 S

The comparisons of the normalized power (P/P0) and reactivity as predicted during the REA transient by APOLLO3®/THEDI and SERPENT2/SCF are shown in Figure 22 through Figure 23. A good agreement between the two different solutions has been observed.

For the first phase of the transient until the end of the CR ejection at about 0.1 s one can observe an excellent agreement between the reactivity profiles for the PWR mini-core. In the second phase of the transient, after the power peak time, some discrepancies can be underlined that need further investigations specially devoted to the thermal fuel rod model. This behavior, that may depend on the TH modules and the energy deposition model, is confirmed also by the final set of comparison realized during the last part of the project.

As specified in next paragraph, even if the final part of activities aims at consolidating the comparison at initial steady-state for reactivity prior to the transient, some aspects such as the fuel thermal properties and their modeling ask a dedicated focus in the project follow-up.

As far as the evolution of the normalized power, the shapes of the profiles generated by the different solutions were found to be very consistent one to each other (Figure 22 through Figure 23). For this test case the peaking values predicted by SERPENT2/SCF are higher with respect to the ones calculated by APOLLO3®/THEDI by ~16% for the PWR (see Table 9).

The power peaks times were also found to be in good agreement within the two solutions, the difference being in the order of ~5 ms (see Table 9).

One of the goals within the CAMIVVER project is the development of the proof-of-concept for the APOLLO3®/CATHARE3 coupling [10]. After its recent implementation, this scheme has also been tested on the PWR mini-core case and a good agreement with the APOLLO3®/THEDI solution with regard to the prediction of the power evolution during the REA transient can be observed, as shown in Figure 23. This represents the first demonstration of the applicability of this newly developed scheme and further verifications are planned by the end of the project to consolidate results in 32 FAs small core case but also when to apply to VVER geometry for small, medium and full core sizes as described in next chapter.

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TABLE 9: POWER PEAKING FACTORS AND CORRESPONDING PEAK TIMES PREDICTED BY SERPENT2/SCF, APOLLO3®/THEDI (AP3/THEDI) AND APOLLO3®/CATHARE3 (AP3/C3)

Coupling tool	SERPENT2/SCF	AP3/THEDI	AP3/C3
Peak factor [P/P0]	47.27	40.60	43.00
Peak time [s]	0.115	0.1198	0.1220

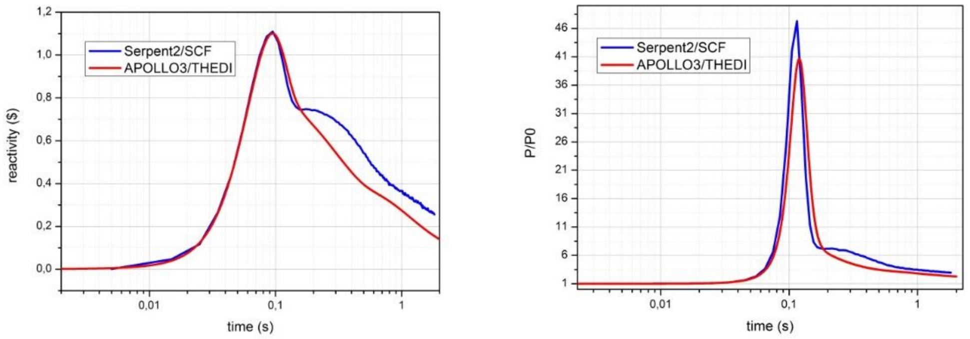

FIGURE 22: PWR MINI-CORE: REACTIVITY AND POWER EVOLUTION

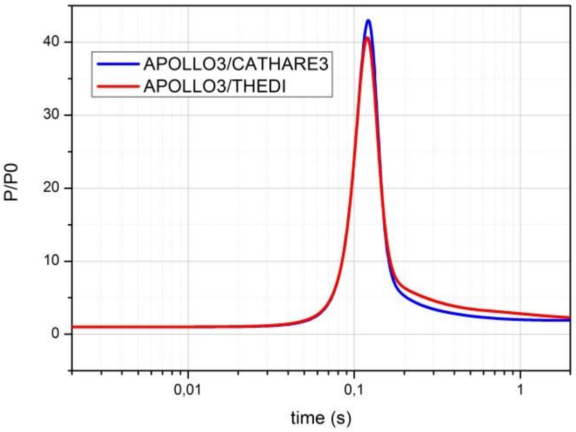

FIGURE 23: PWR MINI-CORE: APOLLO3®/THEDI VS. APOLLO3®/CATHARE3 NORMALIZED POWER COMPARISON

5.2.2. Final analyses and discussions

During the very last months of the project, special attention has been dedicated at consolidating the APOLLO3® based tools and models. In particular, several iterations have been taken place in collaboration with the WP4 to test and provide feedbacks about the very last version of MPOs generated by the NEMESI prototype [7] and its version still under-development, for adjusting XSs interpolation parameters range variation and final debugging for major isotopes.

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Some version improvements have been also realized in the API interfaces of codes and tools involved in pre- and post-processing for APOLLO3® and its couplings.

In Table 21 the delayed fractions and the delayed decay constants for 8 families of precursors have been provided. These data have been provided by KIT for the 32 FAs VVER core case and shared before end 2022. The same data have been adopted for APOLLO3®.

TABLE 10: KINETIC DATA FOR THE 32 FAS CORE CASE

Mini core case	32PWR	
Precursor families	BETA (pcm)	Lambda (1/s)
1	21.5	0.0125
2	104.4	0.0283
3	62.3	0.0425
4	137.6	0.1330
5	233.8	0.2925
6	80.5	0.6665
7	67.4	1.6348
8	25.1	3.5546
Total (1 effective group)	732.5	0.472

After first preliminary MPOs given by WP4, at the beginning of last comparisons a consolidated version of MPOs has been provided with some improvement in modeling. At assembly level a very good agreement was achieved between SERPENT and APOLLO3® (version 2.3.0) associated to NEMESI (v0.2) as confirmed in Table 11.

TABLE 11: COMPARISONS SERPENT/APOLLO3® ON KINF VALUES AT ASSEMBLY LEVEL FOR THE 32 FA CORE ASSEMBLY

	APOLLO3®	diff [pcm]
AIC	0.88665	102
B4C	0.80692	
ARO	1.30568	72

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At core level, an improvement of steady-state operating condition before transient has been achieved thanks to preliminary analyses and sensitivities that enable progresses in consolidating input options as shown in Table 12 thanks to different MPOs versions with different parameter variation.

TABLE 12: COMPARISONS SERPENT2/APOLLO3® ON STEADY-STATE MAIN CORE PARAMETERS FOR THE 32 FAS CORE

First results Steady-state	AP3 sensi 1	AP3 sensi 2	AP3 sensi 3	AP3 in NEMESI 0.1 last 2022
keff	1.1834	1.11510	1.00651	1.00340
beta	734	734	734	730
Xe	0	0	Eq.	0
CR weight [pcm]	887	898	922	728
CR weight $	1.20	1.22	1.25	1.0*
Crpos du haut [cm]	130	130	130	130
bore	**600**	**1300**	**2400**	**2800**
mass flow [kg/s]	1417	1417	1417	1417

When the new set of MPOs was then provided before the final transient analyses, at first a new cycle of new comparisons at steady-state conditions among SERPENT2 and APOLLO3® at core level have been realized.

Some discrepancies still remain at steady-state core level and further investigations and improvements are needed to better compare results and support the affordable industrialization of the APOLLO3® core solver.

During the project a complementary analysis consisting in running both APOLLO3® and SERPENT2 using a fuel assembly control rod in B_4C instead of AIC has been also carried out in order to profit of a complementary sensitivity on the control rod material (Table 13) more than on boundary conditions, main parameters range variation, etc.

During the last months of the project a continuous improving of MPOs and modeling options in APOLLO3®/THEDI has been encouraged.

In Table 14 the comparison between SERPENT2/SCF and APOLLO3®/THEDI on main core parameters is provided with the very last version of data. Some iterations have been necessary among Framatome, CEA and KIT in order to converge on the very final set of values providing the final results of the CAMIVVER project for the task 5.3.

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TABLE 13: COMPARISONS SERPENT2/APOLLO3® ON KEFF AND CR WEIGHT FOR THE 32 FA CORE ASSEMBLY AIC AND B4C BASED CR

K_{eff} Sensitivity at core level FRA/KIT 2022			
	AP3	SERPENT/SCF	diff [pcm]
AIC	1.00360	0.99896	464
B4C	0.99950	0.99896	54
ARO	1.01105	1.00874	231

CR Weight Sensitivity at core level FRA/KIT 2022			
	AP3	SERPENT/SCF	diff [pcm]
AIC	727	864	-137
B4C	1129	971	158
ARO	-	-	-

It is worth mentioning that this improvement in the description of the steady-state put in evidence some discrepancies for instance in the effective neutron multiplication factor (keff) but also in the control rod weight of the rod to be extracted.

An analysis for each source of discrepancy is also provided but these axes of improvement will be investigated deeply during the project follow-up.

TABLE 14: COMPARISONS BETWEEN LAST VERSIONS SERPENT/APOLLO3® ON STEADY-STATE MAIN CORE PARAMETERS FOR THE 32 FA CORE ASSEMBLY

First results Steady-state	SERPENT/SCF	NEMESI Latest 2023
Keff	**1.00002**	**1.00357**[5]
CR weight [pcm]	864	729[6]
Beta [pcm]	731	731[7]
Beta for REA scenario [pcm]	731	644[8]
CR weight $	~1.1	~1.1
Cr Pos Top [cm]	130	130
Xe	0	0
Boron [ppm]	2791	2800
mass flow [kg/s]	1417	1417

Analysis of residual discrepancies between SERPENT and APOLLO3®:

---

[5] This difference in keff should be investigated but possible causes are for instance the reflector model, minor differences in initial boron concentration and the radial discretization.

[6] Difference in CR weight at assembly level has been already identified. This discrepancy impacts mainly at core level the REA scenario. For this reason, the value of beta was penalized before transient in order to keep constant the 1.1$ inserted reactivity.

[7] The present version of MPOs generated by WP4 the kinetic data are not included and they are read by the core solver in a dedicated function. The main impact is that the beta effective value is calculated once and remains constant for the whole transient. A modification will be proposed for the follow up of the project.

[8] Value penalized in order to get an agreement with proposed scenario for REA an inserted reactivity of 1.1$.

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- Difference in keff should be investigated but possible causes are for instance the reflector model adopted, the radial discretization, minor differences in initial boron concentration, etc. The discrepancy is acceptable for this first comparison.
- Some discrepancies in CR weight between SERPENT and APOLLO3® at assembly level have been identified. This discrepancy impacts at core level the CR weight too and this parameter impacts the REA scenario. For this reason
  - the value of beta was slightly penalized in order to keep constant the 1.1$ of inserted reactivity
  - in near future sensitivity should be done in order to understand this difference, for instance:
    - an activity oriented to use an MPOs generated by SERPENT should be realized in order to distinguish the source of error. Similar consideration has been extended to B4C rods too.
    - A first coupling APOLLO3®/SUBCHANFLOW, possible via the C3PO coupling engine, may also help understanding the role of TH feedbacks
- In the present versions of MPOs generated by WP4 the kinetic data are not included and they are read by the core solver in a dedicated function. The main impact is that the beta effective value is calculated once and remains constant for the whole transient. Possible evolutions will be proposed for the follow up of the project.
- A penalized version of the beta effective parameter is proposed with a slight penalization in order to assure a certain coherence in the comparison of codes behavior during transient REA scenario keeping fixed an inserted reactivity of 1.1$.

This analysis of the keff and control rod weight values asked a deeper analysis of cross sections and their tabulation provided by NEMESI v0.2 but also of input options of APOLLO3® and of the POC AP3/C3 coupling input decks.

Again, even if further improvement is requested before realizing industrialization and assuring automatized safety analysis with such tools, a globally good agreement has been achieved in steady-state for both SERPENT2 and APOLLO3® based tools (Table 14).

The effective neutron multiplication factors for rodded and unrodded conditions, and comparison, is proposed for APOLLO3®/THEDI and the coupling APOLLO3®/CATHARE3 too, see Table 15.

TABLE 15: KEFF ADDITIONAL COMPARISONS WITH APOLLO3®/CATHARE3 COUPLING FOR THE 32 FA CORE

keff	BORON 2800
APOLLO3®/THEDI	Rodded =1.00357 Unrodded = 1.01098 CR weight = 730 [pcm]
APOLLO3®/C3	Rodded = 1.00021 Unrodded = 1.00776 CR weight = 749 [pcm]

Based on these very last input configurations, the transient scenario defined in CAMIVVER [3] has been performed. In Figure 24 and Figure 25 transient behavior for normalized power (P/P0) and reactivity indicated in ($) as predicted during the REA transient by APOLLO3®/THEDI, the POC APOLLO3®/CATHARE3 and SERPENT2/SCF are shown.

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A sufficiently good agreement between the different solutions is confirmed on the whole transient in this last comparison.

As observed before, for the first phase of the transient until the end of the CR ejection at about 0.1 s an excellent agreement is experienced between the reactivity profiles available, see Figure 24.

In the second phase of the transient, after the power peak time, the discrepancies persist and their origins may be identified in thermal properties, the fuel rod model adopted and fluid closure laws. This point will be investigated during the follow-up of the project and internal R&D activities.

Moreover, the radial and axial discretization may need further investigations as for these preliminary analyses the choice was not optimized between the one for APOLLO3® neutronic flux modeling realized at the assembly level and the thermal and thermal-hydraulic feedbacks. A first improvement, presented among other complementary activities may be the resolution of a first pin-by-pin radial discretization for power resolution preparing the field to further investigations in the project follow-up.

The tendency for SERPENT/SCF2 on predicting similar values than APOLLO3®/THEDI and APOLLO3®/CATHARE3 coupling during the power transient are confirmed, with globally a similar behavior over the entire duration. The peak power difference in occurrence time is of the order of ~5 ms (see Figure 25).

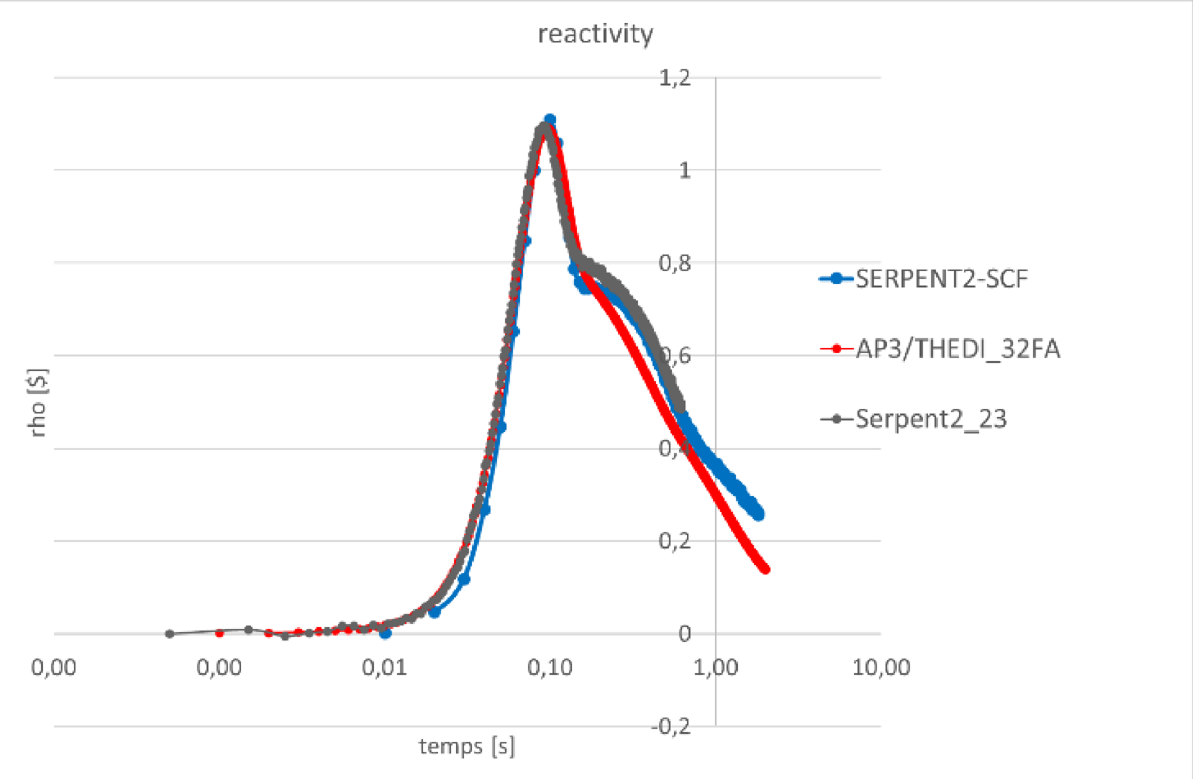

FIGURE 24: PWR MINI-CORE: LAST COMPARISON REACTIVITY TRANSIENT

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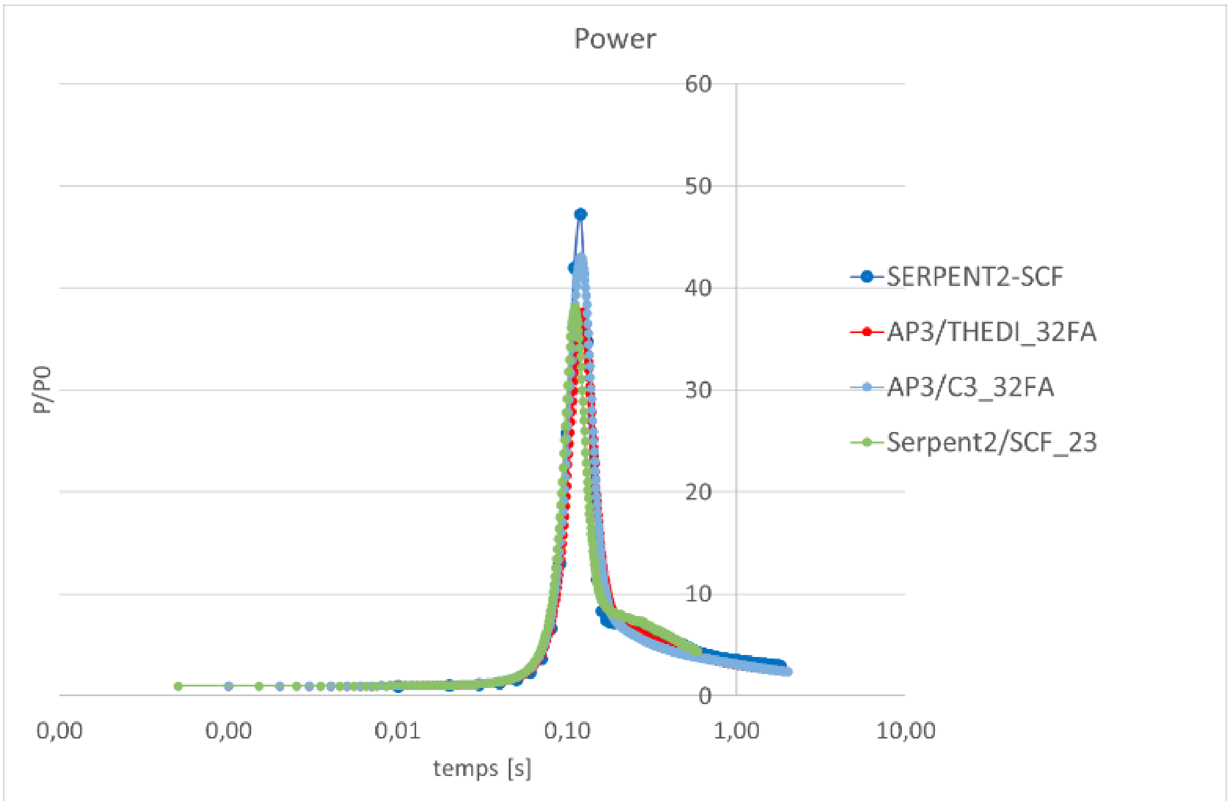

FIGURE 25: PWR MINI-CORE: LAST COMPARISON POWER TRANSIENT

Further analysis concerning the small minicore case should have been addressed to the fuel and coolant temperatures. The impact of thermal and thermal-hydraulic properties is of major importance for such an accidental scenario in all different phases after the power peak. In the project follow-up further investigations are needed for improving the comparison and the codes modeling of neutronic feedbacks as they are of key importance and for the time being a full comparison has not been completed yet.

2D map of fuel and moderator temperature calculated by CATHARE3 and THEDI may be produced, and an example is available in Figure 26 and Figure 27 to provide first elements concerning thermal and thermal-hydraulic behavior of both codes.

The lack of automatized tools dedicated to post-processing for the APOLLO3® core code is a key factor that limits the possibility of performing further investigations in a time compatible with the project duration. Average, minimum and maximum 3D fuel and moderator temperature comparison, as well as radial and axial flux penalization fraction, axial offset, Doppler, moderator feedback coefficients, etc., ask for additional development in APOLLO3® related tools not yet automatized at industrial level.

For the POC AP3/C3 further investigation concerning transient reactivity are also needed, with similar consideration about fuel and moderator temperatures.

The industrialization of the NEMESI prototype being the priority of the CAMIVVER project, all effort was provided firstly in this task to test MPOs and supporting the MPOs verification for WP4.

Nevertheless, the availability of automatized MPOs generator enables the possibility of realizing several sensitivity analyses for steady-state 32 FAs PWR core. Among those sensitivities at the core level, the most important were the one adopting B4C rods and pin-by-pin calculations that have been realized as complementary activities, see §7, where a first APOLLO3® stand-alone deck (without feedbacks) for pin-

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by-pin neutronic calculations has been realized and compared at steady-state to the coarse radial mesh solution of APOLLO3®.

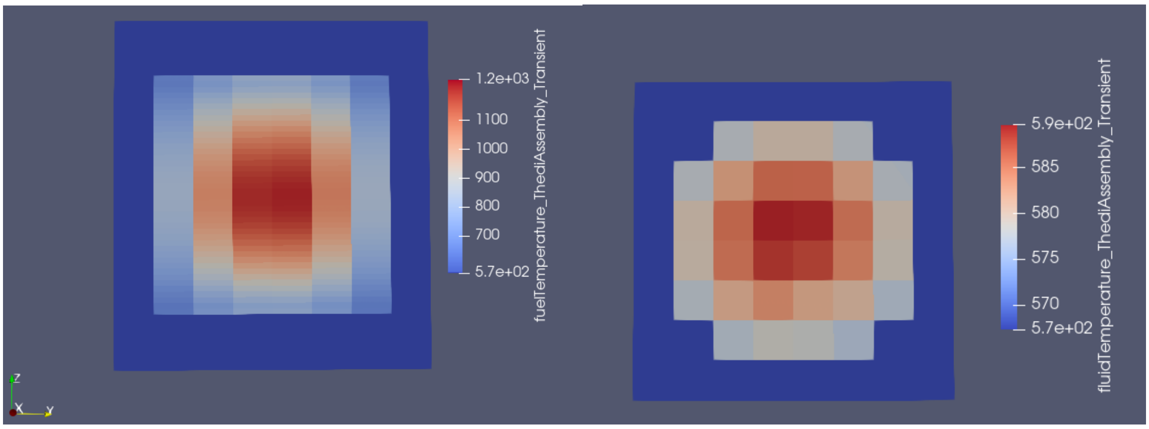

FIGURE 26: FUEL AND MODERATOR TEMEPRATURE MAPS - THEDI

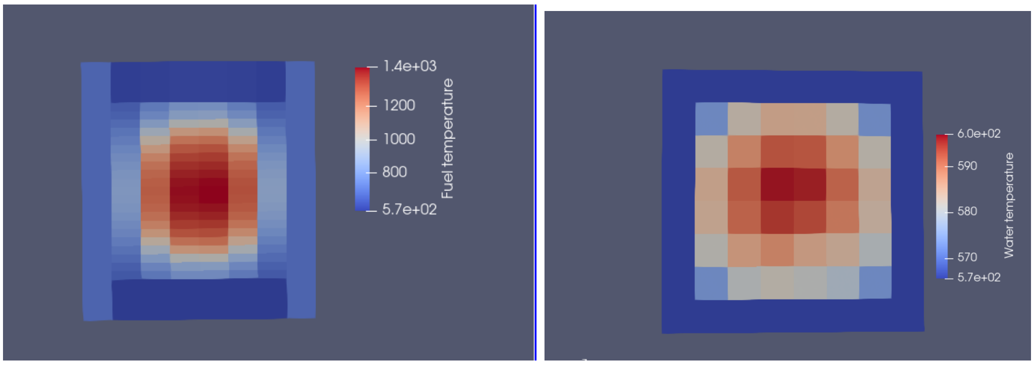

FIGURE 27: FUEL AND MODERATOR TEMEPRATURE MAPS - CATHARE3

5.2.3.SERPENT2/SCF sensitivity analysis and additional results.

A sensitivity analysis related to the time bins has been carried out in the last months of the project and presented in this section. Time bins are used in SERPENT2 for population control, but affects also the time steps in SCF and of course the number of times in which TH parameters are updated via the coupling in the neutronic code. Table 16 presents the three different cases analyzed which mainly differ in the different time bins selected for the transient problem. In cases 2 and 3 the transient simulation was cut up to 1 second due to the huge demand of computational resources.

TABLE 16: SUMMARY OF THE TEST CASES FOR THE SENSITIVITY ANALYSIS

Case	Primary particles	Batch	Number of MPI	Primary particles/batch/MPI	Time bin
A	1E+07	10	20	5E+04	10 ms
B	1E+07	10	20	5E+04	5 ms
C	1E+07	10	20	5E+04	1 ms

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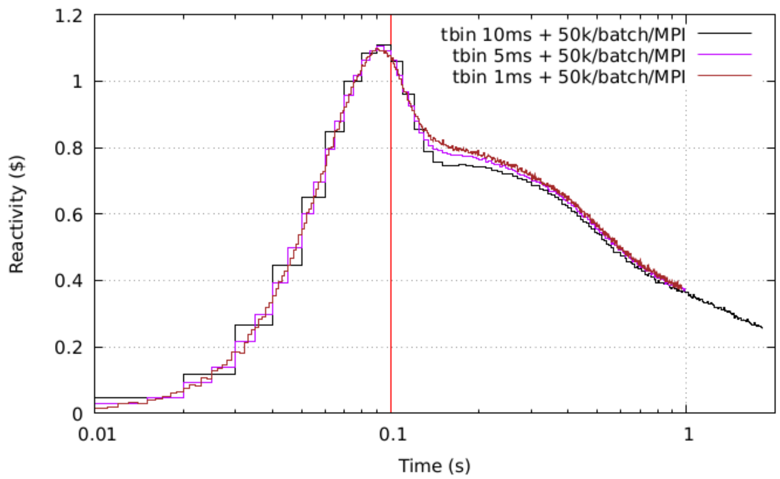
Figure 28 present core reactivity evolution in time for the three cases, no big differences are observed in terms of reactivity, but more details can be observed with the lower time bin, especially just before the control rod going totally extracted (represented in the plots as a vertical red line at $100\ ms$). It can be observed that reactivity starts to drop at $90\ ms$, which means that power is increasing and TH feedback is starting to take into account, as it can be observed in the fuel temperature evolution in Figure 34 and Figure 35. The starting increase of the fuel temperature from $90\ ms$ to $100\ ms$ of transient is transferred to the neutronic code 1, 2 and 10 times respectively for the three cases, which explains again the starting drop in reactivity and therefore affecting the core power evolution, as observed in Figure 29. Mainly the peak power value is affected, which in case C is ~20% lower than case A. Peak values are summarized in Table 17.

TABLE 17: PEAK VALUES OBTAINED DURING THE TRANSIENT

Case	Peak Reactivity (pcm)	Time bin at Peak Reactivity (s)	Relative Peak Power	Time bin at Peak Power (s)
A	811 ± 1	[0.09-0.10]	47.3 ± 0.6	[0.11-0.12]
B	808 ± 1	[0.090-0.095]	41.6 ± 0.7	[0.110-0.115]
C	803 ± 3	[0.090-0.091]	37.4 ± 0.5	[0.109-0.110]

Regarding uncertainty results, Figure 28 shows that shorter time bins lead to an increase in the uncertainty, due to that less particles are simulated in shorter time bins. Also, the uncertainty decreases close to the peak value because more particles appear due to the supercritical state bringing better statistics. Figure 30 and Figure 32 show radial power distribution at the beginning and at peak power time of the transient for case C. Figure 31 and Figure 33 show the radial power map uncertainty distribution, peripheral regions present less interaction of particles bringing higher uncertainty values.



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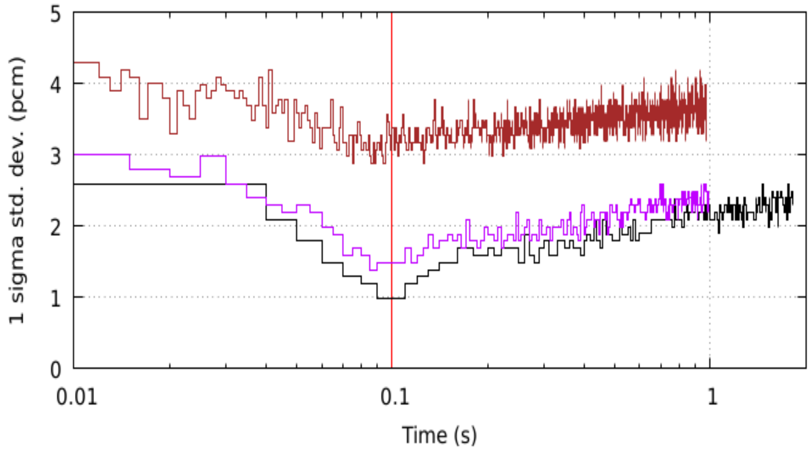
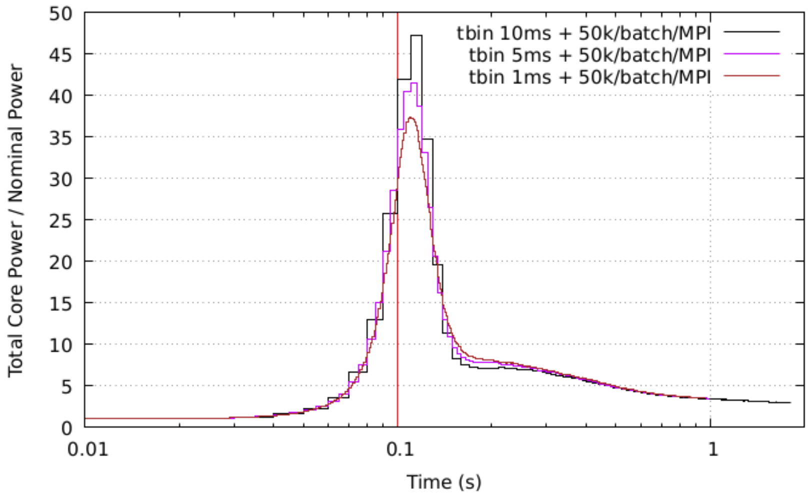


FIGURE 28: (TOP) CORE REACTIVITY EVOLUTION IN TIME[9]. (BOTTOM) STANDARD DEVIATION ASSOCIATED TO THE MONTE CARLO SIMULATION. VERTICAL RED LINE MARKS THE TIME WHEN THE CONTROL ROD C1 IS TOTALLY EXTRACTED



[9] Constant β_{eff} of 731 pcm obtained during the steady state calculations is used to express reactivity in dollars.

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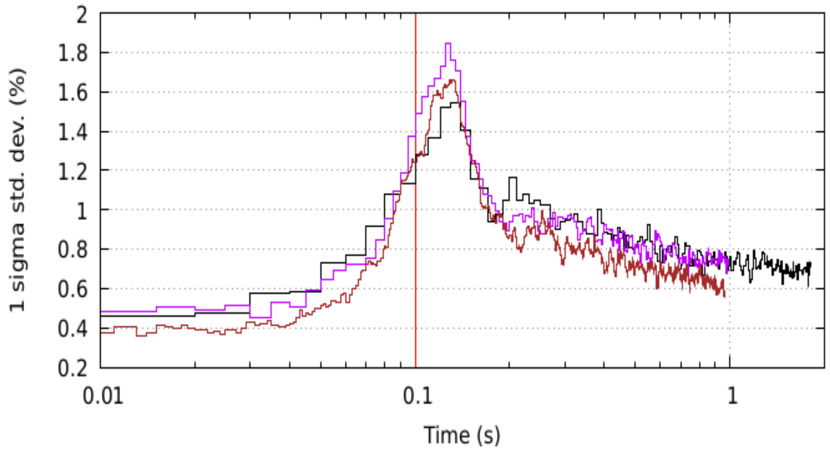

FIGURE 29: (TOP) NORMALIZED CORE POWER EVOLUTION IN TIME. (BOTTOM) STANDARD DEVIATION ASSOCIATED TO THE MONTE CARLO SIMULATION. VERTICAL LINE MARKS THE TIME WHEN CONTROL ROD C1 IS TOTALLY EXTRACTED

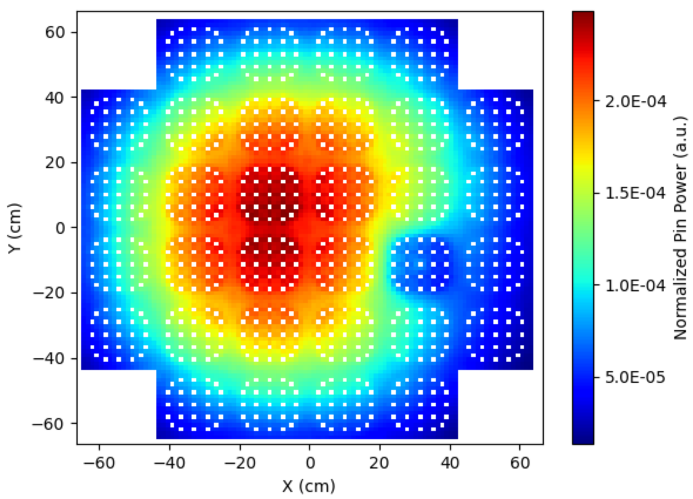

FIGURE 30: AXIALLY INTEGRATED NORMALIZED PIN POWER BEFORE THE TRANSIENT (CASE C)

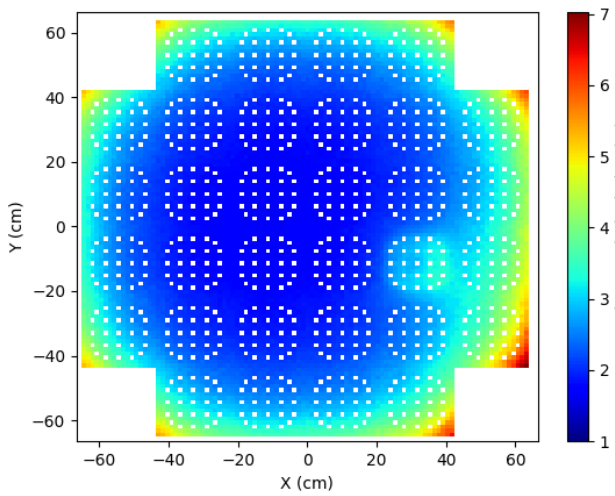

FIGURE 31: AXIALLY AVERAGED 1 SIGMA STANDARD DEVIATION BEFORE THE TRANSIENT (CASE C)

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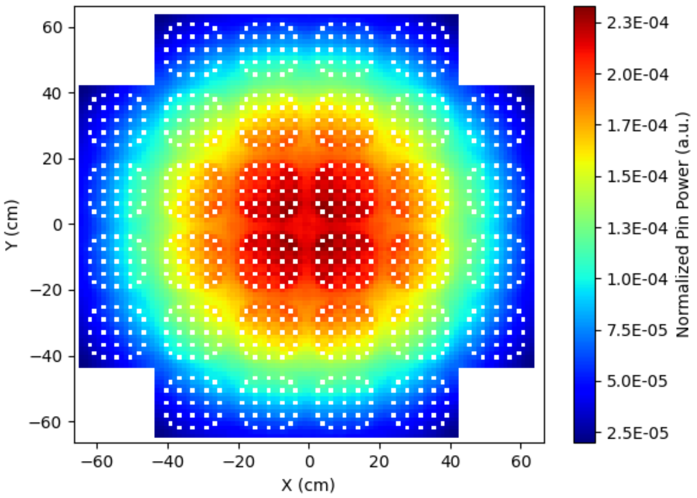

FIGURE 32: AXIALLY INTEGRATED NORMALIZED PIN POWER AT PEAK TIME (CASE C)

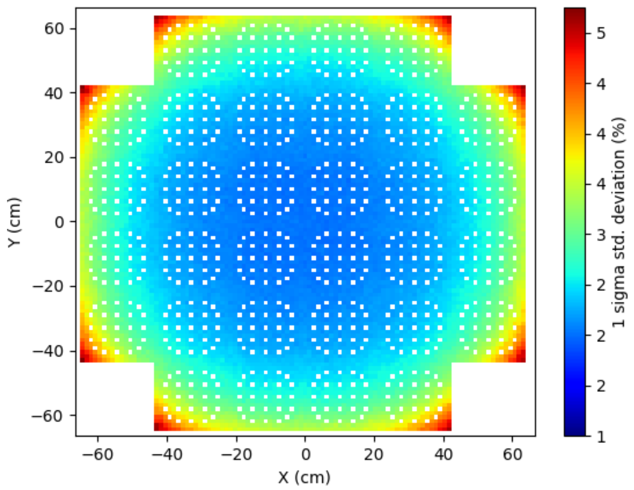

FIGURE 33: AXIALLY AVERAGED 1 SIGMA STANDAR DEVIATION AT PEAK TIME (CASE C)

As explained in the model section, 9248 rods and 10368 channels are simulated, each divided into 26 axial cells, leading to a total of 240448 rod-elements and 269568 channel-elements, respectively. Some TH parameters are selected from that level of detail, and maximum or critical values are presented in the following figures. Figure 34 and Figure 35 show the maximum fuel temperature evolution in time in the centerline and on the pellet's outer surface. Fuel temperature increases even before CR1 goes totally extracted, inserting negative reactivity into the system and counter-resting the supercritical state. The fuel temperature increases very fast up to $\sim 160\ ms$, then a change in the slope is observed because the coolant starts to remove the heat and therefore coolant temperature starts to increase, as can be observed in Figure 40. Figure 36 and Figure 37 show fuel temperature map distribution at the beginning and at $\sim 1s$[10] of the transient for the case C.

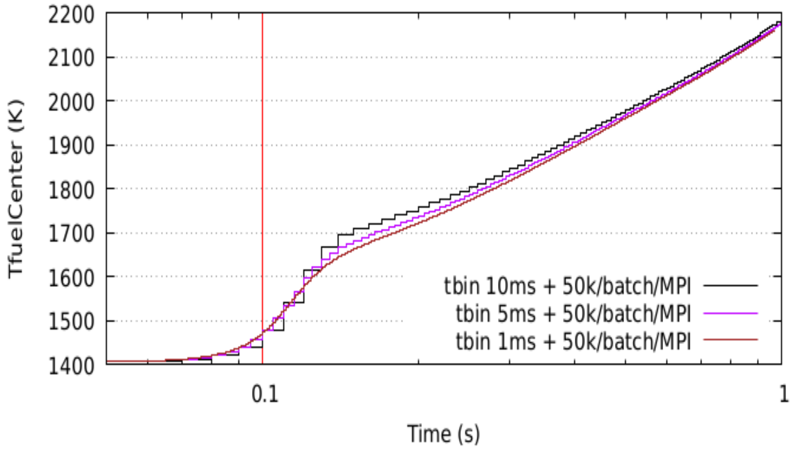

FIGURE 34: MAXIMUM FUEL CENTERLINE TEMPERATURE EVOLUTION IN TIME

[10] Due to wall-clock time limitation of the KIT-Horeka cluster, simulation was only possible up to 0.968 s of the transient for case C.

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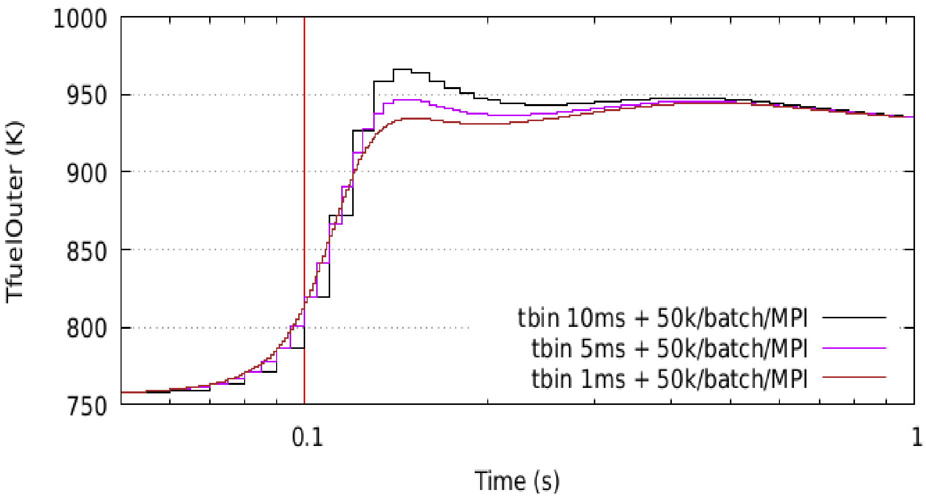

FIGURE 35: MAXIMUM OUTER SURFACE FUEL SURFACE TEMPERATURE EVOLUTION IN TIME

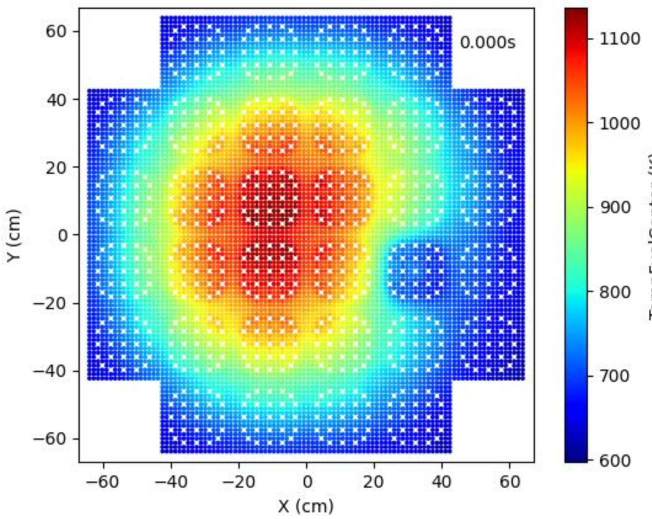

FIGURE 36: ROD AXIALLY AVERAGED FUEL CENTERLINE TEMPERATURE BEFORE THE TRANSIENT (CASE C)

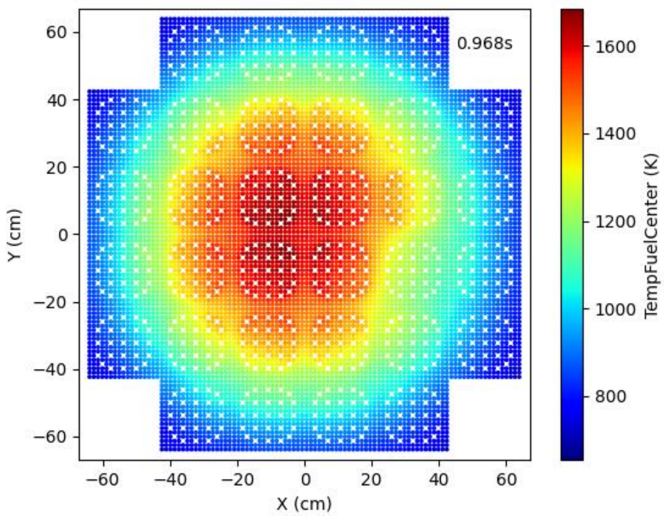

FIGURE 37: ROD AXIALLY AVERAGED FUEL CENTERLINE TEMPERATURE AT 0.968 SECONDS (CASE C)

Figure 38 and Figure 39 show maximum cladding temperature evolution on the inner and outer surfaces. A similar behavior as the fuel is observed for the cladding temperature, the quick increase in temperature is stopped due to the transmission of the heat into the coolant. It is interesting to observe that cladding temperature on the outer surface does not have a smooth behavior and some jumps are observed in cases A and B, but not in case C.

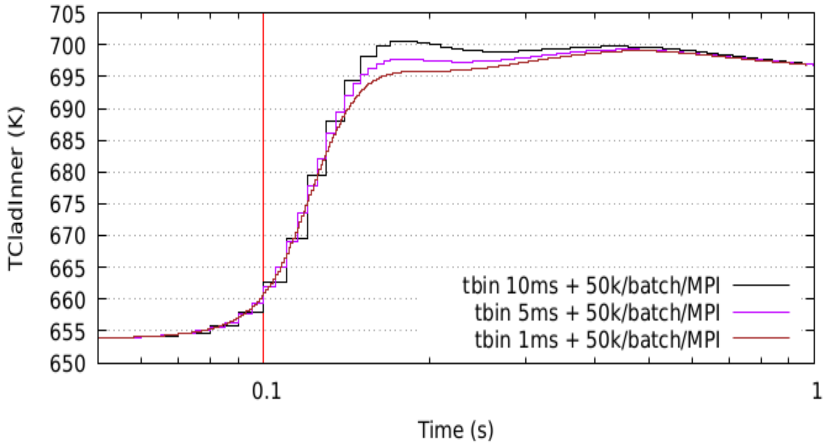

FIGURE 38: MAXIMUM INTERNAL SURFACE CLADDING TEMPERATURE EVOLUTION IN TIME

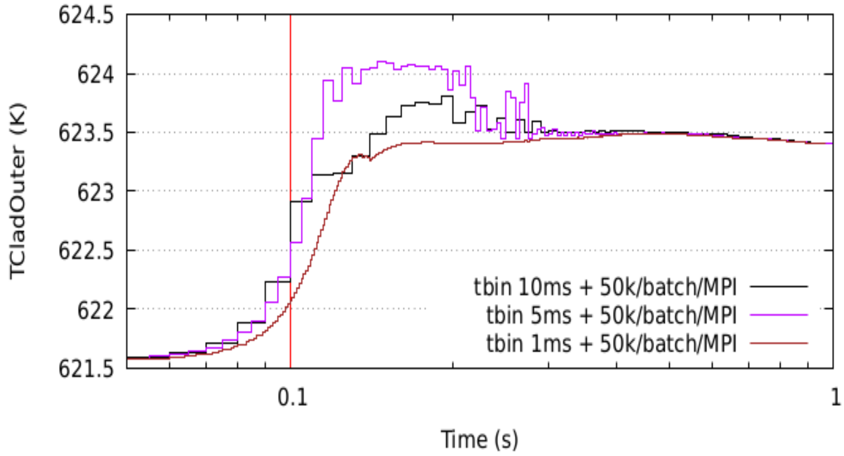

FIGURE 39: MAXIMUM EXTERNAL SURFACE CLADDING TEMPERATURE EVOLUTION IN TIME

Figure 40 shows the maximum coolant temperature evolution in time. As explained before, coolant temperature starts to increase at $\sim 160\ ms$, removing the heat generated in the pellets and inserting extra negative reactivity into the system. It is interesting to observe that saturation temperature is achieved at $\sim 0.4\ s$ of the transient, so it is expected to find some saturated vapor in the core. Figure 41 and Figure 42 show coolant temperature maps distribution at the beginning and at $\sim 1s$ of the transient for case C. Additionally, void fraction maps are presented in Figure 43 and Figure 44. According to the transient definition, a monophasic condition was expected during the transient evolution, so this should be considered in the following studies.

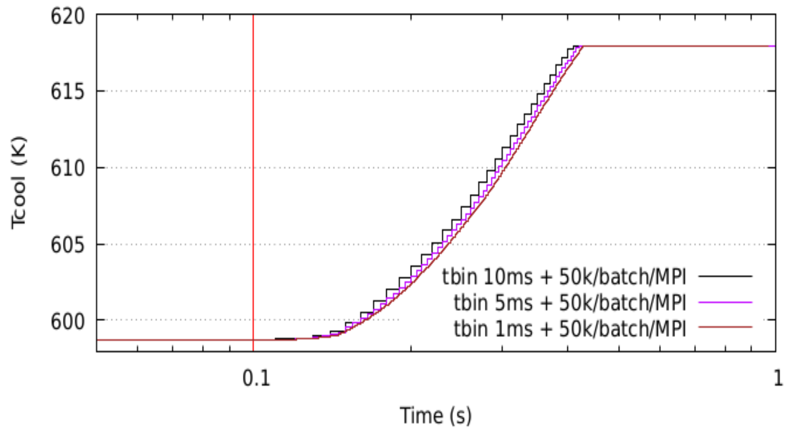

FIGURE 40: MAXIMUM COOLANT TEMPERATURE EVOLUTION IN TIME

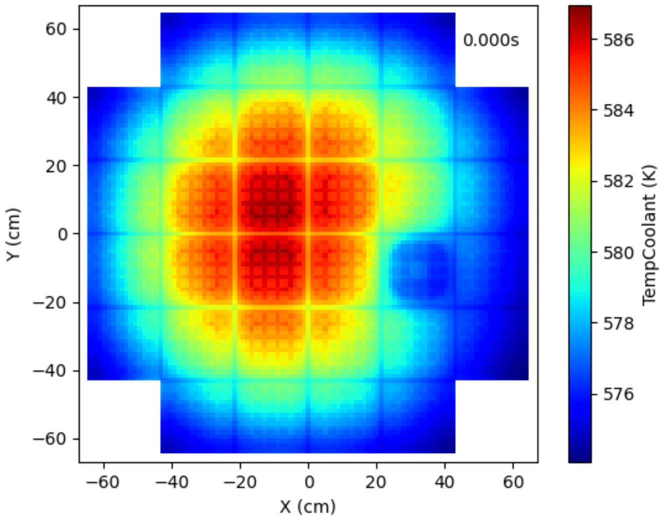

FIGURE 41: SUBCHANNEL AXIALLY AVERAGED COOLANT TEMPERATURE BEFORE THE TRANSIENT (CASE C)

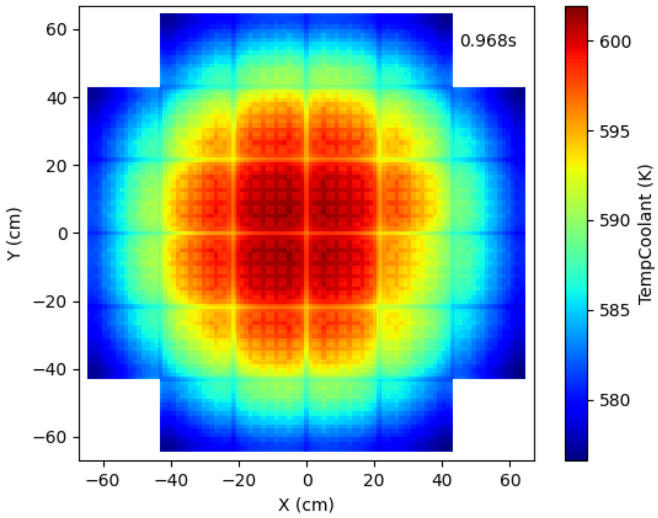

FIGURE 42: AXIALLY AVERAGED RADIAL COOLANT TEMPERATURE AT 0.968 SECONDS OF THE TRANSIENT (CASE C)

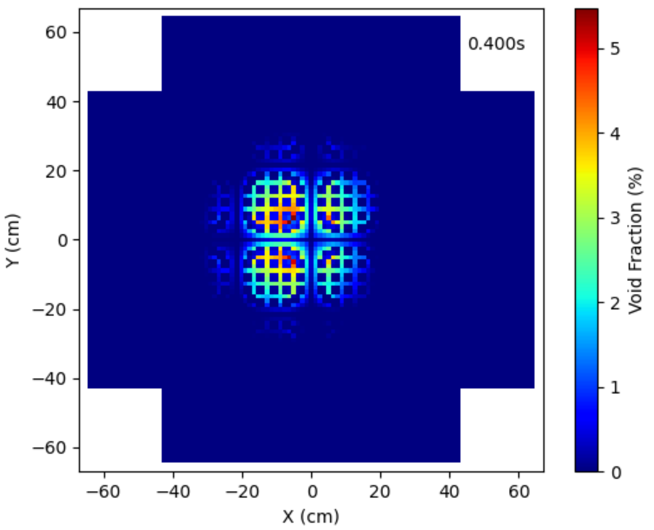

FIGURE 43: SUBCHANNEL AXIALLY AVERAGED VOID FRACTION AT 0.4 SECONDS OF THE TRANSIENT (CASE C)

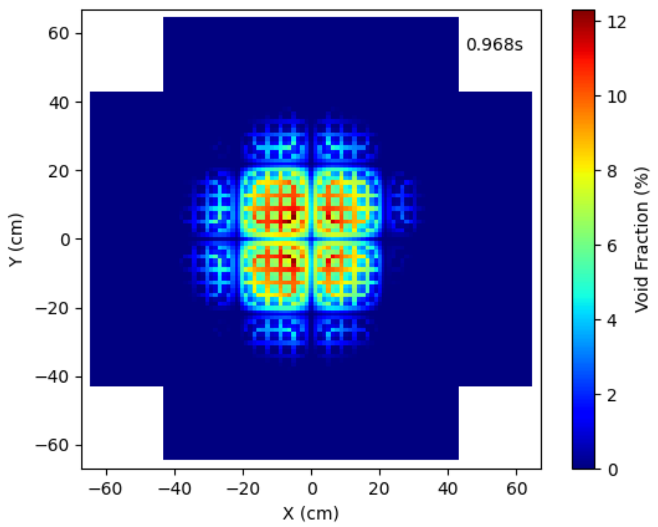

FIGURE 44: SUBCHANNEL AXIALLY AVERAGED VOID FRACTION AT 0.968 SECONDS OF THE TRANSIENT (CASE C)

Lastly, DNBR (departure from nuclear boiling ratio) evolution in time is presented in Figure 45. The minimum value obtained during the transient was 1.03 (very close to the critical heat flux).

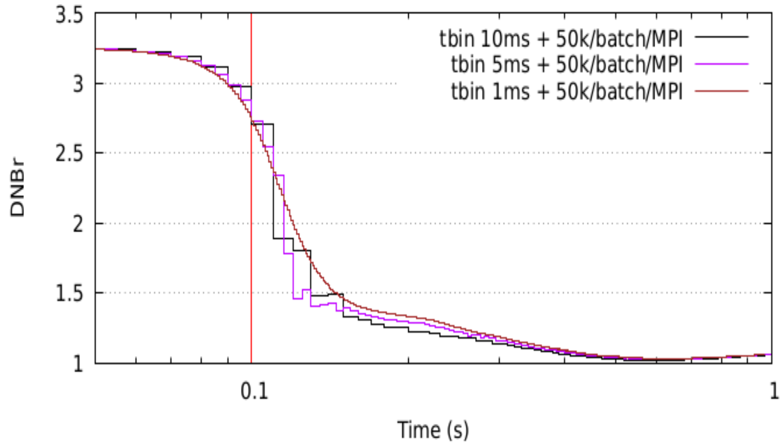

FIGURE 45: MINIMUM DNB RATIO EVOLUTION IN TIME

A summary of the computational resources and simulation times are summarized in Table 18. Simulations are performed in the Horeka high-performance computing cluster [13]. Each CPU is an Intel Xeon Platinum 8368 with 76 cores per node.

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TABLE 18: COMPUTATIONAL RESOURCES AND SIMULATION TIMES

Case	MPI	OMP	Transient analyzed	Wall-clock simulation time
A	20	76	[0 – 2s]	2 days
B	20	76	[0 – 1s]	1 day 19 hours
C	20	76	[0 – 0.968 s]	3 days

The analysis showed that the choice of the time bins for SERPENT2 (time steps for SCF) has a significant influence in fast transients (e.g., control rod ejection transients), especially in the power peak values, and the reason is mainly due to the rate in which fields between the codes are interchanged. Also, shorter time bins in SERPENT2 lead to an increase in the uncertainties as observed in cases A, B, and C. So, an increase of the primary particles also should be considered in future analysis to get reference solutions[11].

[11] This work was performed on the Horeka supercomputer funded by the Ministry of Science, Research and the Arts Baden-Württemberg and by the Federal Ministry of Education and Research.

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6. Summary of major results for the 7 FAs VVER test case

Besides the 32 FA PWR test case, WP5 participants greatly contributed to results for the 7 FAs VVER small core test case (Figure 46). As a consequence, D5.3 [5] is fully oriented to VVER core modeling with APOLLO3® and here it may be found the short description of WP5 VVER activities that contributes to the consolidation of APOLLO3®/THEDI VVER modeling but also to first functionalities applying the APOLLO3®/CATHARE3.coupling schemes to VVER too, for both steady-state and transient.

Some elements are presented here to provide a description of first results with intermediate codes and MPOs versions available at end of 2022. With this concern, in the next deliverable D5.4 any information concerning synergies with PWR applications for both APOLLO3®/THEDI and APOLLO3®/CATHARE3 coupling are available.

Most of the effort provided by WP5 concerning APOLLO3® core activities were spent mainly to consolidate input decks, pre- and post-processing tools and providing feedbacks on first attempt MPOs delivered by the WP4. Having access to a small core numerical benchmark, sufficiently representative of real applications this was a precious exercise to contribute to the industrialization of the NEMESI automation of APOLLO3® for PWR but also for VVER core modeling (see Figure 46).

The 7 FAs small core was initially described in [2] and all results directly contributes to the task 5.2 [5].

Major information concerning the geometry and composition of fuel assemblies is provided in [3].

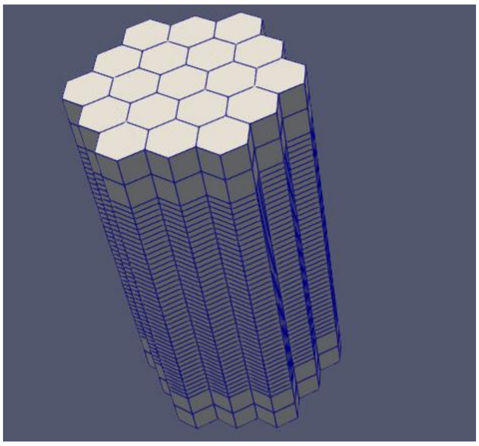

FIGURE 46: 7 FAS VVER MINI-CORE

6.1. The 7 FAs VVER core test case

In accordance to the 32 FAs core case, a short summary of the 7 FAs VVER core benchmark is provided here underlying some additional details not yet available in D5.1 [3], see Table 19 and Table 21, such as:

- Control rod material definition: B4C;
- Control rod position: intermediate at 51 cm from the top;
- Boron concentration = 403 ppm;
- Control rod ejection time = 80 ms;
- Kinetic data (see Table 21);
- Fresh fuel composition (BU=0 GWd/tiHM).

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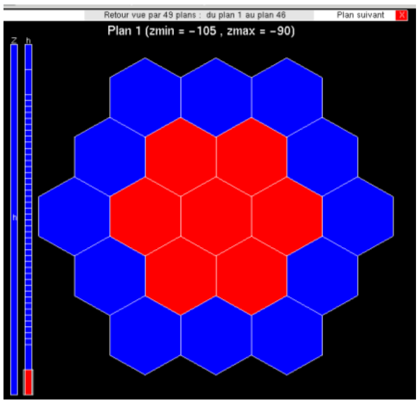
TABLE 19: 7FAS VVER CORE INFORMATION

Reactor power [MWth]	55
Inlet Water temperature [K]	562.15
Output Pressure [bar]	157
Inlet mass flow [kg/s]	784.5
Control rod position	Partially Inserted (34%)
Rod ejection time	0.08 s
Control rod composition	B_4C
Boron concentration [ppm]	403
Core Height [cm]	150
Reflectors Height [cm]	Lower = 30 Upper =30
Thermal properties	See D5.1 [3]

TABLE 20: GEOMETRIC DATA CONSOLIDATION

Geometrical data consolidation	
Total Flow area [m^2]	0.18
Total core cross section area [m^2]	0.34
heated perimeter [m]	62.44
wetted perimeter [m]	67.7



As already mentioned, D4.3 and D5.1 do not include kinetic data information. In Table 21 the delayed fractions and the delayed decay constants for 8 families of precursors have been provided, based on JEFF3.1.1 data. These data have been provided by KIT (see next section for more information) for the 7 FAs VVER core case.

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TABLE 21: KINETIC DATA FOR THE 7 FAS CORE CASE

Mini core case	7VVER	
Precursor families	BETA (pcm)	Lambda (1/s)
1	23.3	0.0125
2	109.6	0.0283
3	65.5	0.0425
4	144.3	0.1330
5	245.3	0.2925
6	81.4	0.6665
7	68.2	1.6348
8	25.6	3.5546
Total (1 effective group)	763.1	0.464

6.1.1.*The APOLLO3®-based solutions*

For the VVER test case two different approaches for multi-physics solutions have been tested by Framatome and described:

- APOLLO3®/THEDI core calculations used in order to improve knowledge around the new generation code APOLLO3® core solver when applied to VVER.
- APOLLO3®/CATHARE3 proof of concept developed in CAMIVVER for investigating the thermal-hydraulic core capabilities of the CATHARE3 code, improving knowledge of new code features and providing feedbacks around its usage for multiphysics couplings.

As already mentioned in §4 and §5, the proof-of-concept APOLLO3®/CATHARE3 is based on the C3PO engine [28] and this new tool for multiphysics analysis has been tested on a VVER core, too.

For the steady-state and transient VVER cases analyzed, the multi-parametric cross section libraries have been generated specially for the CAMIVVER project by using APOLLO3® encapsulated in the NEMESI prototype [7]. To succeed a consolidated version of MPOs for VVER geometries and compositions, the last year of the project has been devoted to continuous feedbacks to test and propose modifications to previous tentative MPOs for VVER (see Appendix 1 – MPOs tests during the project). Results are still preliminary as the APOLLO3® encapsulated in the NEMESI prototype is still under development and improvements are expected to increase its level of industrialization.

This effort toward industrialization and consolidation of physical results is needed and it should be continued during the follow up of the project.

6.2. Results and discussions

In the following paragraphs the comparison of the steady-state and REA transient's solutions generated by KIT and Framatome for the VVER small core test case with the tools previously presented are briefly discussed and summarized.

6.2.1.Preliminary analyses of mid-term point comparisons

The steady-state core operating conditions before transient are described in §6.1. These hypotheses are summarized in Table 19 in previous sections.

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Core geometrical feature and control rod location, with the specification of the ejected one, are provided in Table 20.

According to the transient scenario specifications and beginning from the initial conditions in the mini-core test case described in the previous sections, the CRs are ejected at constant velocity. At the beginning of the REA transient, since the CR worth targeted is about ~1.2$.

During the first part of the benchmarking exercise the comparison among CR worth enables the verification of such targeted reactivity insertion. Despite an important difference detected between APOLLO3® based tools and SERPENT2, and in order to keep the comparison satisfactory even during transient, a penalization on the beta effective has been adopted in order to be as closed as possible to the targeted reactivity insertion as detailed below. In a way similar to the PWR case described before, an extremely rapid exponential power increase is observed. The increase of the fuel temperature first and the decrease of the moderator density subsequently will counteract the reactivity increase with some delay due to the energy deposition mechanisms. At this point also the delayed neutron production will be needed to sustain the chain reaction and consequently the power will decrease until the delayed neutron generation is strong enough to sustain the fission chain again.

The SERPENT2/SCF axially integrated pin-power map distributions normalized to the nominal powers at the steady-state prior to the transient and at power peak time are shown in Figure 47 for the 7 FAs VVER case, in which the power hot spots close to the ejected CRs can be highlighted. The maximum and average statistical uncertainties associated to the pin power calculations is below 3%.

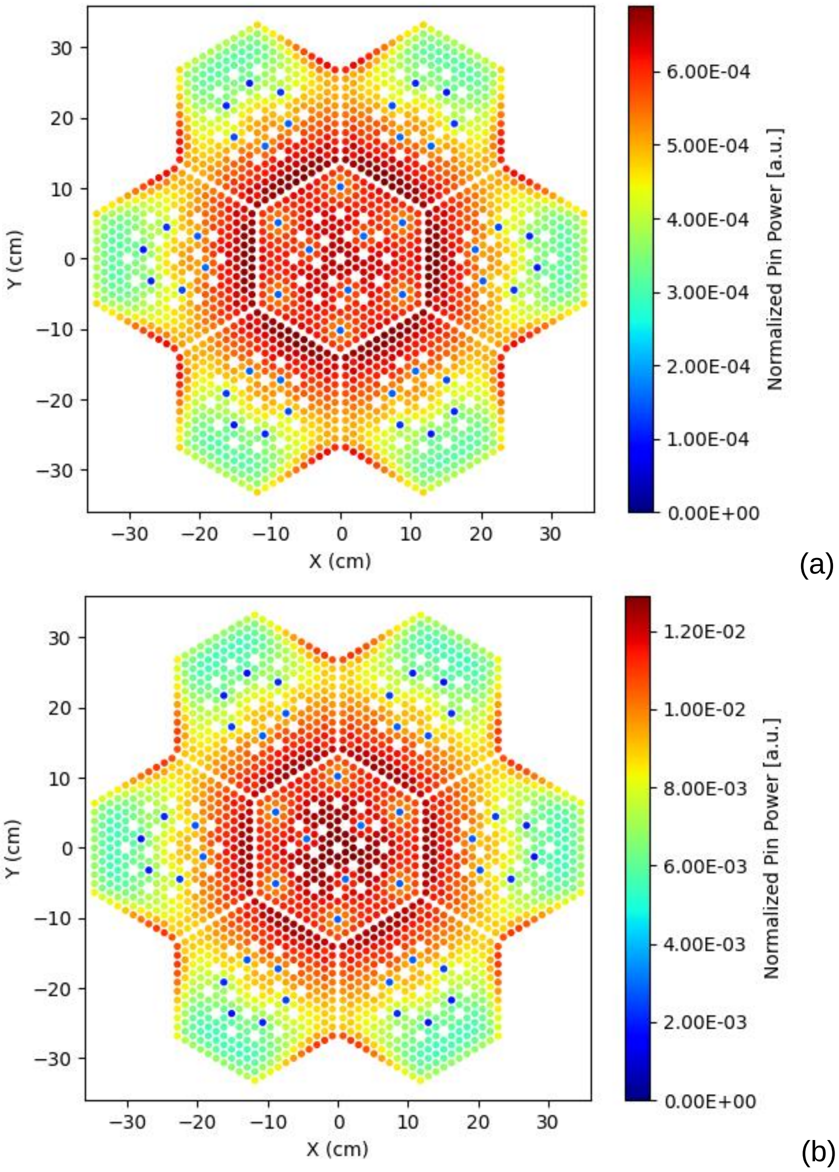

FIGURE 47: VVER MINI-CORE: SERPENT2/SCF AXIALLY INTEGRATED NORMALIZED PIN RADIAL POWER DISTRIBUTION FOR THE STATE BEFORE THE TRANSIENT (A) AND AT PEAK TIME (B)

The axial distributions of the center fuel temperature and coolant temperature at power peak times are also provided in Figure 48. This provides an example of the high-resolution capability of the SERPENT2/SCF tools which allows the prediction of reactor fuel and moderator temperature at the local level.

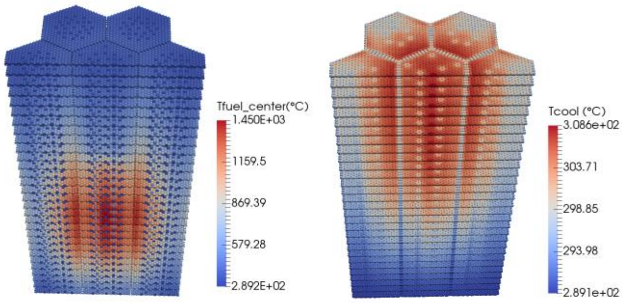

FIGURE 48: VVER MINI-CORE: SERPENT2/SCF CENTER FUEL TEMPERATURE (LEFT) AND COOLANT TEMPERATURE (RIGHT) DISTRIBUTION AT T=0.12 S

The first comparisons of the normalized power (P/P0) and reactivity as predicted during the REA transient by APOLLO3®/THEDI and SERPENT2/SCF are shown in Figure 49. A good agreement between the two different solutions can generally be observed.

For the first phase of the transient until the end of the CR ejection at about 0.08 s one can observe an excellent agreement between the reactivity profiles for the 7 FA VVER mini-core. In the second phase of the transient, after the power peak time, some discrepancies can be underlined. This behavior, that may depend on the TH modules and the energy deposition hypothesis (distribution of the energy deposition during transient between fuel pin and coolant), is similar to the one observed for the 32 FAs case and confirmed also by the final set of comparison realized during the last part of the project.

As specified in next paragraph, the final part of activities aims at consolidating the comparison at initial steady-state for reactivity prior to the transient, some aspects such as the fuel thermal properties and modeling needing in a dedicated focus in the project follow-up.

As far as the evolution of the normalized power, the shapes of the profiles generated by the different solutions were found to be very consistent one to each other, the peaking values predicted by SERPENT2/SCF are higher with respect to the ones calculated by APOLLO3®/THEDI by ~10% for the VVER (see Table 22).

The power peaks times were also found to be in good agreement within the two solutions, the difference being in the order of ~5 ms (see Table 22).

TABLE 22: VVER CASE POWER PEAKING FACTORS AND CORRESPONDING PEAK TIMES PREDICTED BY SERPENT2/SCF, APOLLO3®/THEDI (AP3/THEDI)

Coupling tool	SERPENT2/SCF	AP3/THEDI
Peak factor [P/P0]	19.55	17.74
Peak time [s]	0.095	0.0895

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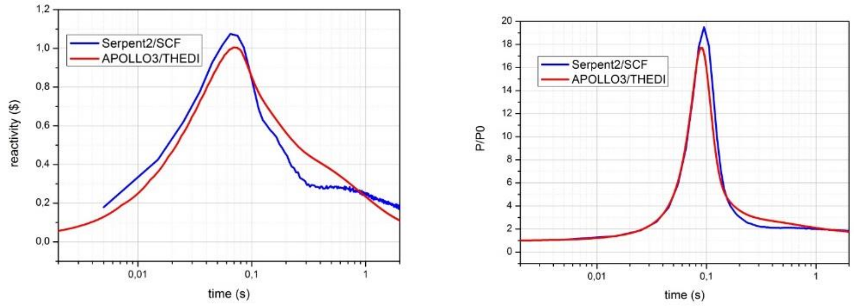

FIGURE 49: VVER MINI-CORE: REACTIVITY AND POWER EVOLUTION

6.2.2.Last discussions and improvements

Several iterations have been done during the last months of the project around APOLLO3® encapsulated in the NEMESI prototype for VVER applications [7] in order to adjust parameters range variations and final debugging for secondary isotopes. Some version improvements have been also realized in the API interfaces of codes and tools involved in the APOLLO3® based solutions.

Several iterations have been also necessary with WP4 and the development team of the NEMESI APOLLO3® preprocessor to improve the robustness of proposed MPOs for VVER reactor types.

Preliminary results, with a first selection of available MPOs, have been obtained before end 2022 (in line with the milestones fixed at WP4 and WP5) with some improvement in modeling. At assembly level very good agreement was achieved for VVER assemblies between SERPENT2 and APOLLO3® (version 2.3.0dev) as confirmed in WP4 achievements (see details in D4.4 [44] and Table 23).

TABLE 23: COMPARISONS SERPENT2/APOLLO3® ON KINF VALUES AT ASSEMBLY LEVEL FOR THE VVER 7 FA CORE

	APOLLO3® via NEMESI	diff [pcm]
B4C (390GO)	0.99132	-
DY203 (390GO)	1.05496	-165
ARO (390GO)	1.24749	-55
ARO (30AV5)	1.13810	-61

At core level, several sensitivities at boundary conditions, main parameters range variation, transient scenario main options have been tested during the first months of the project as the ones proposed in Table 24.

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TABLE 24 : COMPARISONS SERPENT BETWEEN APOLLO3® SENSITIVITIES ON STEADY-STATE MAIN CORE PARAMETERS FOR THE VVER 7 FAS CORE

First results steady-state	APOLLO3® via preliminary sets of FA cross sections	APOLLO3® Via NEMESI 0.1 last 2022
keff	1.05621	1.0569
beta	760	763
Xe	0	0
CR weight [pcm]	888.5	785
CR weight $	1.17	1.03
CR position from the top [cm]	46	51
bore	**400**	**400**
mass flow [kg/s]	4382	4382

As it was described for the 32 FAs core case, a new set of MPOs was then realized between the end of 2022 and beginning 2023, accompanied by a cycle of new comparisons at steady-state conditions among SERPENT2/SCF and APOLLO3® at core level.

During the last months of the project a continuous improving of MPOs and modeling options in APOLLO3®/THEDI and the POC AP3/C3 coupling has been encouraged. In Table 25 the comparison between SERPENT2/SCF and APOLLO3®/THEDI on main core parameters has been realized as well with the very last version of data. Some iterations have been necessary among Framatome, CEA and KIT in order to converge on the very final set of values providing the final results of the CAMIVVER project for the task 5.2.

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TABLE 25: COMPARISONS BETWEEN LAST VERSIONS SERPENT2/APOLLO3® ON STEADY-STATE MAIN CORE PARAMETERS FOR THE 7 FA CORE ASSEMBLY

First results steady-state	SERPENT2/SCF	APOLLO3® via NEMESI Latest 2023
Keff	1.00004	0.99127[12]
CR weight [pcm]	**921**	**970**[13]
Beta [pcm]	**763**	**763**[14]
Targeted CR weight $	~1.2	~1.2
CR Pos Top [cm]	51.4	51
Xe	0	0
Bore [ppm]	**403**	**403**
mass flow [kg/s]	784.5	784.5

The keff calculated with the control rod at critical position, with the rodded and with the unrodded conditions at steady-state for both SERPENT2 and APOLLO3® is presented in Table 26 with in addition the keff of first attempt calculated with the coupling APOLLO3®/CATHARE3.

[12] This difference in keff should be investigated deeper. Minor modification since the last final workshop is provided here with agreement in boron concentration comparing SERPENT2/SCF and AP3 based tools.

[13] Difference in CR weight at assembly level has been already identified. In the first part of comparisons, a very low penalisation has been adopted for the beta value in order to keep the target ~1.2$ inserted reactivity. It has been recently verified that for the APOLLO3®/THEDI case this penalization is not necessary. A possible minor discrepancy between CR worth calculation automatic procedure in APOLLO3® as indicated in the table and the value recalculated on the basis of keff has been detected and need further investigations (see for more details Appendix A).

[14] In the present version of MPOs generated by WP4 the kinetic data are not included and they are read by the core solver in a dedicated function. The main impact is that the beta effective value is calculated once and remains constant for the whole transient. A modification will be proposed for the follow up of the project.

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TABLE 26 : KEFF COMPARISONS AMONG APOLLO3®/THEDI, APOLLO3®/CATHARE3 AND SERPENT2 FOR THE 7 FA VVER CORE

keff	BORON concentration equal to 403 ppm
APOLLO3®/THEDI	Critical rod height = 0.99127 Unrodded =1.00089
APOLLO3®/C3	Critical rod height = 0.99343 unrodded =1.00191
SERPENT2	Critical rod height = 1.00006 unrodded = 1.00936

On the basis of these very last input configurations, the transient scenario defined in CAMIVVER task 5.1 [3] has been performed as well. In Figure 50 and Figure 51 transient behavior for normalized power (P/P0) and reactivity indicated in ($) as predicted during the REA transient by APOLLO3®/THEDI, the POC APOLLO3®/CATHARE3 and SERPENT2/SCF are shown. A quite good agreement between the different solutions is confirmed for the 7 FAs VVER small core case for the overall transient.

It should be mentioned that for both approaches, SERPENT2/SCF and the APOLLO3®/THEDI, two different sets of solutions have been obtained with a major modification proposed (see Appendix A of [5]) in Figure 50 and Figure 51):

- SERPENT2_SCF: first set of results for SERPENT2/SCF, SERPENT_SCF_23: last set of results.
- AP3_THEDI_7FA: first set of results for APOLLO3®; AP3_THEDI_7FA_no_penalisation: last set of results.

As observed for the 32 FAs core case, in the second phase of the transient, after the power peak time, some discrepancies persist even after double checking the thermal properties. The coherence in the different approaches proposed among the definition of energy fraction deposited in the fuel should also further investigated.

Moreover, the radial and axial discretization is not the same with an APOLLO3® neutronic flux modeling realized with homogeneous assembly mesh approach.

The POC APOLLO3®/CATHARE3 coupling [10] developed for PWR applications, has been extended to VVER geometries too, as shown in Figure 51, where results obtained on the 7 FA VVER case for prediction of the power evolution during REA transient are presented.

More information concerning the improvement and debugging of SERPENT2/SCF coupling will be provided in the project follow-up.

As already mentioned, in support to Task 7.4 the proof-of-concept for the APOLLO3®/CATHARE3 coupling has been applied to a full core analysis, too. The Kozloduy NPP Unit 6 3D core modeling and loading corresponding to a 1st cycle at steady-state conditions have been realized in collaboration between WP5 and WP7. More details are provided in §6.3.

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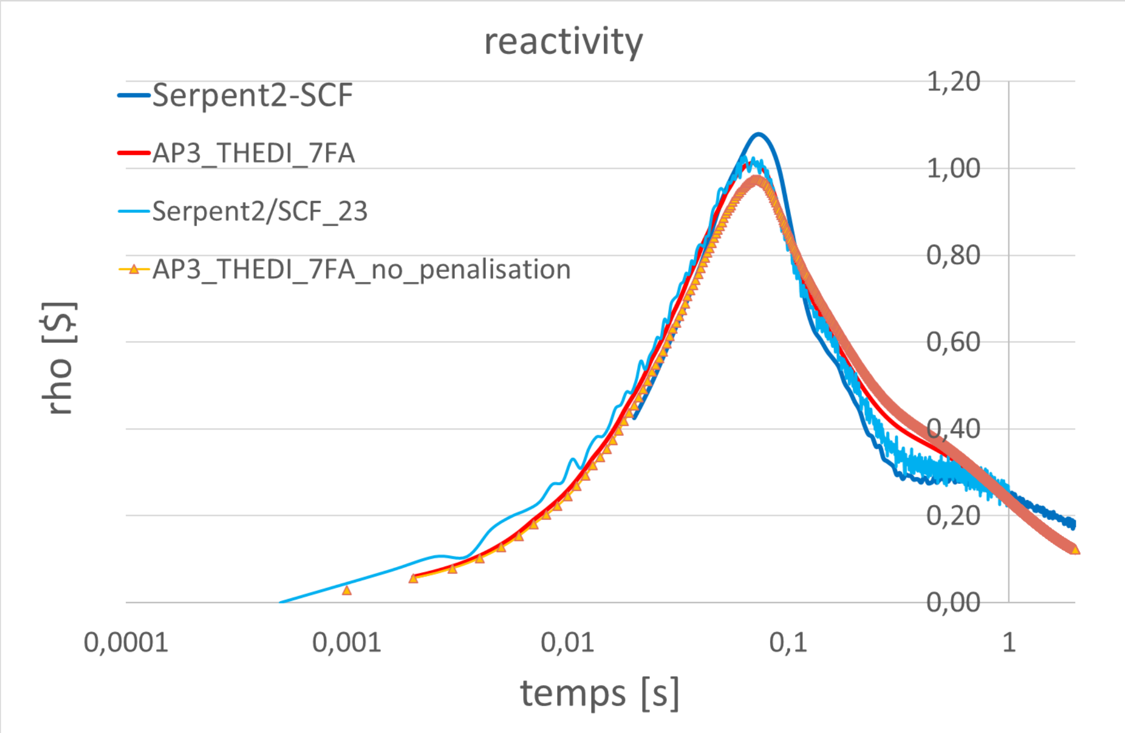

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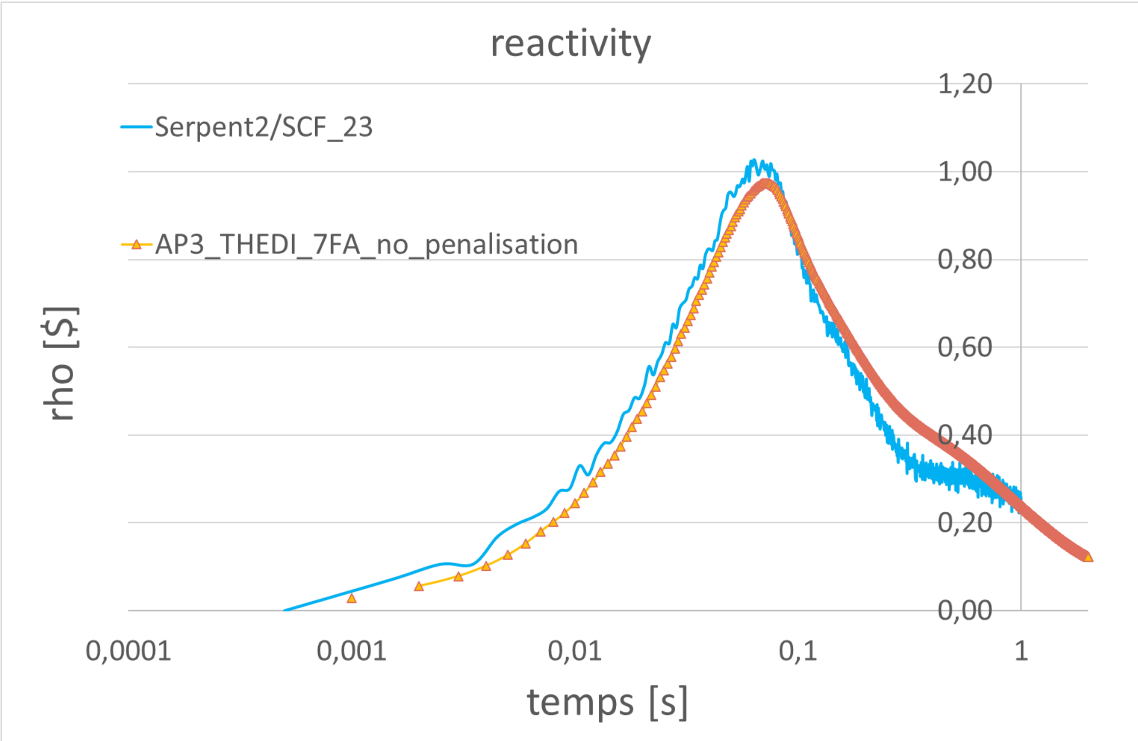

(B)

FIGURE 50: 7 FAS VVER MINI-CORE: LAST COMPARISON REACTIVITY TRANSIENT WITH FIRST AND FINAL RESULTS (A) AND A ZOOM ON FINAL RESULTS (B).

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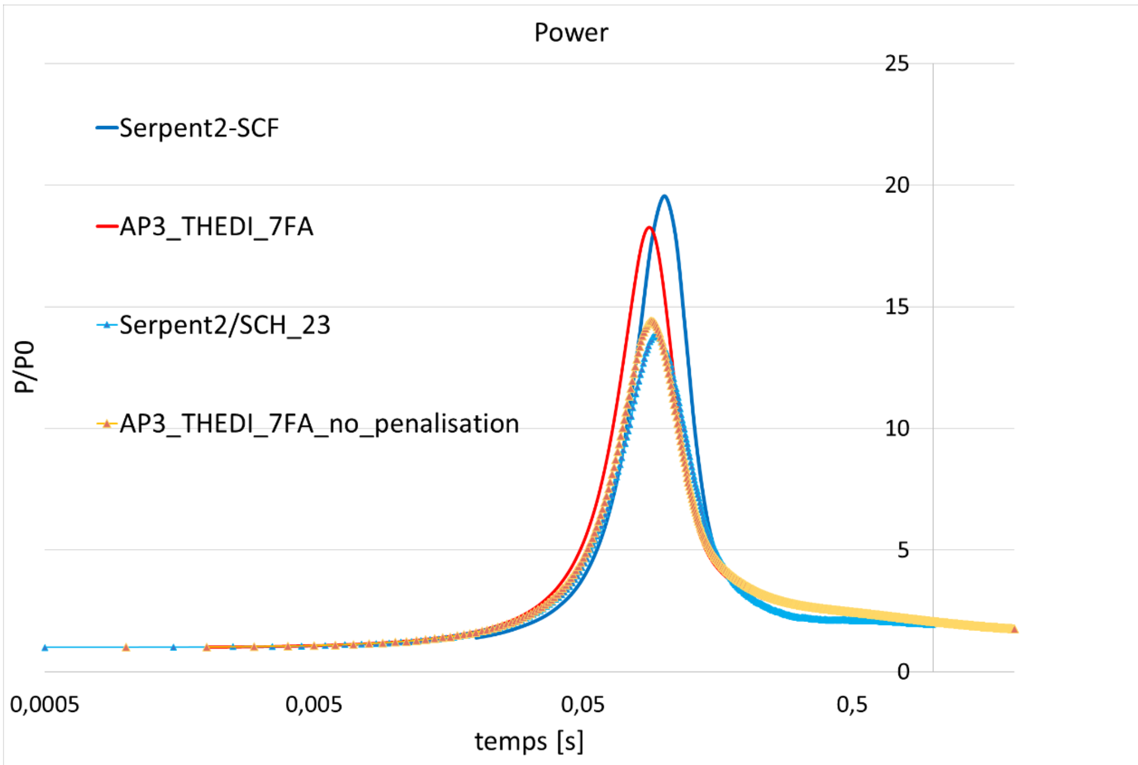
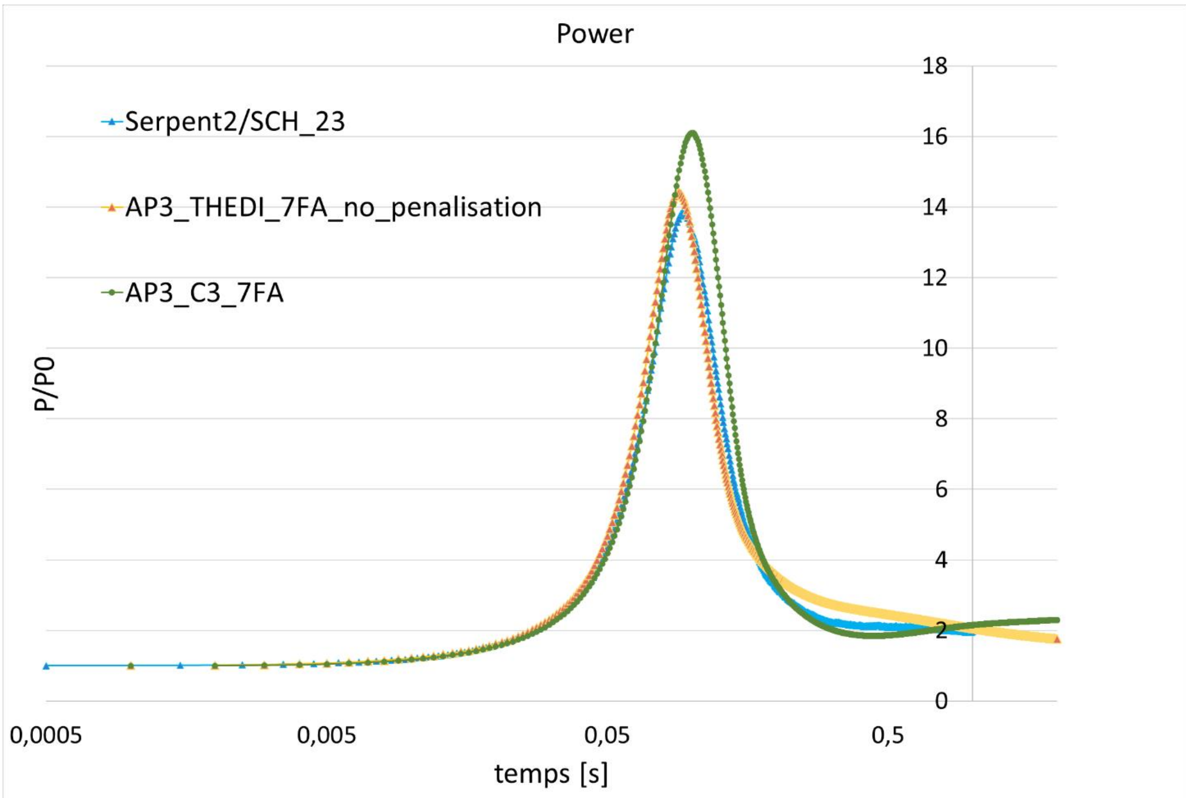


(A)



(B)

FIGURE 51: 7 FAS VVER MINI-CORE: LAST COMPARISON POWER TRANSIENT WITH FIRST AND FINAL RESULTS (A) AND A ZOOM ON FINAL RESULTS WITH THE APOLLO3®/CATHARE3 CONTRIBUTION(B).

6.3. The KZLD6 163 FAs VVER core test case

The present section summarizes the core definition and associated neutronic data needed for the MSLB exercises proposed in Task 7.4, as well as major hypotheses considered for the core modeling with both the APOLLO3®/THEDI and the APOLLO3®/CATHARE3 coupling.

It has been decided that for the full core VVER benchmark MSLB case analyzed in Task 7.4, the beginning of cycle 1 instead of cycle 8 as in the previous NEA benchmarks has to be considered. The boundary conditions for the MSLB transient have been defined and updated by INRNE and they are the object of a dedicated update of D3.2 [41].

In the project organization (see ref. [1]), the Task 7.4 was proposed for testing the coupling and 3D capabilities of the current codes against a transient of interest for Safety Analysis as MSLB. In the past, this transient has been analyzed in an international benchmark using 1D models [42].

The interest on moving to a 3D modelling and more advanced coupling has pushed the partners to choose a configuration that requires small efforts on cross-section preparation and may allow to reduce the sources of discrepancies due to burnup models. During the Task 7.4 meeting, it was decided to use the core data of Task 7.3 MCP-Restart benchmark [42]. This choice is not impacting the interest on this first comparison proposed in the CAMIVVER project.

As it will be detailed in Task 7.4 for the first application of the APOLLO3®/CATHARE3 coupling, the fact that a full primary and secondary system CATHARE3 stand-alone input deck was not yet available before the very final months of the project limited the possibility to attain a full primary/secondary/and core unique modeling for the MSLB configuration. Anyway, the functionality and the feasibility of such exercise is already available while adopting the existing CATHARE3 deck for the MCP-Restart benchmark.

Further evolution to simulate boundary conditions in primary and secondary systems thermal-hydraulics fully representative of the defined MSLB benchmark will be continued in the follow up of the project, taking advantaging in all evolution in MPOs foreseen applying newest version of NEMESI.

In the following subsections a short description of the core loading and operational conditions at steady-state for BOL (cycle1) Kozloduy NPP Unit 6 core, in support to Task 7.4 activities, is presented.

6.3.1.Core Neutronic models for cycle 1

For Task 7.4, it was decided to use the core geometry and definitions provided in reference [42] as starting point to define a reference design for the VVER-1000 for CAMIVVER partners starting from reactor geometry and some operational data of the Kozloduy NPP Unit 6.

6.3.1.1. Core model

The core model, provided as an example by APOLLO3 preprocessor in Figure 52, is characterized by 163 FA and 48 reflector assemblies. Axially, the reactor core has a total active core height of 355 cm. The upper and lower axial reflectors have a thickness of 23.6 cm. Zero flux boundary conditions are specified on outer reflector surface for both radial and axial reflectors.

Fuel assemblies with different U235 enrichments are present in the core. This is the first cycle for NPP Kozloduy Unit 6 and all assemblies are fresh.

The proposed grouping is shown in Table 27 and the radial core layout is presented in Figure 53.

Two types of CRs are considered:

- Partial length CR (group V): control rods with neutron absorber only in its lower half
- Fully (groups I-IV and VI-X)

The CR are represented as well in Figure 53 and Table 28.

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For any further specification and details the information will be provided by Task 7.4.

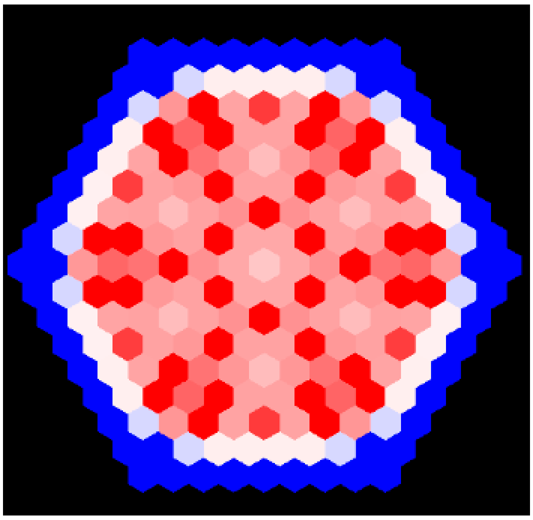
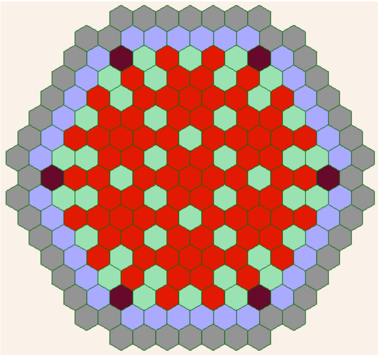


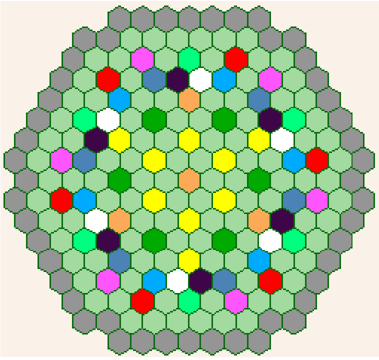
FIGURE 52: KOZLODUY-6 NPP CORE [41]

TABLE 27: CYCLE 1 TYPE OF ASSEMBLIES

Assembly type	Enrichment, w/o	Colors in Figure 53
1	2.0	
2	3.0	
3	3.3	
4	3.3 profiled	
5	Reflector	



a)



b)

FIGURE 53: A) CORE LAYOUT CYCLE 1 AND B) CR LOCATION [41]

TABLE 28: CYCLE 1 CR POSITION

Assembly type	Purpose	Colors in [41]
I	Safety	
II	Safety	
III	Safety	
IV	Safety	
V	Partial-length	

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VI	Safety	
VII	Safety	
VIII	Safety	
IX	Safety	
X	Regulation	

6.3.1.2. Major contribution to task 7.4 and relationship with task 7.3

In next sections the summary of most important hypotheses taken to improve the core modeling for the Kozloduy-6 Cycle 1 NPP with codes and first analyses at core level are presented.

Preliminary results for KINF evolution as a function of burnup are presented with APOLLO3® and SERPENT2 in §6.3.1.2.3 to test MPOs of first attempt and helping to consolidate further comparison has been realized, too.

6.3.1.2.1. Assemblies and grids models

The core model is shown in Figure 53. Radially, the core is divided into hexagonal cells with a pitch of 23.6 cm, each corresponding to one fuel assembly (FA), plus a radial reflector (shaded area) of the same size. There are a total of 211 assemblies, 163 FA and 48 reflector assemblies. Axially, the reactor core is divided into 10 layers with a height (starting from the bottom) of 35.5 cm, adding up to a total active core height of 355 cm.

The available gap width is 0.08 mm (distance between pellet surface and inside clad wall). For the neutronic problem, each of the FAs is homogeneous.

Assembly data are available at D4.3 [2].

Grids are not explicitly modeled in a first approach, but their modeling could be considered in order to extend comparisons to experimental data coming for instance from Kozloduy-6 power plant.

6.3.1.2.2. Reflectors

An average fuel temperature value equal to 600 K is used for the radial reflector cross-section modelling in both the initial steady-state and transient simulations, and the average coolant density for the radial reflector is equal to the inlet coolant density. For the axial reflector regions, the following assumptions are made: for the bottom reflector the fuel temperature is equal to the inlet coolant temperature (per T-H channel or cell) and the coolant density is equal to the inlet coolant density (again per channel); for the top reflector the fuel temperature is equal to the outlet coolant temperature (per channel) and the coolant density is equal to the outlet coolant density (per channel).

For a first guess comparison a major hypothesis shared among partners corresponds to keep for the reflectors (top, bottom and radial) the same compositions as moderator.

An update with heavy reflector may be realized during the follow-up project. Some actions have been already proposed for starting to improve the reflector models as indicated in Appendix 2 – Improved reflectors modeling.

6.3.1.2.3. First analysis of VVER MPOs generated by NEMESI

In correspondence of the resolution of this discrepancy a first comparison has been realized between AP3 and SERPENT for kinf evolution vs burnup for two assembly cases (390GO and 30AV5) using 600 ppm boron concentration

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Major results are provided below in Figure 54. The comparison shows good agreement and minor discrepancies are analyzed in the framework of the WP4.

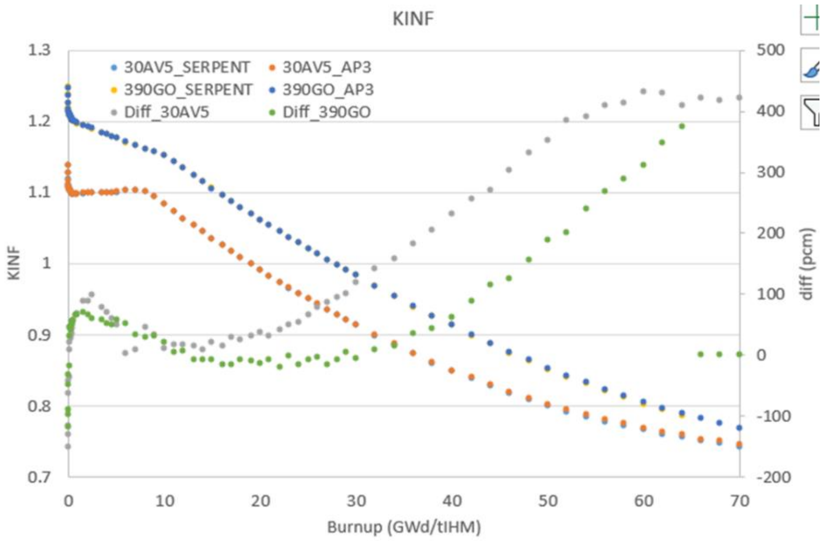

FIGURE 54: APOLLO3 AND SERPENT COMPARISON OF KINF EVOLUTION VS BURNUP FOR TWO ASSEMBLY CASES (390GO AND 30AV5)

6.3.1.2.4. Boundary conditions and steady-state conditions before transient

The newly defined hypotheses concerning core and assemblies and reflectors compositions change the core state at the beginning of the transient.

A core model is provided by KIT and Framatome to perform sensitivities oriented to define the steady-state operating conditions before transient.

Some effort was spent to find optimal conditions to reach criticality and some sensitivities have been performed by KIT with SERPENT, confirmed by Framatome with APOLLO3, to provide a suitable configuration for boron concentration and control rod banks positions.

To fix conditions to be shared before any comparison, a first scenario may have the boron concentration fixed to 1200 ppm, the core operated at hot full power with xenon in equilibrium. Critical state may then be achieved tuning control rod banks IX and X, as previously defined in Table 28.

First sensitivities oriented to define a more realistic as possible pre-accidental condition close to criticality already realized by KIT and Framatome are presented here after.

As final specifications are still ongoing till the very last period of the project they will be integrated to the last revision of documentation.

At the beginning the generation of 2 groups homogenized XSs to feed the core simulations with APOLLO3 to consolidate first KIT analyses has been realized providing MPO generated via NEMESI prototype (WP4).

After some comparisons at assembly level (ARO and B_4C) see Table 29, comparison between SERPENT (KIT) and APOLLO3® (FRA) at core level has been realized.

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TABLE 29: COMPARISONS AT ASSEMBLY LEVEL (KINF AT BOL WITHOUT XENON) FOR THE 4 KZL6 FAS

	FA2_F	FA3_F	FA3_3_F	FA3_3_G
SERPENT2 (KIT)				
HFP, NULL XENON, ARO	1.09810	1.22105	1.24675	1.24054
HFP, NULL XENON, ARI	0.82319	0.94299	0.96966	0.96294
NEMESI (FRA)				
HFP, NULL XENON, ARO	1.09832	1.22121	1.24682	1.24061
HFP, NULL XENON, ARI	0.82330	0.94327	0.96987	0.96314
Discrepancy A-S (pcm)				
ARO	18	11	5	5
ARI (=B4C)	15	32	22	21

In addition, several tests have been carried out between KIT and Framatome in order to consolidate practices around core modeling for the Kozloduy-6 NPP, see Table 30.

TABLE 30: COMPARISONS AT CORE LEVEL - KZL6

STATE	BOR ON	SB1-8	SB9	CB10	SERPENT2 KEFF	PARCS KEFF ADF OFF	PARCS KEFF ADF ON	AP3	DIFF AP3/S2, pcm	DIFF SERP/PARCS ADF OFF, pcm	DIFF SERP/PARCS ADF ON, pcm
HFP	1200	A	R	O	1.04800	1.04635	1.04651	1.05306	505	-150	-136
HFP	1200	100%	100 %	0	1.04012	1.03751	1.03825	1.04433	421	-242	-173
HFP	1200	100%	0	100%	1.04223	1.04069	1.04104			-142	-110
HFP	1200	100%	0	0	1.03227	1.02955	1.03064	1.03613	385	-256	-153
HFP	1200	A	R	I	0.95481	0.94903	0.95303	0.95655	175	-637	-196

As it could be observed in Table 30, in order to target Keff = 1 the control rod should be drastically moved without proposing too high boron concentration responsible for unacceptable modification in moderator feedbacks, see Table 31 as example.

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TABLE 31: RELASHONSHIP BETWEEN SAFETY BANKS POSITION AND BORON CONCENTRATION

STATE	XE	SP. GRID	BORON (ppm)	Others SB	SB10
HFP	NO	NO	1630.	100%	20%
HFP	NO	NO	1692.	100%	80%

Optimum configuration in still under discussion and will be presented by Task 7.4 adopting tools and models provided in collaboration with WP4 and WP5.

Among contribution to be pursued by WP4 it could be mentioned the improvement enabling the Xenon feedbacks by ad hoc parametrization.

Concerning WP5 contribution, APOLLO3® core loading with rod bank modeling will be continued till the end of the project. An additional contribution will be the development and consolidation of core interfaces enabling the coupling between the core modeled with APOLLO3®/CATHARE3 Multiphysics coupling and the full primary and secondary systems Kozloduy-6 CATHARE3 input deck realized in the framework of the CAMIVVER for the Task 7.3. Its improvement to attain the final boundary conditions enabling a MSLB transient will be continued till the end of the project and pursued in the project follow up.

6.3.1.2.5. First coupling core 3D neutronics and full system thermal-hydraulics

During the CAMIVVER project it has been possible to take the deck CATHARE3 produced in the framework of the task 7.3 for the Main coolant start-up test and adapted it in order to couple the full system thermal-hydraulics to the core 3D neutronic solver of APOLLO3®, thanks to the C3PO engine.

First results of such a coupling are presented in Figure 55 below.

Currently, before the end of the project the same exercise in ongoing in order to prepare the CATHARE3 input deck for the MSLB KZLD6 transient and propose a 3D neutronic coupling with APOLLO3® also on this heterogeneous transient. If all components are available for the CAMIVVER project and a first feasibility has already been performed for the MCP start-up test, the fulfillment of the coupling for the MSLB transient will be completed for the project follow-up.

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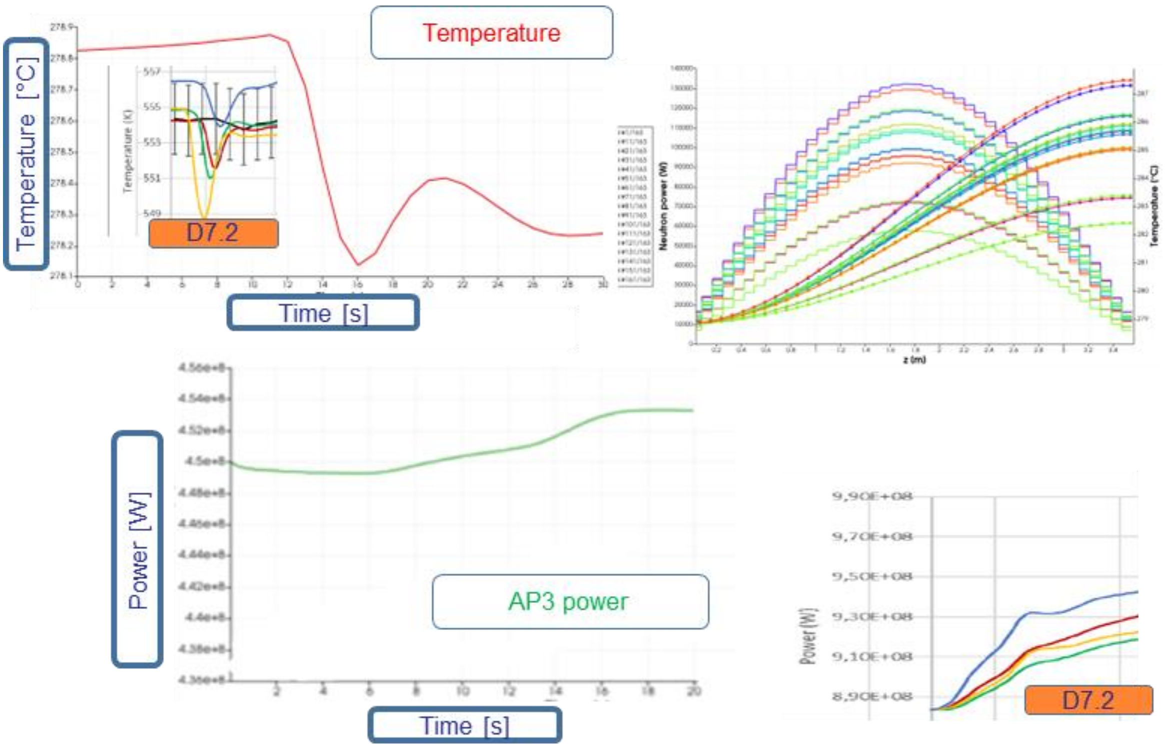

FIGURE 55: MCP START-UP SIMULATION CATHARE3 DECK (TASK 7.2) CORE + SYSTEM THERMAL HYDRAULIC SIMULATION – FEASIBILITY OF THE FULL SYSTEM PLUS 3D NETRONICS COUPLING

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7. Complementary analysis for PWR and VVER applications

In this chapter a summary of complementary analyses performed in the framework of the CAMIVVER project is presented, consolidating the application of APOLLO3 core solver and the Multiphysics couplings to PWR and VVER cases. The contribution of this part has been relevant in supporting the development of the NEMESI encapsulating APOLLO3® (pre/post processor) and to test the associated MPOs in small and full core applications.

In this chapter some comparison between APOLLO3® based solutions and SERPENT are also proposed by Framatome.

7.1. 32 FAs core pin-by-pin calculations

In order to improve the PWR core modeling benchmark and to enable, at least in the project follow-up, a better understanding of some discrepancies observed in previous chapter, a pin-by-pin input deck for core calculation with APOLLO3® in stand-alone mode, without feedbacks, has been realized. This model helps improving comparisons with a reference calculation as the one provided by SERPENT2/SCF in the project follow-up and consolidating the high fidelity solution.

The pin-by-pin input deck implements steady-state and transient calculations. It needs special MPOs enabling pin-by-pin calculations. To succeed a first exercise, the available MPO with pin-by-pin discretization, was created with the 2022 NEMESI version, corresponding to results provided in Table 13. Results may undergo limited evolution with further version of tools under development.

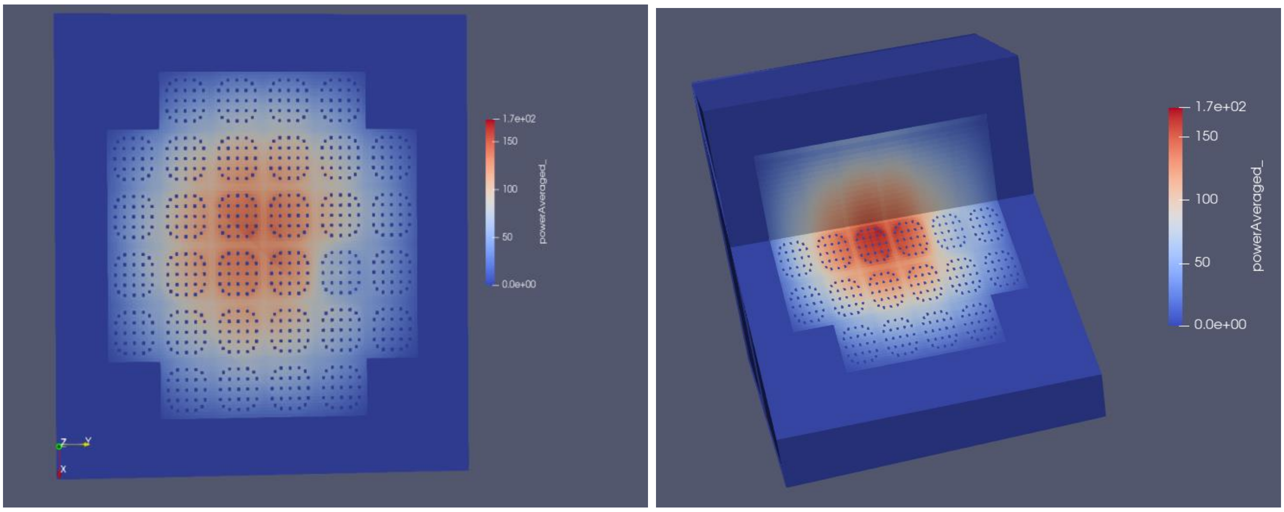

FIGURE 56: PWR 32 FA MINI-CORE: APOLLO3 PIN-BY-PIN MODELING.

Comparisons among APOLLO3/THEDI version and the APOLLO3® PbP approach but also a in-house version of the SERPENT code have been possible for the steady state configuration at different boron concentration, see Table 32. The results are satisfactory as first step of this activity in the framework of the CAMIVVER project. Before any application to safety analysis further tests are necessary and deeper comparisons.

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TABLE 32 : KEFF COMPARISONS AMONG APOLLO3/THEDI IN COARSE MESH, APOLLO3 PBP AND SERPENT FOR THE 32 FA CORE

keff	BORON 600
APOLLO3/THEDI	Rodded =1.18972 unrodded =1.20098
APOLLO3 PbP	Rodded =1.19939 unrodded =1.20600
SERPENT (Own Framatome model)	Rodded =1.20285

7.2. Other PWR analyses

In support to WP4 activities and to test capability of the APOLLO3® code of modeling different core geometries and isotopic compositions, other calculations have been realized for cluster of assemblies, small core with MOX FA and full core calculation as examples of future industrial applications.

Next test cases have been treated in supporting sensitivity analysis (for instance oriented to core size, core loading heterogeneities in case of MOX, impact of core size to code and couplings performances, etc.) in preparation of next steps for the industrialization of APOLLO3® as it will be presented briefly in next chapters:

- 3x3 FAs cluster
- 52 FAs KAIST 3D core
- PWR full cores:
  - 241 FAs GEN III core
  - 177 FAs TMI core.

Similar analyses exist also for the VVER geometry.

7.2.1. 3x3 pin-by-pin cluster of assemblies test case

This case has been developed in order to test and verify implementation and sensitivity analysis for neutronic and thermic/thermal-hydraulic models and numerical options.

In this cluster a REA may be simulated with a control rod initially inserted in central FA ejected, as in previous test case in 0.1 s, see Figure 57. Nominal initial power is scaled consequently as boundary conditions, too.

Main achievement of this activity is that steady-state and transient calculations may be realized successfully on a cluster of assemblies in pin-by-pin radial configuration.

Preliminary keff values are proposed in Table 33.

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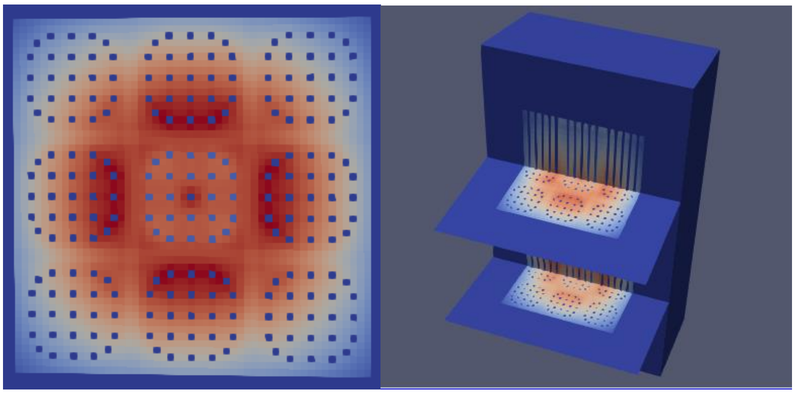

FIGURE 57: PWR 3X3 FA CLUSTER - APOLLO3® PIN-BY-PIN MODELING.

TABLE 33 : KEFF COMPARISONS AMONG APOLLO3®/THEDI IN COARSE MESH, APOLLO3® PBP AND SERPENT FOR THE 32 FA CORE

3x3	Boron 600 ppm
APOLLO3 PbP	Rodded = 1.02343 Unrodded = 1.06465

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7.2.2. The 52 FAs 3D “KAIST” APOLLO3®/THEDI test case

This optional PWR configuration based on the KAIST 1A benchmark [37] is described in D4.3 [2].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 briefly summarized below. For any further detail the reader is encouraged to refer to D4.3 [2] for material isotopic composition. As indicated in D4.3 [2] a transient scenario may be associated to the 3D core version but due to lack of time this step as well as all application at industrial level of Advanced 2D reflector model.

7.2.2.1. Core description

The square unit, fuel and guide tube with absorber pin cells are all described in D4.3 [2]. Geometry and material specifications are shown too for each cell with details on the material isotopic compositions.

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.

Concerning the FAs description there are five (5) types of FAs:

- UOX-1: Homogeneous FA with UO2 (2.0% ^{235}U) Fuel Pins
- UOX-2: Homogeneous FA with UO_2 (3.3% ^{235}U) Fuel Pins
- UOX-2 (BA-16): Heterogeneous FA: 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 with three plutonium content zones: 8.7%, 7.0% and 4.3%
- MOX-1 (BA-8): MOX FA 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.

Before modelling 3D core during accidental transient, the active length needs to be clarified starting from [2] and in [4].

The core loading map is described in Figure 58. Here we could notice that a quarter of the 52 FAs PWR minicore layout 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, see Figure 59 and [2].

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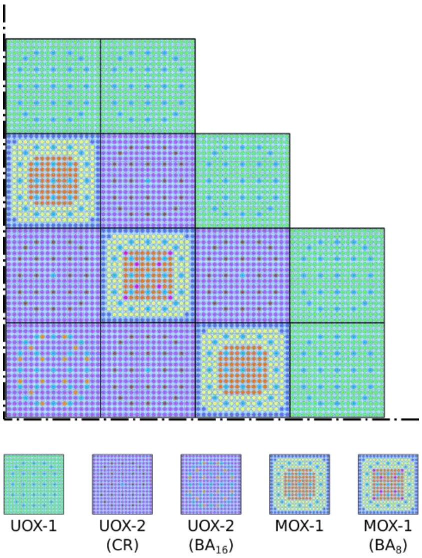

FIGURE 58 52 FAS PWR MINICORE LAYOUT (BASED ON [2])

Concerning the advanced modeling of the radial reflector important progress has been realized in Task 4 of WP4. The implementation of such advanced modeling in WP5 will take further time and is not compatible with the end of the CAMIVVER project and this progress needs to be completed in project follow-up. For the CAMIVVER project WP5 needs, the radial reflector to be retained for the optional 52 FA core calculation needs is in this first approximation the approach proposed for the 32 FAs minicore case. The same is true for the axial reflector that may be consistent with the 32 FAs PWR minicore.

The thermophysical properties as well have been defined in [3].

7.2.2.2. Transient Scenarios

As in the reference cases, the initial condition of a possible transient scenario can be a neutronic-thermal-hydraulics coupled steady-state calculation at nominal conditions, as shown in Table 34. Nominal conditions for the 52 FAs PWR minicore are specified in [3]. Total power is set to 15% of the nominal power of 900 MWth [3].

TABLE 34 HOT FULL POWER (HFP) INITIAL CONDITIONS FOR THE 52 FAS PWR MINICORE [3]

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 59
Boron	Critical Search
Irradiation	Fresh FAs

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The same or similar scenarios as for the reference cases (Section §5) can be used in case this minicore is calculated and more detail are available in [3].

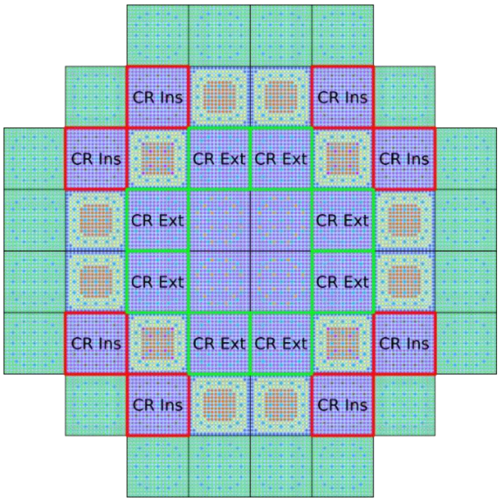

FIGURE 59 NOMINAL CORE CONFIGURATION. INSERTED (INS) AND EXTRACTED (EXT) CRS ARE INDICATED (BASED ON [3])

It has been possible to produce a 3D core deck for APOLLO3®/THEDI modeling the neutron diffusion approximation with a coarse radial discretization in steady state.

This exercise enables first feedback to the WP4 for verifying and improving the MPOs produced for MOX and Gd based fuel assemblies.

In Figure 60 and Figure 61 the APOLLO3® preprocessing of the KAIST core case for core loading and CRs position.

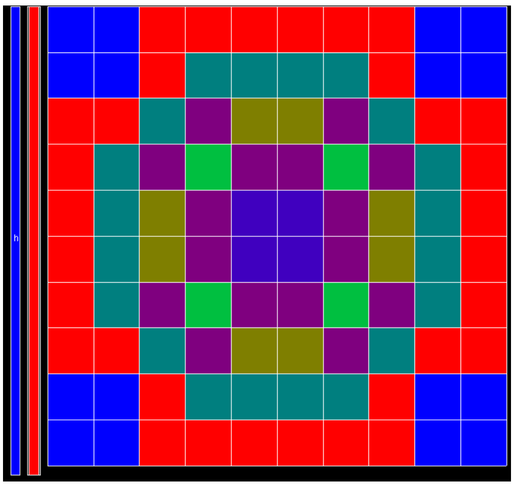	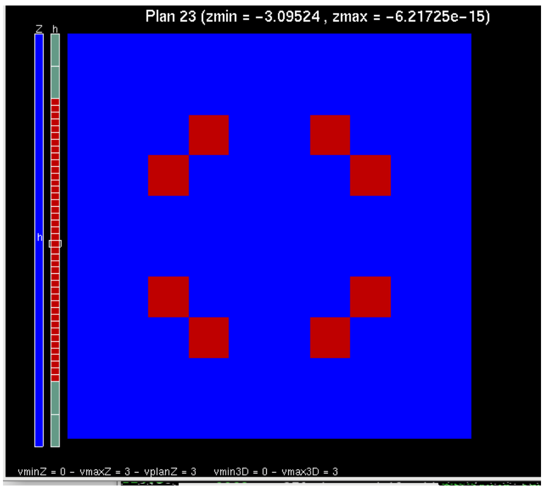
FIGURE 60: KAIST - APOLLO3®/THEDI MODELING.	**FIGURE 61: KAIST - APOLLO3®/THEDI CRS POSITION.**

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7.2.3. Full core PWR simulations with APOLLO3®

This section brings a complementary contribution to state about the industrialization of APOLLO3® and its associated tools with a feasibility analysis of full core PWR modelling.

Two examples have been considered, for which main specifications are available in open literature such as the TMI core [38] and the GEN III core [39].

7.2.3.1. TMI full core PWR modelling

The PWR TMI-1 [40] is often used a reference test case for benchmarking at international level. This core unit is provided with 177 FAs each presented a 15x15 fuel lattice.

The APOLLO3®/THEDI model is presented in Figure 62 Core loading map and CRs location pattern (see Figure 63) is the one described in [38].

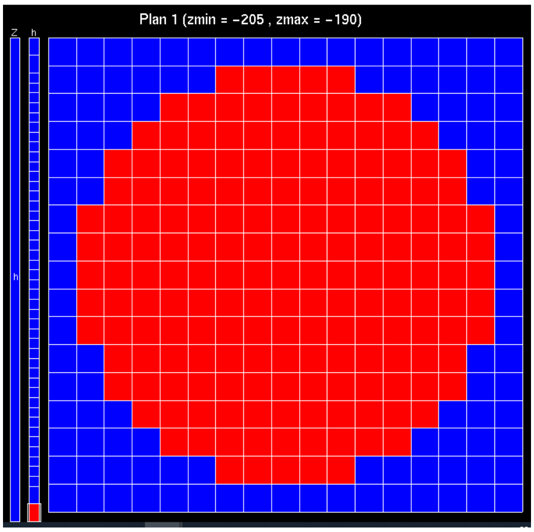

FIGURE 62: PWR TMI - APOLLO3/THEDI MODELING.

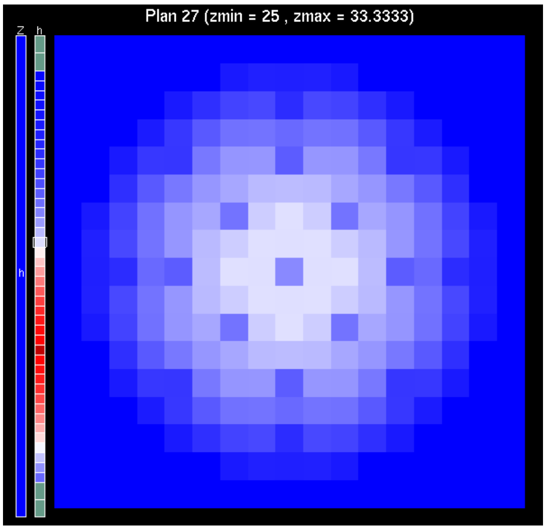

FIGURE 63: PWR TMI - APOLLO3/THEDI MODELING WITH CRS POSITION.

Initial steady-state conditions before transient are described in Table 35. First calculation has succeeded Figure 64 and first keff calculations using the APOLLO3®/THEDI core solver for diffusion approximation and a coarse radiale meshing discretization have been realized.

TABLE 35: 177 TMI CORE INITIAL CONDITION

Primary circuit	177FA	
Pressure	1.55E+01	MPa
Coolant temperature	5.73E+02	K
Coolant flowrate	79214.80466	m3/h
Core power	1.35E+02	MWth
Density	729.5	kg/m3

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Mass flowrate 177 FA	16052.0	kg/s

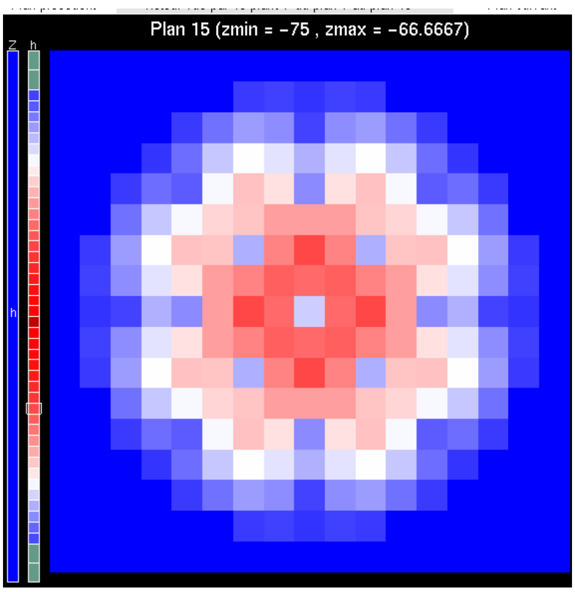

FIGURE 64: PWR TMI - APOLLO3®/THEDI CORE STEADY-STATE CALCUALTION.

7.2.3.2. GEN III full core PWR modelling

Initially provided for the OECD/NEA LWR benchmark [39] a core test case representative of designs for Generation 3 PWR (GEN-III) is considered here in order to provide the APOLLO3®/THEDI of a complex LWR model containing both Uranium Oxide (UOX) and Mixed Oxide (MOX) fuels.

Initial steady-state conditions before transient conditions are described in Table 36.

TABLE 36 : 241 FAS PWR GEN III CORE TEST CASE INITIAL CONDITION

Primary circuit	241 FAs	
Pressure	1.55E+01	MPa
Coolant temperature	5.73E+02	K
Boron	1400	ppm
Tfuel_moy	627	K
Core power	1000E+06	MWth
Density	717.0	kg/m3
Mass flux	3000	kg/m2s

The APOLLO3/THEDI model for the GEN III 241 FAs core is presented in Figure 65. Core steady-state heterogeneous power calculation is shown in Figure 66.

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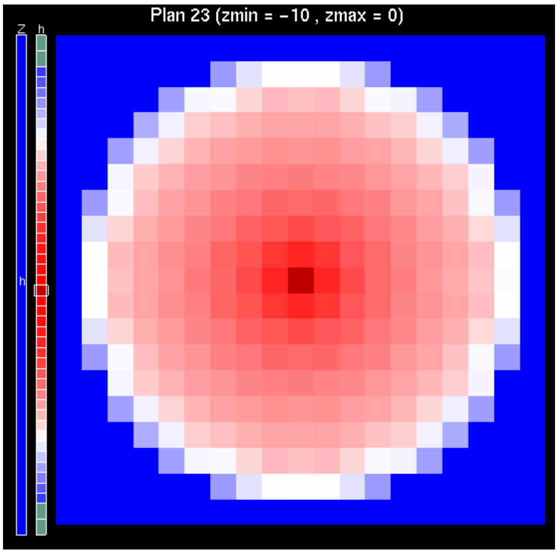	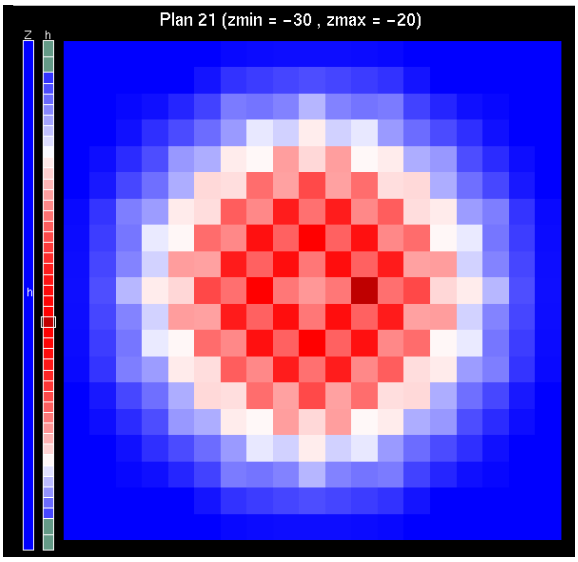
FIGURE 65: PWR GEN III - APOLLO3®/THEDI MODELING.	**FIGURE 66: PWR GEN III - APOLLO3®/THEDI 2D CORE POWER MAP.**

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7.3. VVER oriented complementary analyses

As already mentioned, the WP5 contains three main tasks, as established in the project proposal [1] specially conceived to support multiphysics core calculations.

Task 5.2, in agreement with associated chapters in D5.1 [3] and its consolidated version in D52 [4], consists in supporting the VVER reduced size core reference test cases definition and their modeling following the corresponding initial and boundary conditions.

In Task 5.2 for evaluating the aforementioned transient scenarios with VVER [5] geometries with coupled neutronics and closed channel thermal-hydraulics tools (APOLLO3®, SERPENT2/SCF, PARCS/TRACE).

Special attention has been devoted to support WP4 in succeed the target of being able to provide lattice calculation and MPOs dedicated to VVER reactors.

In CAMIVVER project WP5 it was decided to mainly focus on comparison among scientific tools starting from a small core test case.

In this section a summary of complementary tests and feasibility analysis performed applying APOLLO3® core code to VVER:

- Small core at different sizes: 19, 37 FAs VVER core,
- VVER 1000 full core: the X2 VVER benchmark core [43].

7.3.1. The 19 and 37 FAs VVER core test case

In the present section intermediate size cores 19 Figure 67 and 37 Figure 68 modeling with APOLLO3/THEDI is provided.

The same core may also be model with the coupling APOLLO3®/CATHARE3.

Major achievement is related to the versatile application of APOLLO3® based core tools and the POC APOLLO3®/CATHARE3 coupling.

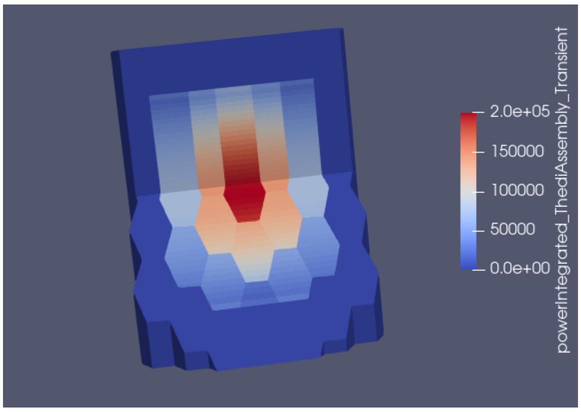

FIGURE 67: VVER 19 FAS CORE MODEL

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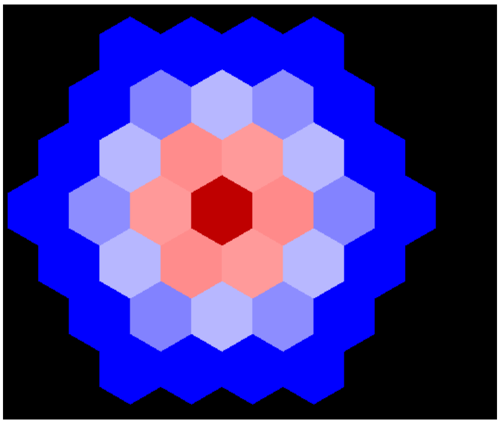

FIGURE 68: VVER 37 FAS CORE MODEL

7.3.2.The X2 VVER core benchmark

The publicly available data for such validation, particularly for VVER-1000 reactors, is very limited. The OECD NEA benchmarks Kalinin-3 (Tereshonok et al., 2009) and Kozloduy-6 (Ivanov et al., 2006) describe VVER-1000 operational transients, but their specifications missing of fuel geometry and materials definitions and fuel cycle operational data, providing libraries of homogenized fuel properties instead. During the 19th and 20th AER Symposium (‘‘AER,’’ 2019) in 2009 and 2010, a new VVER-1000 core benchmark was proposed (Lötsch et al., 2009, 2010). The benchmark was based on the VVER-1000 operational data of the second unit of the Khmelnitsky Nuclear Power Plant (NPP) located in Ukraine. The unit was put in operation in 2004 and was one of first VVER-1000 unit fully loaded with fresh TVSA fuel type. The benchmark was called ‘‘X2’’ where ‘‘X’’ stands for ‘‘Kh’’ in Ukrainian transcription and ‘‘2’’ stands for the unit number. All information available here comes from reference [43]. On this basis the APOLLO3® core model has been realized as shown in Figure 69 .

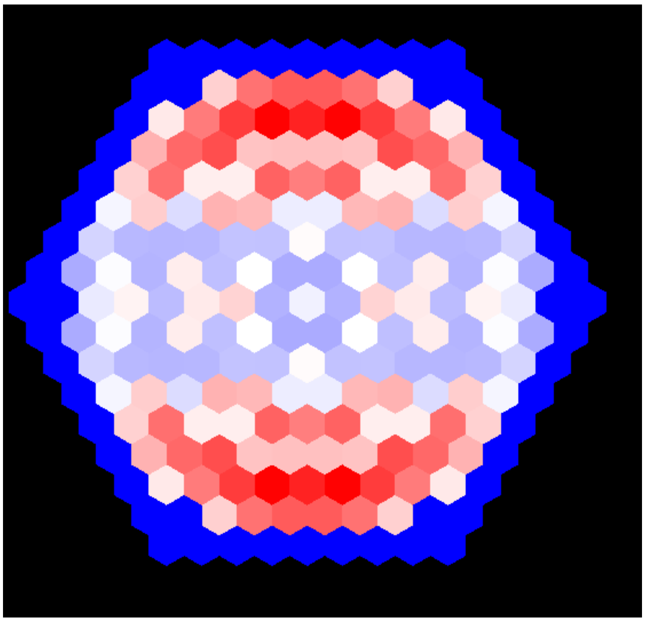

FIGURE 69: X2 VVER-1000 APOLLO3® CORE MODEL [43]

```
#input for sensitivities
MPO = True
NFUELASS = 163
Puissa_Watt = 3000e6
BORE_ppm = 1208. #sensi: 0 , 600, 800, 1000, 1140, 1200
CR_H_Top = 0.# 130. #355.  #355. #51. #46. # to be fixed!
MassFlux = 4224.31 #sensi mass flux : 10000 # 4224.31 #6382.31#
tot_times = 0.2#2.0#0.2
Ejt_time_CR = 1e-1 #0.8e-1 #
Twater_Inlet_K = 560.15
Twater_moy_C = 387.0 #
Water_densi = 0.725 # 0.730
Tfuel_moy = 740620
Keff = 0.99290
```

8. Conclusions

This document constitues the deliverable D5.4 of the CAMIVVER project.

It is mainly dedicated to present APOLLO3® core solver based solutions and tools gather during these years to perform calculations and benchmarks with both APOLLO3®/THEDI and the POC APOLLO3®/CATHARE3 advanced multiphysics coupling on a small and full cores for both PWR and VVER configurations.

The C3PO coupling engine, associated to ICoCo norm, has been used for the APOLLO3®/CATHARE3 3D multiphysic coupling and a first simulation of a reactivity insertion transient on a small 32 FAs core has been performed.

All comparisons with SERPENT2 stand-alone and with SERPENT2 coupled with SCF (KIT) [10] show a generally good agreement. Some discrepancies have been underlined and further improvements axes have been identified and they will be addressed in the follow-up of the project.

Mainly these first results confirmed the successful developpement of a first prototype of advanced 3D multiphysic coupling managed under GitLab and released on the CRONOS HPC cluster for Framatome as detailed in the present report.

8.1. Perspectives

APOLLO3® core code needs to be extensively tested and used by experimented users with industrial vision to improve its deployment up to a final industrial level. Nevertheless, main functionalities are already available, compatible with both Cartesian and hexagonal fuel assembly geometries.

A users friendly interface (IHM) is still missing and important work has to be done in order to automatize preprocessing and post-processing asking for improvements in input and output options.

The 3D coupling between APOLLO3®/CATHARE3 includes some functionalities but needs further development to include expected improvements in input and output options, but also in its industrialization level as well as the APOLLO3®/ core one.

The scenarios proposed here started and facilitate discussions among partners and ease the verification process, but those efforts need to be continued further on in the project follow up.

Fuel assemblies geometry and multi-parametric data libraries MPOs have been an input option from WP4 and WP5 provided feedbacks to WP4 developers. Such interaction is vital for succeeding benchmarks.

Among all other improvement, the coupling will have to take into account evolutions of singular codes version (e.g. APOLLO3®, THEDI, CATHARE3, C3PO, ICoCo).

During last project years, 2022 and 2023, first comparison with MonteCarlo codes and results from partners were expected in steady-state, possibly evolution and transient conditions. This object purpose was globally attained.

An improvement of accident procedures is for these purposes expected too.

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Appendix 1 – MPOs tests during the project

The multi-parametric cross section libraries have been generated by using APOLLO3® encapsulated in the NEMESI prototype [7] that has been developed as part of the CAMIVVER project. The scheme adopted is based on the Method of Characteristics, MOC, and TDT-solver for flux resolution over a refined 2D assembly geometry.

The last year of the project has been passed to test and to propose feedbacks to the tentative MPOs newly generated by NEMESI for PWR and VVER cases. The feedbacks provided with core applications were useful in supporting WP4 activities on NEMESI development and verification process. Several tests of MPOs have been generated and tested as well as several iterations have been needed since 2021 testing also APOLLO3® releases from V2.0.1 up to V2.3dev currently used as indicated in Figure 70.

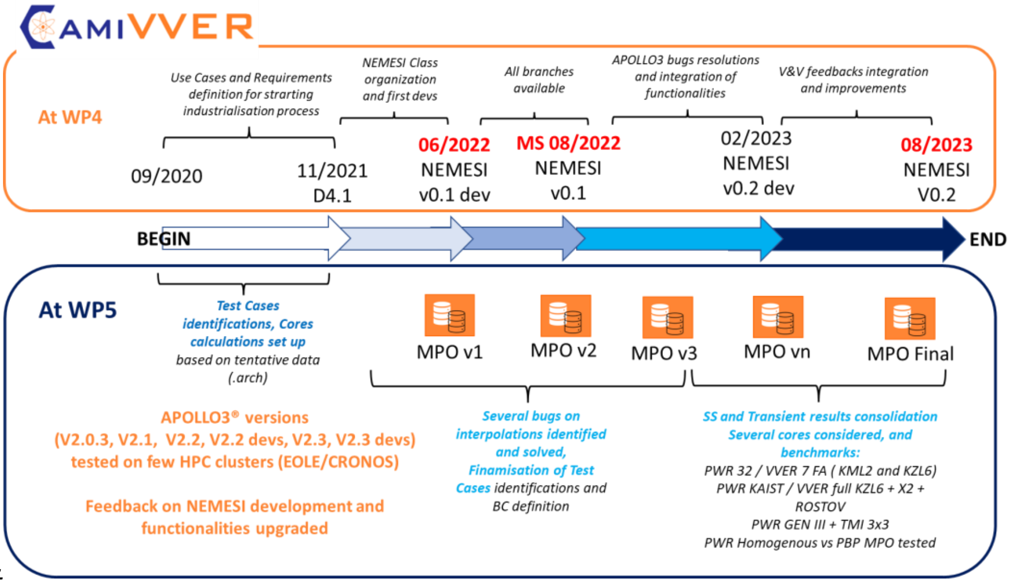

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FIGURE 70: NEMESI EVOLUTION AND TESTING MPOS AT CORE LEVEL

Appendix 2 – Improved reflectors modeling

In order to improve the model used for reflectors in preparation to the follow up project, several activities have been carried out at Framatome using the tools and the approaches implemented in CAMIVVER WP4 and WP5.

Two internships' projects have been started with the aim to automatize the creation of geometries for lattice calculations based on ALAMOS tool that may be used for reference studies and for producing cross-sections for core analysis:

- The first one is dedicated to the development of a Python based library for the generation of PWR Cartesian unstructured FA geometries with ALAMOS tools to be inserted in NEMESI environment (work done by Mathieu Robin in collaboration with Université de Grenoble – PHELMA - France).
- The second one is dedicated to the development of a Python based library for the generation of PWR and VVER unstructured reflectors geometries with ALAMOS tool as first step for preparing improved reflectors cross-sections to be used at core level and feeding reference 2D calculations (work done by Fabio Inzirillo in collaboration with Politecnico di Milano - Italy and Polytechnique Montreal - Canada).

In this appendix, few elements concerning this second work are presented knowing that more details will be made available in other project deliverables.

The choice on the development of a Python based library for the generation of VVER unstructured reflectors geometries has been carried out by taking into account since the beginning the needs to be applied to different reactors size and different reflector types (water and heavy reflectors included). So, several generic classes have been considered and organized as indicated for instance in example shown Figure 71.

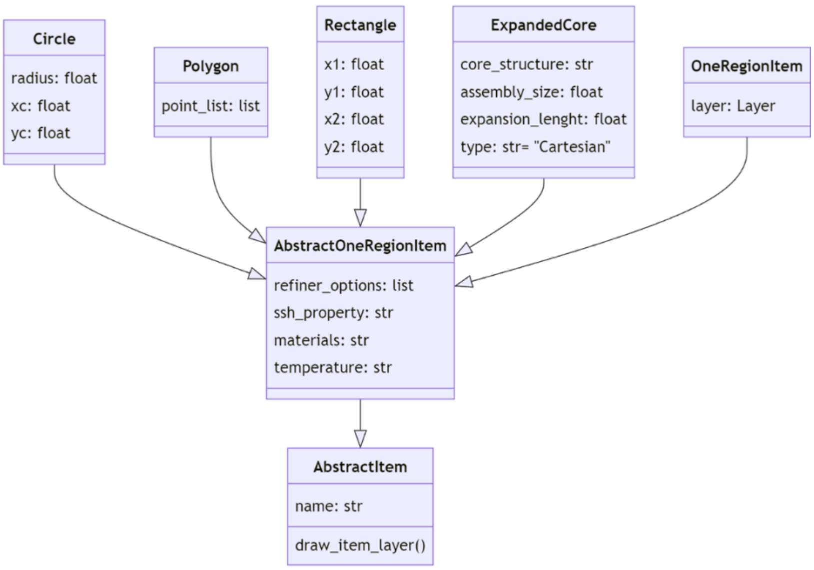

FIGURE 71: EXAMPLE CLASSES ORGANIZATION (INTERNSHIP ON REFLECTORS - ONGOING)

This Python library will allow to automatize the generation of the reflector geometry for any type of reactor and make sensibility on the meshing structure.

Examples of the application to the KAIST-like reactor described in ref. [2] and VVER KML2 configurations are shown in Figure 72 and Figure 73 respectively.

In order to create a full core model, the two Python libraries have been combined and first application to the KAIST-like core performed. The work on FA hexagonal library is ongoing.

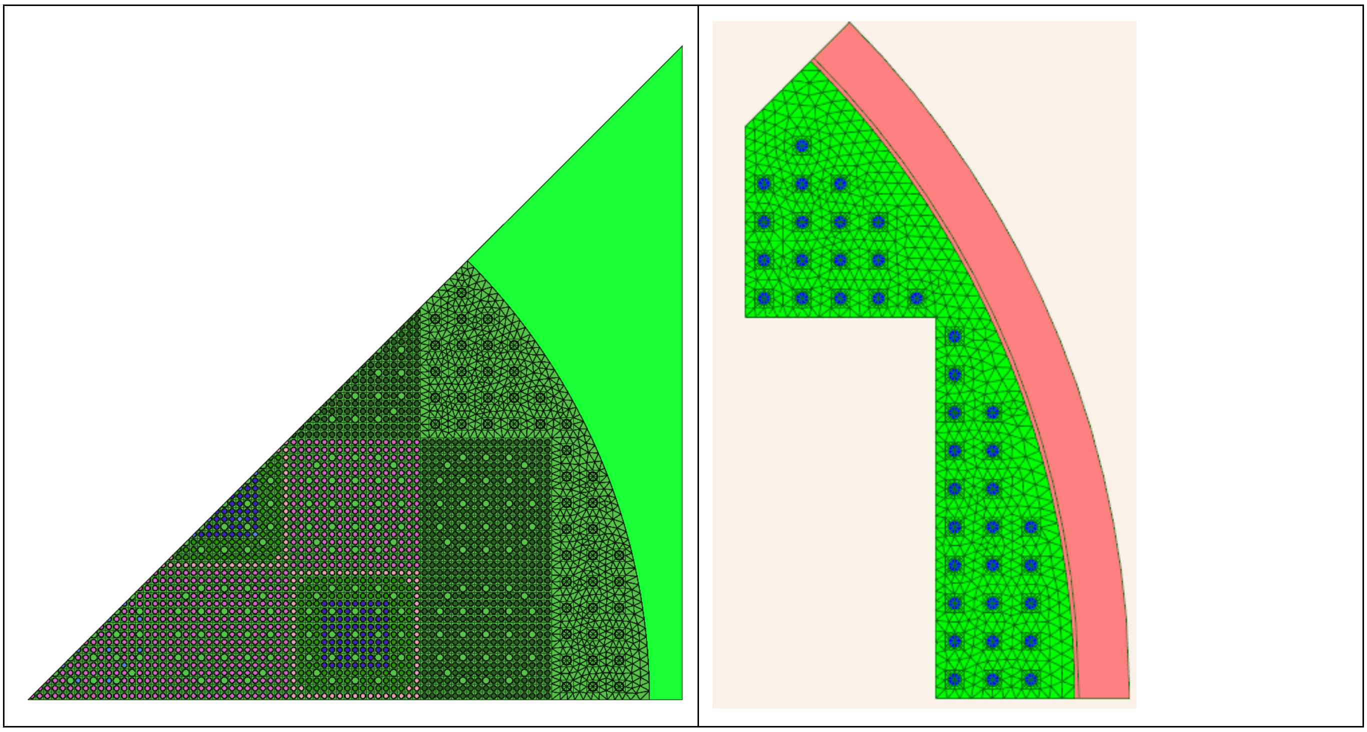

FIGURE 72: EXAMPLE KAIST-LIKE REFLECTOR GENERATED WITH PYTHON LIBRARY – ONGOING

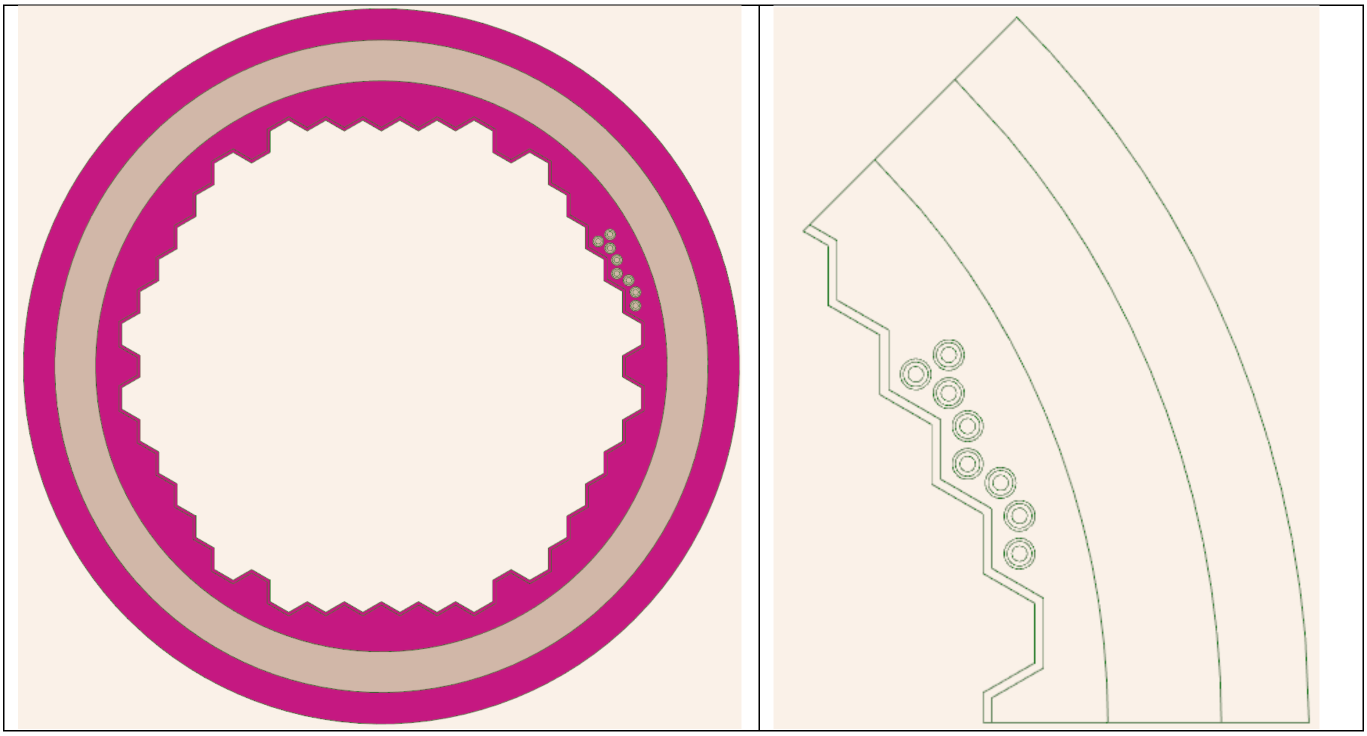

FIGURE 73: EXAMPLE KML2 REFLECTOR GENERATED WITH PYTHON LIBRARY - ONGOING

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