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REVIEW ARTICLE

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Codes and methods improvements for safety assessment and LTO: varied approaches

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Abstract. Nuclear safety has always been at the heart of the concerns of nuclear power plant operators and developers, as well as of various nuclear research organizations and regulatory authorities. Over the last decades, all these nuclear actors have developed and integrated a large number of calculation codes and other tools into their safety work. From the system approach to the local understanding of a phenomenon on a given component, from neutronics to operation optimization for long-term operation, these methods and codes have been constantly evolving since their appearance, in order to be able to integrate new plant designs and components, to improve the results of modeling physical phenomena or quantify and thus reduce the uncertainties on these results. Currently, several H2020 Euratom projects are working on the improvement of these codes and methods. This article will focus on three of these projects: CAMIVVER (Codes And Methods Improvements for VVER comprehensive safety assessment), APAL (Advanced PTS Analysis for LTO), and sCO2-4-NPP (innovative SCO2-based heat removal technology for an increased level of safety of Nuclear Power Plants) in order to illustrate our thinking on the improvement of calculation frameworks. First, we will present the work and the approach adopted with regard to the different calculation codes and methods used in each of these three projects. We will then conclude with an overall analysis of these three approaches, highlighting the difficulties and successes of these three projects, and identifying areas of work for the general improvement of the calculation codes.

1 Introduction

Nuclear safety has always been at the heart of the concerns of nuclear power plant operators and developers, as well as of various nuclear research organizations and regulatory authorities.

Over the last decades, all these nuclear actors have developed and integrated a large number of calculation codes and other tools into their safety work.

Currently, several H2020 Euratom projects are working on the improvement of these codes and methods. Our article will focus on three of these projects: CAMIVVER (Codes And Methods Improvements for VVER comprehensive safety assessment), APAL (Advanced PTS Analysis for LTO), and sCO2-4-NPP (innovative SCO2-based heat removal technology for an increased level of safety of Nuclear Power Plants) in order to illustrate our thinking on the improvement of calculation frameworks.

2 Euratom Projects presentation

2.1 The APAL project

The reactor pressure vessel (RPV) is a key component of a nuclear power plant (NPP), and its integrity must be ensured throughout its entire operating lifetime including long-term operation (LTO) in accordance with applicable regulations.

The dominant degradation mechanism of the RPV material is embrittlement due to neutron irradiation, especially in the core (beltline) area. If a flaw of critical size existed in an embrittled RPV and if a certain severe system transient occurred, the flaw could propagate very rapidly through the vessel, possibly resulting in a through-wall crack, which challenges the integrity of the RPV.

The pressurized thermal shock (PTS) analysis is one part of an RPV structural integrity assessment. PTS is characterized by rapid cooling (i.e., thermal shock) of the reactor downcomer and internal RPV surface, followed sometimes by re-pressurization of the RPV. Thus, the PTS event poses a potentially significant challenge to the structural integrity of RPV in pressurized-water reactors

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(PWRs) and water-cooled water-moderated energy reactors (WWERs).

Currently, in the European Union, PTS analyses are based on deterministic assessments and conservative boundary conditions. The PTS analyses of this type are reaching their limits in demonstrating the safety of PWRs and WWERs facing LTO, and they need to be enhanced. However, inherent safety margins exist, and several LTO improvements applicable to the NPP, as well as advanced methods of PTS analyses, may be able to increase these safety margins. Additionally, the quantification of the safety margins in terms of risk of RPV failure by advanced probabilistic assessments becomes more and more important because the probabilistic methods ensure more comprehensive assessments in PTS analysis, and they enable the quantification of uncertainties in the results.

To address this challenge, the project Advanced PTS Analysis for LTO (APAL) has been launched in October 2020 with a duration of four years. The main objectives of the APAL project are the development of advanced probabilistic PTS assessment methods, the quantification of safety margins for LTO improvements, and the development of best-practice guidance. The project will address multidisciplinary and multi-physics challenges related to the RPV safety assessment of PTS. The planned work to achieve these objectives is divided into six technical work packages (WPs), presented in Figure 1.

The first work package (WP1) consists of an extensive literature review and collection of partners' experiences to identify the state of art of LTO improvements that may have an impact on the results of PTS analysis.

After establishing the LTO improvements, thermal-hydraulic (TH) calculations are performed, including uncertainty quantification relevant to the PTS assessment (WP2). The impact of both LTO improvements and human factors on the results of TH analysis will be quantified and later assessed by subsequent structural mechanics and fracture-mechanics benchmarks within WP3 and WP4.

The third work package (WP3) consists of performing deterministic structural and fracture-mechanics analyses to quantify the safety margins related to both LTO improvements and uncertainties in TH analyses. The analyses to be used for deterministic margin assessments by the APAL partners will first be tested on a common deterministic benchmark.

In the fourth work package (WP4), probabilistic margin assessments based on probabilistic fracture-mechanics analyses will be performed. They will enable the quantification of safety margins in terms of the risk of RPV failure. An appropriate benchmark for the probabilistic fracture-mechanics analysis will be defined in accordance with the benchmark performed for deterministic margin assessment.

In the fifth work package (WP5), recommendations and conclusions will be gathered from the work to define the best practices for advanced PTS analysis for LTO. Close cooperation with APAL Advisory Board (AB), regulatory bodies, and end users (NPP owners, suppliers, etc.) during the project will help to increase the acceptance of the best-practice guidance. For that purpose, several workshops will be organized (WP6) to discuss the best-practice guidance with regulatory bodies and the end users in order to analyze potential barriers, integrate feedback, and obtain broad acceptance of the best-practice guidance for an advanced PTS analysis for LTO within the nuclear community.

"Fracture mechanics"

2.2 The CAMIVVER project

The European nuclear fleet is composed of Gen. II and Gen. III reactor types. This fleet is currently going through LTO upgrades and it remains an important challenge for the European Community. As several VVER reactor units are planned for construction – or are currently under construction. It's realistic to think that VVER-type reactors will keep playing a strategic role in the European energy and economic stability, its decarbonation strategy, and Europe's safety in general. In this framework, the Euratom Supply Agency underlines as a matter of concern the 100% reliance on a single Russian supplier and therefore an issue for all EU countries operating VVER reactors [1]. Dependence on a single supplier constitutes a significant risk and qualifying an alternative supplier could take several years because of licensing and testing requirements.

In order to support the development and the qualification of fuel and more generally to provide the required elements for the safety analysis report (SAR), an important place is reserved for the development, improvement, verification, and validation of computer codes and methods used in the VVER safety analysis. The codes and methods continuous update needed for answering the regulatory requirements for reactors LTO is the basis of CAMIVVER (started in September 2020), for the improvement of codes and methods for VVER comprehensive safety assessment in support of other activities, carried out concerning VVER fuel development and qualification. CAMIVVER is oriented to the VVER-1000 reactor type.

The CAMIVVER project activities (Fig. 2) have been built to reach four main objectives:

- the improvement of scientific computer codes, models, and methods to be used at an industrial level for the comprehensive safety assessment of Generation II and III reactors.
- The promotion of 3D neutronics-thermalhydraulics coupled calculations to improve the safety assessment by a better representation of the physical phenomena (e.g., accidental transient characterized by strong heterogeneities in power or coolant fields), an important aspect for the LTO upgrade when considering the evolution of margins with respect to safety criteria.
- The promotion of the use of advanced mathematical methods (metamodels, deterministic sampling, etc.) for the assessment of uncertainty propagation within numerical simulations.
- The integration of the VVER context (VVER-1000), slightly different from western PWR but with some common features, challenges the robustness of codes and methods and their validation strategy.

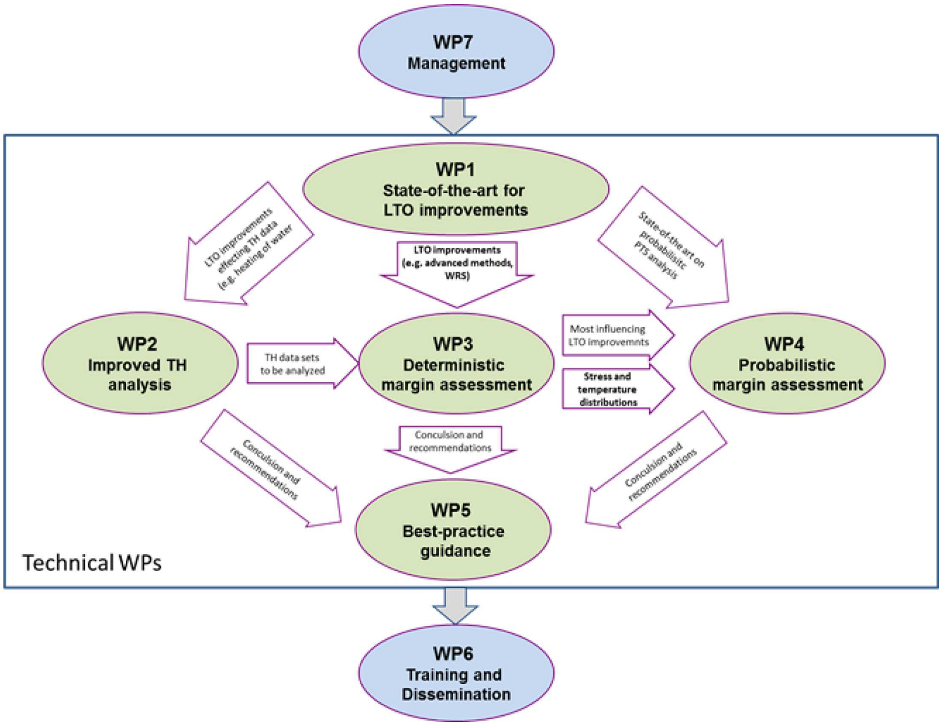

Fig. 1. APAL Project structure.

The project is organized into 7 Work Packages (WP2–WP8). Each WP is dedicated to a specific part of the safety assessment calculation chain, except WP2 dedicated to Project Management, WP3 dedicated to VVER data collection and WP8 dedicated to Communication, Dissemination, Educational, and Training activities. This structure has been chosen following the type of codes used in each technical WP (lattice codes in WP4, core neutronics, and thermal-hydraulics codes in WP5, CFD codes in WP6, and systems codes in WP7), the skills to be involved, and the dependency between the different actions. WP8 is dedicated to communication, dissemination, and education. This structure allows maintaining an overall consistency through the technical links existing between each WP, as indicated in Figure 2 while keeping separate the implementation of work programs and therefore limiting the risk of strong dependencies that may result in planning fulfillment delay.

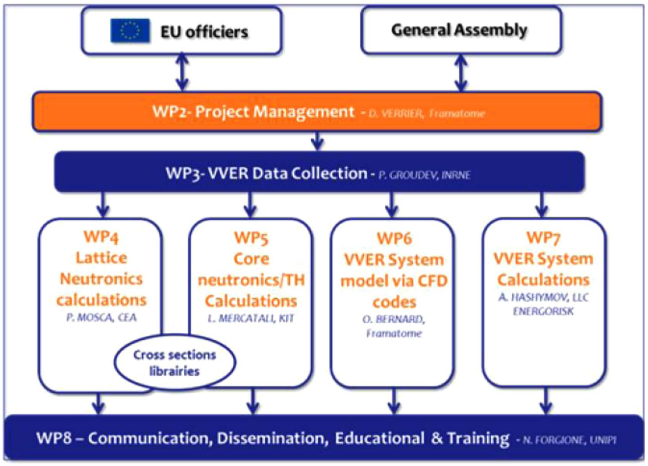

Fig. 2. CAMIVVER Project structure.

2.3 The sCO2-4-NPP project

The Fukushima Daiichi nuclear accident demonstrated the vulnerability of NPP to the loss of electrical power and the loss of the ultimate heat sink (UHS) events. Among the lessons learned to overcome the above-mentioned vulnerability was the need for safer and more reliable fuel heat removal solutions. Safety standards have hence been improved at an international level requiring the development of new technologies for improving the safety of both existing and future nuclear reactors.

New innovative heat removal technologies are currently being developed for different types of energy production sources (nuclear, solar, fossil, etc.). Among these, technologies based on the use of supercritical CO_2 (sCO_2) can significantly increase the level of safety in the case of accidents, since sCO_2 is non-flammable and non-toxic and, when attached to an NPP as a backup cooling system, delays the need for human intervention. In addition, it can potentially lower the costs of energy production and subsequent recovery of the reactor thanks to the compact size of the equipment. The compact size and high energy density of the system also mean an overall smaller plant footprint.

The former Horizon 2020 project sCO_2-HeRo developed and proved the concept of a heat removal backup

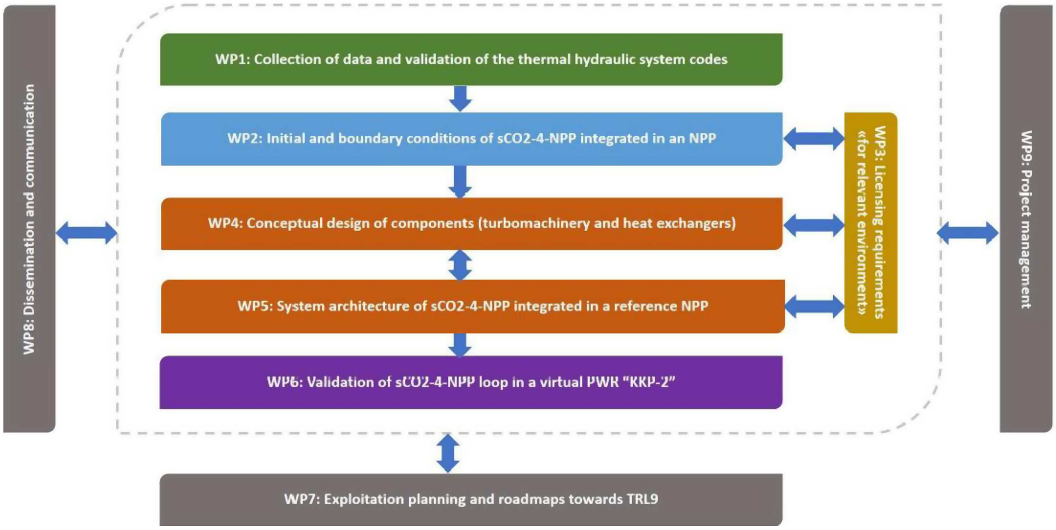

Fig. 3. sCO2-4-NPP Project structure.

technology based on sCO_2 making it an excellent backup cooling system for the reactor core in the case of a station blackout (SBO) and loss of UHS. The concept consists of several modular sCO_2-systems, attached to the existing heat removal system, to remove decay heat from the reactor.

By bringing this technology closer to market, sCO2-4-NPP (started in September 2019, for 3 years) offers a new solution to the various NPP operators that will improve plant safety in the case of an accident with minimal impact on existing reactors. The sCO2-4-NPP solution can potentially also lead to improvements in energy efficiency in other energy and industrial sectors.

The project is organized into seven technical work packages as shown in Figure 3. WP1 carried out the experiments at the 200 kW sCO2-HeRo cycle attached to the glass model in Essen, Germany, in order to obtain initial data on the performance of the sCO2-based system, as well as to validate the simulation models in the ATHLET and CATHARE codes. This WP finished in June 2020.

The output of this WP fed WP2 to specify the initial and boundary conditions of the sCO2-4-NPP modular system integrated into a real NPP. The results from WP2 (finished in June 2021) allowed the improvement of the design of components and their necessary adaptations to the nuclear environment in WP4.

The optimized design specifications from WP4 were integrated into WP5 for updated technical specifications of the components of the system. Prior to this, WP5 delivered the system's overall architecture when integrated into a reference NPP. With the system architecture and the improved component specification, the models in ATHLET, ATHLET/Dymola, and CATHARE were updated and simulation of sCO2-4-NPP modules integrated into a real NPP will be carried out.

The Dymola results will be used to build the real-time simulator of the sCO2 heat removal system for coupling to the existing KONVOI simulator. WP6's objective is to validate the sCO2-4-NPP system in the virtual KONVOI NPP.

In parallel with WPs 2–5, WP3 will document regulatory requirements and provide input to those WPs regarding the specific requirements to be considered in the design of components and the system as a whole.

Similarly, in parallel to the work in WP1–WP6, WP7 will develop the technological, regulatory, financial, and organizational roadmaps for reaching TRL9.

3 Numerical codes and related work

3.1 Numerical codes used in APAL

3.1.1 Codes and methods descriptions

Several codes and software are used in APAL, in order to reach the objectives of the project. These tools can be categorized following the different approaches studied in the PTS analyses. The PTS analyses are performed using various types of sophisticated software. The full PTS analysis consists of three specific consecutive analyses.

- *System thermal-hydraulic analysis*

It's the analysis of the behavior of the whole NPP system (primary and secondary circuits, emergency core-cooling systems, auxiliary systems, etc.) from the thermal-hydraulic point of view. The resulting parameters include, among others, temperatures, pressures, flow rates, velocities, and heat transfer coefficients in all modeled components and piping. The goal of the system thermal-hydraulic calculations is, in addition to the coolant pressure calculation, to give the initial and boundary conditions for thermal-hydraulic mixing calculations. In some cases, the system thermal-hydraulic calculations directly provide the boundary conditions for structural analyses.

For this analysis, APAL partners use RELAP5, ATHLET, and TRACE software.

- *Mixing thermal-hydraulic analysis*

It's the detailed analysis of coolant mixing inside the reactor, namely in the reactor downcomer. The resulting parameters include detailed distributions of coolant temperature in the reactor downcomer and/or detailed distributions of both inner surface RPV wall temperature and heat transfer coefficients at the RPV inner surface. There are two types of TH mixing codes – (1) codes based either on engineering models or regional mixing models, and (2) codes based on Computational Fluid Dynamics (CFD). The goal of the thermal-hydraulic mixing codes is to give the boundary conditions for structural analyses.

The thermal-hydraulic codes used for this analysis are GRS-MIX, KWU-MIX (regional mixing codes), and FLUENT (CFD code). There is no development of both system and mixing TH codes expected within APAL. Some still existing TH models were adjusted or transferred to other TH codes for application within APAL.

- *Structural and fracture mechanics analyses*

The structural and fracture-mechanics analyses can be performed using either a deterministic or a probabilistic approach. The software tools for both approaches significantly differ.

– Deterministic approach

For structural analysis, commercial "general" finite-element method (FEM) software tools are used. Among many capabilities of general FEM codes, the solutions of heat-transfer problems and mechanical problems (either linear-elastic or elastic-plastic) are used for PTS analysis. The results from thermal-hydraulic mixing analyses (see above) serve as boundary conditions for solving the heat-transfer problem with the FEM code. Results of the heat-transfer problem solution (time-dependent temperature field in the RPV wall) serve as the load for the mechanical problem together with the load due to pressure (which is the result of system TH analyses under point 1). The mechanical problem is usually solved by the same software and on the same FEM mesh as the heat-transfer problem. The results of the mechanical problem solution are time-dependent displacements, strains, and stresses in the RPV wall (calculated in all nodes of the FEM mesh).

The fracture-mechanics analysis is generally performed in two different methods.

The first method is based on the formulae from standards, which allow for calculating fracture-mechanics parameters (namely stress intensity factor, K_{I}) based on stresses exported from the FEM model. In this method, the FEM model of the RPV does not contain any cracks. These fracture-mechanics calculations are usually performed by in-house auxiliary software, together with the final assessment of RPV integrity (comparison of stress intensity factor with its allowable value, establishing the maximum allowable transition temperature, preparing the resulting graphs and tables, etc.).

The second method of performing the fracture-mechanics analysis is based on the FEM model of the RPV with the assessed crack included in the FEM mesh. Fracture-mechanics parameters (J-integral or energy release rate, G) are calculated directly in the post-processor of the commercial FEM software. All major commercial FEM software has this capability. Some in-house auxiliary codes (or EXCEL spreadsheets) are used only for the final assessment of RPV integrity.

In APAL, the codes used for this deterministic approach are ABAQUS, ANSYS, SYSTUS, etc.

There is no development of commercial FEM codes expected within APAL. New FEM models will be created by all partners for application within APAL.

– Probabilistic approach

The probabilistic approach differs from the deterministic one by taking into account the randomness and uncertainties of input data and calculating probabilities of crack initiation or RPV failure. Because commercial software is not suitable for this type of analysis, a specific software especially for the fracture-mechanics assessment, frequently created in-house, is used. Sometimes commercial FEM software can be used as a pre-processor for structural analysis (calculation of temperature and stress fields). In other cases, the specific or in-house software has its own pre-processor for this purpose. The structural assessment is usually based on a deterministic approach and treatment of uncertainties on temperature and stresses requires additional investigations. The main task of the probabilistic software for fracture-mechanics analysis is sampling some of the input data, which are treated as statistically distributed, and to calculate the conditional probability of crack initiation or RPV failure. Usually, a Monte Carlo method or FORM/SORM method (First Order Reliability Method/Second Order Reliability Method) is used for this purpose.

Most APAL partners plan to use the FAVOR code (developed by Oak Ridge National Laboratory for the United States Nuclear Regulatory Commission (USNRC) and available upon request to the USNRC). PROVER, SIF-Master, ISAAC, PASCAL, PROST, and other in-house codes will be used by other APAL partners. Significant modifications of almost all used probabilistic codes are expected within APAL, as some formulae or data prescribed for APAL benchmarks are different from those used in probabilistic PTS analyses performed routinely by APAL partners.

3.2 Numerical codes used in CAMIVVER

3.2.1 The ambition

CAMIVVER's ambition for reaching its objectives is to push new generation codes and methods towards an industrial use for VVER and PWR safety assessments. The selected new generation codes, namely APOLLO3® [2] and CATHARE3 [3], are still under development at the laboratory level. Their industrialization process is ongoing and CAMIVVER is directly contributing to this effort. This laboratory-to-industry process is illustrated in Figure 4. The CAMIVVER project is identified as one

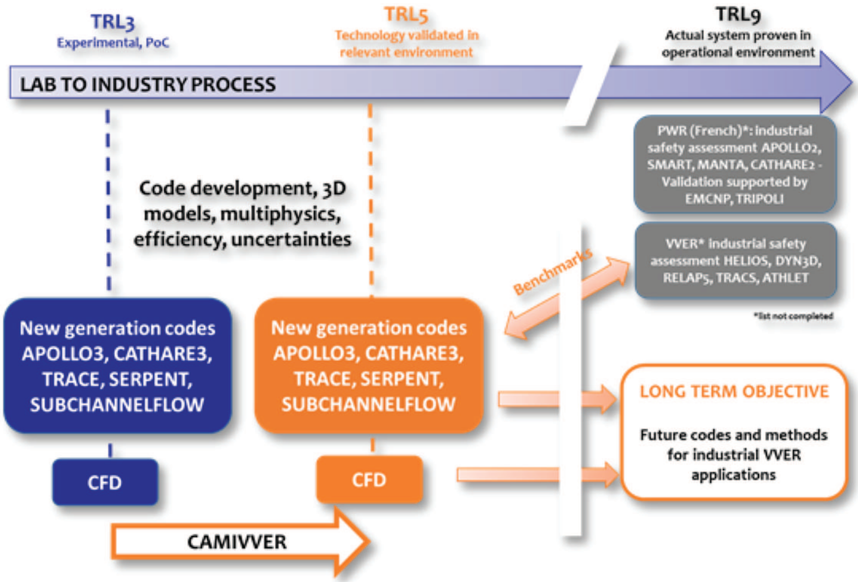

Fig. 4. Codes development within CAMIVVER.

step in that process. Post-CAMIVVER steps could be considered in the frame of the next EU R&D programs.

To achieve that significant progress, CAMIVVER relies on:

- performing code development of a neutrons library generator prototype based on APOLLO3® code and of a proof of concept of an innovative coupling based on APOLLO3®/CATHARE3 codes.
- Benchmarking those new generation codes against codes currently used for VVER and PWR safety assessment and high-fidelity calculations based on Monte Carlo codes (TRIPOLI-4 and SERPENT, [4–6], coupled with subchannel codes (SUBCHANNELFLOW) for steady state and transient calculations.
- Performing methods development based on 3D modeling to improve system thermal-hydraulics modeling of the VVER plant, especially by challenging the robustness and validation of CATHARE3 against reference RELAP5 and TRACE models.
- Performing methods development based on 3D modeling and uncertainty propagation in CFD analyses, using partners codes (STARCCM+, CFX, FLUENT, TRIO-CFD).

Both APOLLO3® and CATHARE3 bring potential advantages and improvements to the safety analysis studies with respect to the codes currently used in France. The developments of these codes have been initiated several years ago and are achieved outside the CAMIVVER framework. Within the CAMIVVER scope, essential adaptations of APOLLO3® required for VVER applications are implemented in WP4, focusing on the industrialization of the lattice part, and in WP5, by coupling neutronics with thermal-hydraulics models. In that respect, CAMIVVER will include a demonstration of the feasibility of the APOLLO3®/CATHARE3 coupling.

CATHARE3 development and validation are also involved regarding VVER plant system thermal-hydraulics. Within CAMIVVER that code is benchmarked with updated RELAP5 and TRACE codes on some selected transients: MCP (main circulation pipeline) start-up, LOCA (loss-of-coolant accident), and MSLB (main streamline break).

CFD modeling of VVER is addressed in WP6 of CAMIVVER especially as regards mixing phenomena in the primary vessel. Specific works within CAMIVVER are consisting of calculations based on the Kozloduy-6 mixing experiment [7]: CFD models development and upgrades by contributing partners, benchmarking results of CFD analyses and performing uncertainty propagation analyses by using the Deterministic Sampling method [7]. The ambition is clearly to improve the validation files.

3.2.2 The progress

Half the way of CAMIVVER has just been crossed recently. It is worth noticing that the project is proceeding normally despite the pandemic. Detailed information can be found in project deliverables, the majority of them being public and available on the project website (`www.camivver-h2020.eu`).

The first technical activities consisted in collecting all necessary reference data to be used by project partners. Those essential tasks have been conducted within WP3 and have been achieved since the summer of 2021.

In WP4, the activities are dedicated to setting up the framework (first steps) for the industrialization of a computing platform capable of performing lattice neutronic analysis and generating multi-parameter neutron data libraries based on the new lattice code APOLLO3®, up to now developed mostly as a research computational tool. Two important tasks have been completed in 2021 in relation to the multi-parameter library generator: the definitions of test cases for the verification phases, and the definition of representative use cases and specification requirements. Work is now progressing with the aim to have the first version of the library generator this summer and perform the validation steps against an existing validated generator (APOLLO2) and reference Monte Carlo calculations.

WP5 is tightly connected to WP4 and consists of three main tasks: (1) the definition of the VVER and PWR reduced size core reference test cases with their corresponding initial and boundary conditions; (2) the evaluation of the test cases with coupled neutronics and closed channel thermal-hydraulics tools (APOLLO3®, SERPENT/SUBCHANFLOW, PARCS/TRACE); (3) the development of a 3D neutronics-thermal-hydraulics reference calculation based on APOLLO3®/CATHARE3 coupling based on the outputs from (1) and (2). The first task has been successfully completed in 2021: the VVER and PWR test cases have been specified with all necessary information: geometries, materials, thermophysical properties, transient scenarios (initial/boundary conditions), and output parameters to be observed. Test cases consist of so-called "mini cores" of 7 fuel assemblies for the VVER case and 32 fuel assemblies for the PWR case. Such small configurations have been chosen to limit necessary calculation resources and times. Information related to those WP4 and WP5 activities has been recently published [8].

Works performed in WP6 during the first half of the project consisted of the development of the VVER-1000 vessel CFD models by each of the five contributing partners to the benchmark exercise, each with his own calculation tool. This task has been completed in 2021. Steady-state conditions have been simulated and compared between models and results have been released at the beginning of 2022. The Kozloduy-6 mixing experiment exercise is now progressing.

A comparable progression was achieved in WP7 in the field of system analyses. Each partner has developed his own model and steady-state calculations have been produced in 2021. The first transient calculations have been achieved at the very beginning of 2022. A new document has been recently produced about the Kozloduy-6 MCP start-up transient benchmark, showing consistency of results with test data.

3.3 Numerical codes used in sCO2-4-NPP

3.3.1 Codes and methods description

- *The THERMAL-HyDraulic SYSTEM CODE ATHLET*

The thermal-hydraulic system code ATHLET [9,10] is developed by the Gesellschaft fuer Anlagen- und Reaktorsicherheit gGmbH (GRS). The highly modular code structure of ATHLET includes advanced thermal-hydraulics as well as physical and numerical models.

ATHLET is able to calculate single or two-phase flows. To simulate the thermo-fluid-dynamic behavior of the fluid, the user has to specify the system configuration by connecting basic fluid dynamic elements, the so-called thermo-fluid dynamic objects (TFOs). These TFOs can be divided into several segments, the so-called control volumes (CVs), to refine the simulation's resolution. The user can choose between the classic 5-equation model, also called the 1-M model, (with drift flux approach) and a two-fluid model with separate momentum balance equations for liquid and vapor, also called the 6-equation model or 2-M model.

The ATHLET code system performs spatial integrations based on a finite volume approach, which leads to a set of first-order differential equations, stemming from two mass and energy conservation equations per control volume and one or two momentum conservation equations per junction. The code also distinguishes homogenous CVs, where all phases are distributed uniformly and no directional quantities exist, and mixture-level CVs, which contain a horizontal mixture level. Below the mixture level, only pure fluid with vapor bubbles may exist, and above, only vapor with liquid droplets.

- *The Thermal-Hydraulic Code CATHARE*

The CATHARE (Code Avancé de THermohydraulique pour les Accidents de Réacteurs à Eau) code is a French thermal-hydraulics system code developed since 1979 and extensively validated in collaboration between CEA, EDF, IRSN, and FRAMATOME [11]. It is internationally used in plant simulators and for nuclear power plant safety analysis and licensing. It was originally devoted to best estimate calculations of thermal-hydraulic transients in water-cooled reactors. The CATHARE 2 has then been extended to gas applications in the 2000s. However, the gas was then considered ideal in this version of the code. This is one of the reasons for the development of a new version of the code CATHARE 3 [12] which enables the consideration of real gas instead of an ideal one in simulations. Therefore, the CATHARE 3 code allows expanding CATHARE 2 ability to model nuclear reactors such as new generation reactors with sodium application and closed Brayton cycles [13–16]. Its major feature is the possibility to choose field numbers from one (pure monophasic) to four: two continuous fields (liquid and vapor) and two dispersed fields (droplets and bubbles). Furthermore, CATHARE 3 can use the Equation Of State (EOS) component which enables the calculation of gas properties from several libraries especially the NIST Reference Fluid Thermodynamic and Transport Properties Database (REFPROP).

The CATHARE 3 solves a two-phase six equation model including additional equations for non-condensable gases and radio-chemical components transport. These equations correspond to the local instantaneous mass, momentum, and energy conservation. They are averaged for each phase over a cross-section over time and allow to represent mechanical and thermal disequilibrium between phases. The system of the equations is closed by physical closure laws of momentum and energy transfers between phases. Finally, the global non-linear system is solved using a Newton–Raphson iterative method.

CATHARE 3 allows modeling the coolant circuits of any reactor by assembling axial (1-D), volume (0-D), and three-D (3-D) hydraulic modules. Thermal and hydraulic sub-modules such as thermal walls, heat exchangers, pumps, valves, turbines, a fluid source, and a sink can be added to these main modules.

- *DYMOLA modeling and simulation tool*

To build and simulate the sCO$_2$-loop numerical model, the Dymola [17] modeling and simulation tool was used by the project partner CVR. Supporting the simulation of the models that are written in the Modelica programming language, the sCO$_2$-loop Dymola model was prepared using the Modelica library and ClaRaPlus, TSMedia, ClaRa_DCS Modelica language-based libraries developed by XRG [18] and TLK [19] companies. In this way, the sCO$_2$-loop Dymola model is a 1D model capable of capturing basic characteristics of the non-steady fluid flow and heat transfer based on the finite volume approach. In a case of a two-phase flow, the fluid is treated as a homogenous mixture of liquid and steam. TS Media library also allows for subcooled CO$_2$ and water to be modeled.

3.3.2 Developments and results

- Developments and results for ATHLET
  - ATHLET extensions for the Simulation of sCO$_2$ Cycles

For the modeling of sCO$_2$ cycles, Venker [20] implemented the first version of the thermodynamic and transport properties of sCO2. In terms of enthalpy and density, data points were generated on a temperature-pressure grid with the computationally expensive equation of state for CO$_2$ (developed by Span and Wagner [22]).

In the frame of project sCO2-4-NPP and project sCO2-QA [23], ATHLET was further improved and extended for the modeling of sCO$_2$ cycles [24,25]. The accuracy and the range of the thermodynamic properties of sCO$_2$ were improved by applying a biquadratic spline interpolation on a pressure-enthalpy grid, similar to Kunick [26], and calculating the enthalpy from the inverse function of the temperature. In addition to the temperature, the density, the entropy, and the speed of sound were provided as spline fits. In the subcritical region, this approach was also applied but there and especially in the transition between the regions some numerical issues need further investigation [23]. For the simulation of turbines, the available model for axial steam and gas turbines may be used. For the simulation of radial turbines, a new efficiency correlation was added to this model [27]. Additionally, a new performance map-based turbomachinery model was implemented. This model allows the simulation of compressors as well as turbines and applies a real gas similarity approach [28] to account for changing thermodynamic inlet conditions for the machines. For the simulation of the heat transfer to the UHS in the sCO2 cycle, an additional heat transfer correlation for the finned air side was implemented [25,29]. On the water side, another correlation for the film-condensation [30,31] was implemented and in general, it was found that the available standard heat exchanger modeling approach in ATHLET may also be applied for the modeling of the heat exchangers in the sCO$_2$ cycle [24,25,31].

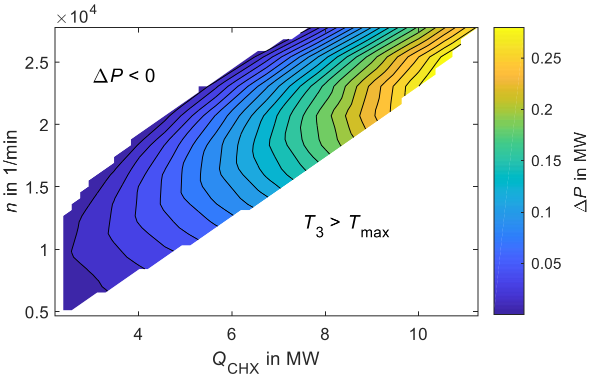

Fig. 5. Excess power output of the cycle at $T_1 = 55$ °C and $T_{\mathrm{air,in}} = 45$ °C with type 2 turbomachinery.

  - Selected simulation results of ATHLET

First, a stand-alone analysis of the sCO$_2$ heat removal system was studied [21,32]. The heat removal system is not designed for efficient electricity generation but for self-propelling heat removal over a wide range of conditions. Therefore, it must be ensured that the cycle operates in a region with an excess power ΔP higher than zero, as shown in Figure 5. The color map indicates that the excess power is decreasing both with decreasing Q'' (power of the compact heat exchanger) and decreasing n (turbomachinery rotational speed). Moreover, Figure 5 shows regions in white where the cycle cannot be operated. First, in the lower right, the operation range is limited by the heat transfer in the CHX (compact heat exchanger) and the maximum steam temperature. Secondly, in the upper left, the operation range is limited because ΔP drops below zero. This is mainly a result of the reduced turbine power caused by the decreased turbine inlet temperature T_3. At the design speed of 23 krpm, the minimum allowable T_3 is 181 °C. With decreasing speed, the minimum allowable T_3 also decreases, e.g. at 13 krpm it is 140 °C. Therefore, it can be concluded that the turbomachinery speed should be decreased with decreasing thermal power input to the CHX.

Thirdly, selected results from the simulation of the sCO$_2$ heat removal system coupled to a pressurized water reactor are shown. A detailed description of the coupled simulations and the results are provided in the reference [33]. During the analyzed SBO scenario, the decay heat is transferred driven by natural circulation, first from the primary loop to the steam generators and then further to the CHXs of the CO$_2$ cycles and finally to the ambient air. In the analyzed case, each of the four steam generators is equipped with one CO$_2$ cycle. Figure 6 shows the decay power compared to the total thermal power of all CO$_2$ cycles of the heat removal system. From an operational readiness state, the CO$_2$ cycles are ramped up (start-up) to their design thermal power. After the equilibrium of the decay power and the removed thermal power, the hot-side temperatures of the nuclear power plant and the CO$_2$ cycles start to decline (cooldown).

- Developments and results for CATHARE
  - Extensions for the simulation of sCO$_2$ cycles

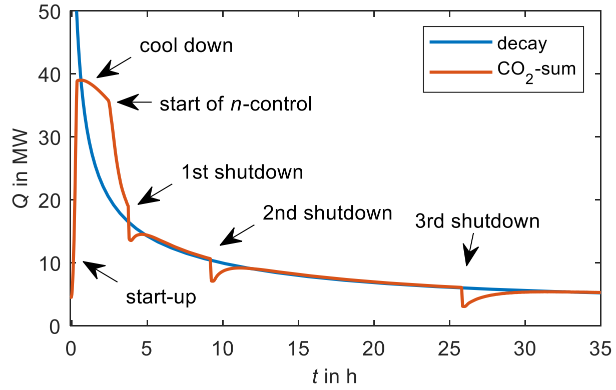

Fig. 6. Decay power and total thermal power removed by the CO_2 cycles over time including different operation modes and the shutdown of single CO_2 cycles.

Many developments have been made in CATHARE 2 to represent all kinds of possible Brayton cycles with turbomachinery [16], a perfect gas turbomachinery module was developed from the CATHARE 2 pump module to describe either a compressor or a turbine that can be coupled to a shaft and an alternator. The behavior of the code has been validated on four real loops. This has therefore demonstrated the ability of the code to accurately represent the dynamic behavior of Brayton cycles in particular the turbomachinery behavior. But the Brayton cycles modeling was then only available for ideal gases.

Therefore, in the framework of the NEPTUNE project [34], REFPROP has been implemented as a new library in the EOS component to use several real gas equations of state in CATHARE-3 such as supercritical CO_2. Thanks to the REFPROP library, CATHARE 3 can compute the real thermodynamic and transport properties of fluids such as supercritical CO_2.

However, the perfect gas turbomachinery model developed in CATHARE 2 was no longer consistent with the new real gas model from REFPROP. Some work has therefore been performed to extend the non-dimensional representation of turbomachinery for a real gas based on turbomachine performance equations. In the perfect gas turbomachinery model, the efficiency is deduced from two reduced values, respectively assessing the flow rate and the shaft rotating velocity. The new real gas turbomachinery model uses the speed of sound of the fluid (instead of temperature) to adequately compute these reduced values without using the ideal law. Performance characteristics are calculated with the real speed of sound and the gas entropy that are available in the REFPROP equation of state.

– Selected results of CATHARE

A stand-alone sCO_2 heat removal system modeling has been performed with the turbomachinery composed of a turbine and a compressor coupled and two heat exchangers CHX (heat source) and UHS (heat sink) (see Fig. 7). The loop is designed to dissipate around 10 MW from one steam generator. Some tests have been done using approximate boundary conditions in the CHX similar to those present in the safety condensers (SACO) of the EPR nuclear plant during a transient SBO scenario. The tests were satisfactory with one or two sCO_2 loops in parallel. Indeed, the power to dissipate on one steam generator is quite high compared to the design of the sCO_2 loop. Therefore, several sCO_2 loops in parallel should be used.

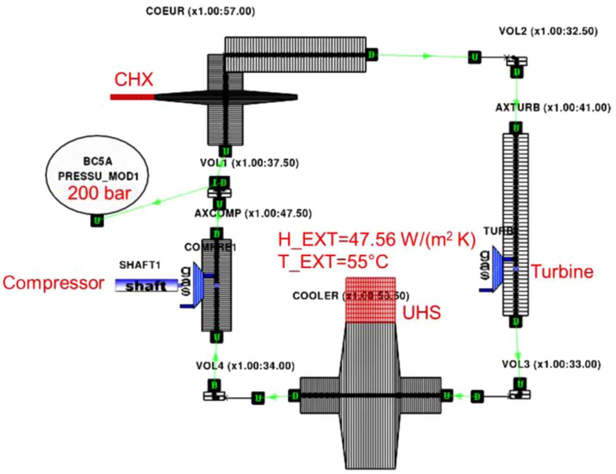

Fig. 7. Layout of the sCO_2 loop modeled with CATHARE 3.

The coupling of the sCO_2 loops with the EPR at the localization of the SACO led to numerical and physical issues. For now, only one sCO_2 has been coupled with one steam generator and there are still numerical issues. The first comparison with an SBO scenario without SACO shows that the sCO_2 loop allows to cool down of the primary circuit but the power dissipated is too low and several sCO_2 loops are needed. A lot of work has still to be done, especially during the regulation phase of the calculation. We think that the initialization and the start-up of the sCO_2 could be the cause of the numerical and physical issues observed.

- Developments and results for DYMOLA
  – Developments for the sCO_2-loop model

Besides the libraries' components, the sCO_2-loop Dymola model comprises new components like turbomachinery and heat exchangers that were built with respect to the project partner's designs under the limiting conditions of the 1D modeling capabilities. As for turbomachinery, the non-dimensional performance curves were implemented to consider changing inlet conditions. When modeling heat exchangers, the 2D nature of the real design was addressed by a proper connection of the hot and cold side heat connectors.

The Dymola sCO_2-loop model needs to be coupled with some external code if we want to simulate the nuclear power plant SBO scenario. Such an external code was ATHLET with the Temelin VVER-1000 nuclear power plant model prepared by UJV. An interface between the Dymola and ATHLET codes was the wall between the CO_2 (Dymola) and steam/water (ATHLET) side of the CHX. To a couple, the Dymola and ATHLET models, the TISC Suite software package (developed by TLK company) was used together with the supervisor code

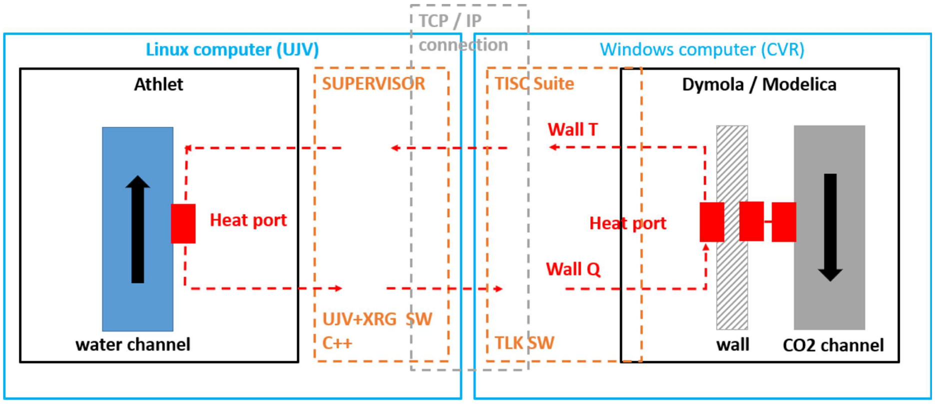

Fig. 8. Dymola-ATHLET coupling schematics.

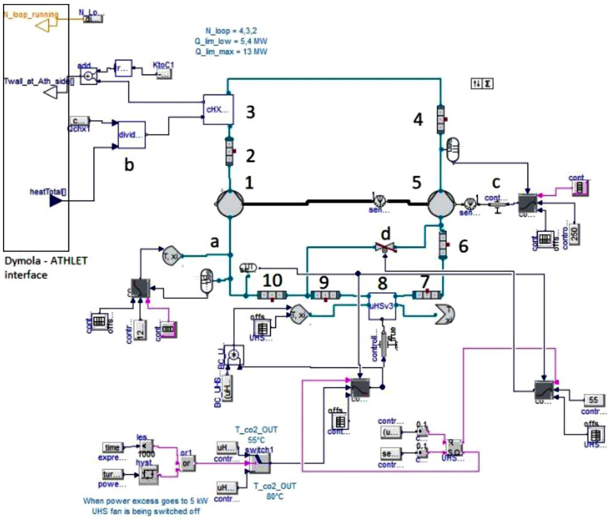

Fig. 9. Dymola model components .

developed previously by UJV for coupling of ATHLET and FLUENT. This supervisor code was adapted for the current application with the help of XRG company. The block diagram of the coupling is depicted in Figure 8.

The Dymola sCO$_2$-loop model basic structure is shown in Figure 9. Here, the basic components are as follows: radial turbocompressor (1), CHX CO$_2$ side (3), radial turbine (5), and UHS (8). As the decay heat gradually decreases with time, so does the number of the sCO$_2$-loops needed to dissipate the decay heat to the atmosphere. As only one sCO$_2$-loop was modeled in the Dymola, the information about the number of the sCO$_2$-loops currently in operation was also transferred between the two codes. For each constant number of running sCO$_2$-loops, the loop thermal capacity was accommodated by the turbomachinery speed of revolution control. Two transient Dymola-ATHLET coupled simulations were performed including that with changing ambient air temperature during the decay heat removal campaign. One of the simulations basic results, namely the comparison of the decay heat and sCO2-loop heat dissipation is depicted in Figure 10. During the whole 72 hours campaign, the maximum core cladding temperature stays within the safety limits.

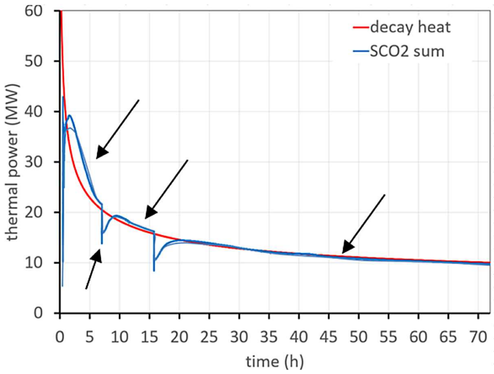

Fig. 10. Decay heat and sCO$_2$ system total heat (ATHLET data).

4 Conclusion

For each of the projects, the work relating to the various numerical codes was initially the subject of a thorough analysis of the characteristics and differences in the treatment of the methods or phenomena studied in the project. These analyses allowed the different consortia to establish comparison grids for the codes used and also the steps to be taken to optimize and harmonize the results of these different codes, for the same phenomenon or the same method analyzed.

It emerges from the work of these three projects, a need to continue to carry out joint work, within the framework of collaborative projects such as the European projects, to be able to:

- undertake the necessary comparisons and harmonizations for these different codes, thus ensuring that the results obtained will be of acceptable quality for the different nuclear studies in cases where keeping different codes is necessary.
- Share new developments related to innovations. Innovations (new components, new systems, new methods) are often associated with new developments of libraries or models in a code. When the sharing of these innovations to a wider audience is desired, this sharing may come up against the fact that the new developments

are only available in a given code, and therefore limit the dissemination of these innovations (for example, the developments related to the system studied in sCO2-4-NPP began in 2015 for the ATHLET code, and only in 2021 for the CATHARE code).
- Moving towards common digital tools. Sharing common developments can also lead the different actors towards the choice of a common tool, and not the multiplication of codes.

Conflict of interests

The authors declare that they have no competing interests in to report.

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Data availability statement

This article has no associated data generated and/or analyzed/Data associated with this article cannot be disclosed due to legal/ethical/other reasons.

Author contribution statement

All *authors contributed* equally.

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