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From past to future: The role of computational fluid dynamics in advancing nuclear safety in Spain and Portugal

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ABSTRACT

This document explores the role of CFD in nuclear safety studies, with a particular focus on advancements in Spain and Portugal. The field of nuclear safety has increasingly included CFD models to address complex safety–critical phenomena, given their ability to capture three-dimensional behavior with high resolution. While traditional one-dimensional codes remain very valuable, they often rely on conservative approximations, making 3D CFD approaches indispensable for accurate predictions across various nuclear scenarios. In the context of Spain and Portugal, this document shows the contribution to CFD applications for nuclear safety research. The topics covered include code development and validation, combustion studies, simulations of nuclear spent casks, fuel assembly analyses, and investigations into containment safety issues. These advances have mainly contributed to improving the predicting capabilities of CFD models for applications in various safety–critical domains. In addition to detailing the achievements and contributions in the field of CFD in Spain and Portugal, readers will find a comprehensive overview of the current challenges and future perspectives of CFD within the domain of nuclear fission technology.

Acronyms	
ATF	Artificially Thickening Flame
AUSM	Advection Upstream Splitting Method
BPG	Best Practice Guidelines
BSC	Barcelona Supercomputer Center
BWR	Boiling Water Reactor
CEA	Commissariat à l'énergie atomique et aux énergies alternatives
CFD	Computational Fluid Dynamics
CNRS	Centre National de la Recherche Scientifique
CSN	Consejo de Seguridad Nuclear de España
CSNI	Committee on the Safety of Nuclear Installations
DCS	Dry Cask Simulator
DNS	Direct Numerical Simulation
ENUSA	Empresa Nacional de Uranio, S.A.
EPRI	Electric Power Research Institute
ETSON	European Technical Safety Organisation Network
EURATOM	European Atomic Energy Community
FADA	Fuel Assembly Drop Accident
FDS	Fire Dynamic Simulation
FEA	Finite Element Analysis
FWP	Framework Programs
FZK	Forschungszentrum Karlsruhe

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Acronyms	
GOTHIC	Generation Of Thermal-Hydraulic Information for Containments
GTRF	Grid-To-Rod-Fretting
HI-STORM	Holtec International Storage Module
iLES	implicit LES
IRSN	Institut de Radioprotection et de Sûreté Nucléaire
ISFSI	Spanish Independent Spent Fuel Storage
KAERI	Korea Atomic Energy Research Institute
KWU	Kraftwerk Union
LES	Large Eddy Simulation
MTES	Modelling of Thermal and Energy Systems Research Group
NEA	Nuclear Energy Agency
NFPA	National Fire Protection Association
NIST	National Institute of Standards and Technology
NPP	Nuclear Power Plants
NRC	Nuclear Regulatory Commission
NS	Nuclear Safety
NUGENIA	Nuclear Generation II and III Association
OECD	Organization for Economic Cooperation and Development
OKBM	Опытное конструкторское бюро Машиностроения (Experimental Design Office)
PAR	Passive Autocatalytic Recombiners
PRA	Probabilistic Risk Analysis
PRISME	Propagation d'un incendie pour des scenarios multi-locaux elementaires
PSI	Paul Scherrer Institute
PSR	Partially Stirred Reactor
PWR	Pressurized Water Reactor
RANS	Reynolds-Averaged Navier-Stokes
SAS	Scale Adaptive Simulation
SMR	Small Modular Reactor
UC	University of Cantabria
UPCT	Universidad Politécnica de Cartagena
UPM	Universidad Politécnica de Madrid
UPV	Universitat Politècnica de València
UQ	Uncertainty Quantification
V&V	Verification and Validation
WGAMA	Working Group on Analysis and Management of Accidents

1. Preface

CFD codes are a powerful tool for simulating fluid behavior and analyzing its interactions with the boundaries. Therefore, for almost half a century, they have been used as a complement to system codes to evaluate the safety of nuclear systems where thermal–hydraulic analyses are relevant. Their greatest advantage in this field is the ability to characterize the phenomenology on a much smaller scale than system codes, which allows for a much more in-depth analysis in many scenarios. However, there is an open debate regarding the credibility of these codes in safety studies, and their use in this sense is still limited to certain applications. CFD codes increasingly use first principles models capable of reproducing the physics of thermal–hydraulic behavior in three dimensions. The growth they have experienced over the last few decades has been significant, in part, thanks to the increase in computing and parallelization capabilities, bringing their use closer to companies, universities, and research centers. However, the requirements for performing accurate high-resolution simulations are still large, especially in multiphase scenarios with mass and energy transfer. CFD represents a truly promising option, but a great effort will be required by the scientific community, industry, and regulatory bodies to fully extend its use in the nuclear field.

In the field of NS, CFD codes represent a major advancement mainly due to the three-dimensional behavior of many of the processes that occur during events of interest in this area (IAEA-TECDOC-1379, 2002). For example, fluid mixing, thermal stratification or more complex phenomena such as liquid–gas or liquid–solid interactions represent mechanisms that can be reproduced using CFD. Additionally, these codes can numerically simulate flows with complex geometries without the limitations inherent to system codes or empirical correlations. In fact, the equations governing fluid motion are independent of the reference scales and thus are theoretically representative for all scales. However, CFD codes still rely in many cases on closure equations that implicitly include dependencies on flow characteristics or length scales. As a result of these advantages, the use of CFD to assess certain phenomena related to safety such as those related to reactor cooling systems, natural circulation, containment or spent fuel cooling has increased in recent years (Smith et al., 2015). In these and other scenarios, pseudo 1-D calculations could lead to erroneous conclusions due to the simplifications they implicitly assume. CFD codes are also a valuable tool that provides information throughout the entire domain, making them highly effective for complementing experimental measurements. Currently, it is common to observe publications on experimental facilities where certain parameters are preliminary foreseen based on validated CFD models (Rivera et al., 2022).

Safety studies require highly reliable CFD approaches to assess their effectiveness. The validation process plays a crucial role in evaluating reliability by comparing CFD results with experimental data, identifying any discrepancies and verifying their accuracy (IAEA NR-T-1.20, 2022). Additionally, the validation process entails comparing predicted and measured data from separate and integral effect tests to understand any deviations. CFD's Verification and Validation process, along with Uncertainty Quantification (commonly known as V&V + UQ), involves selecting models for physical phenomena and developing numerical models for the physical domain and fluid properties. While the scalability of governing equations is not an issue, closure models and the validity range of models can affect the accuracy and uncertainty of results. Additionally, the validity range of the models used may extend beyond the explored domain of the database, which can impact the justification of certain fittings or parameter choices, as well as introduce uncertainty into the results. To make matters worse, adapting UQ methods to CFD remains limited regardless of the efforts done for system-scale analyses. The primary sources of uncertainty are diverse and more complex to analyze than in simplified modeling approaches. Turbulence models, proper representation of boundary conditions, fluid properties, and numerical methods used to solve the governing equations are major sources of uncertainty that affect the confidence of CFD results. The difficulties in performing a holistic uncertainty quantification question the application of CFD simulations to address NS predictions, especially from a regulatory perspective. Significant efforts have been made by the scientific community to develop BPG in order to establish a common and well-thought-out methodology for the use of CFD in NS (OECD/NEA, Mahaffy et al., 2014; NUREG 1934, 2012). This way, errors can be minimized by establishing rigorous steps to follow to obtain better reliability in results.

The inherent complex phenomenology related to NS analyses has motivated the development of nuclear-field codes with 3D capabilities, such as GOTHIC or FDS. Some of these codes are less demanding of computational resources while accommodating the unique characteristics of their respective fields of application. In particular, GOTHIC is a thermal–hydraulic code based on a two-phase, multi-fluid formulation, which solves separate conservation equations for mass, momentum, and energy for three fields: vapor, continuous liquid, and droplets (Harvill et al., 2022). GOTHIC is mostly used for containment safety analysis of light water reactors, but it has also been used for calculating the thermal behavior of waste fuel casks, and it has been extended to tackle liquid-metals phenomena (Lane et al., 2020). In the framework of 3D application-oriented analysis, GOTHIC is seen as a hybrid between CFD and System codes because it does not have the capability of resolving the boundary layer explicitly. The code includes a set of built-in correlations—performing a similar role to wall functions in commercial CFD—cell faces and cell volume porosity factors to model friction, heat, and mass transfer close to the walls. It significantly decreases the computational cost of the simulations, a cost-benefit balance that enables the use of 3D codes in the large (more than 60.000 m^3) and demanding computational domain to obtain variables of pressure, temperature, or hydrogen concentration.

In the same way, as mentioned above, the development of CFD codes has also enabled the integration of multiple physics in problem-solving, allowing the incorporation of phenomena of interest that affect fluid performance. For instance, it is possible to obtain information about the evolution of different species subjected to chemical reactions or predict fire propagation. Since the 1970s, a large amount of computational fire models have appeared to predict fire behavior and try to increase the safety of nuclear power plants. A major milestone in nuclear safety was the publication of the standards NFPA 805 Performance-Based Standard for Fire Protection for Light Water Reactor Electric Generating Plants in 2001. This standard allows the application of computational fire models to support performance-based fire protection and risk analyses, but they must be verified and validated for the specific phenomena analyzed. Although there are three main types of fire models, algebraic models, zone models and field models (CFD based), the last type is more detailed and accurate, and they are applicable to a large number of fire scenarios in nuclear power plants. Inside field models (CFD), FDS is the most widely employed and validated (McGrattan et al., 2023; NUREG-1824, 2016a). This model has been developed by the NIST, and it is a CFD model of fire-driven fluid flow. FDS solves numerically a form of the Navier-Stokes equations, appropriate for low-speed, thermally-driven flows emphasizing smoke and heat transport from fires. This model is useful to analyse all fire phenomena (combustion, fire spread, species generated, smoke, etc.) and the interaction with the fire protection systems (sprinklers, water mist, exhausts, compartmentation systems, etc.). Nevertheless, its application to certain specific phenomena related with fire safety is still to be validated, showing different discrepancies in the results of international benchmarks that remark the necessity to continue working in the validation and the definition of guidelines to model those phenomena (Plumecocq et al., 2023).

This paper outlines Spain and Portugal's contributions to CFD for Nuclear Safety. Section 2 presents a synthesis of the different projects conducted, categorizing the research topics into code development, combustion, nuclear-spent casks, fuel assemblies, containment, and other areas. Following the same structure, Section 3 describes the main outcomes for each research domain. In Section 4, the authors discuss current and upcoming challenges and planned activities for their respective organizations. Finally, the conclusions offer a holistic summary of the paper's main contributions.

2. Research synthesis

2.1. Code development

Since 2002 the **UPCT**, has worked in the development of numerical CFD codes and its validation for nuclear safety applications through different international research collaborations with European institutions. During 2002 and 2003, the Modelling of Thermal and Energy Systems Research Group (MTES) of UPCT worked in collaboration with Commissariat à l'énergie atomique et aux énergies alternatives (CEA) at Saclay, in the development and validation of AUSM+ numerical schemes and other Riemann Solvers under unstructured grids and on the bases of a one-pressure two-fluid model denominated CATHARE Model, in the context of the European Project: Advanced 3D two-phase flow simulation tool for application to reactor safety, from the 5th EURATOM Framework Programme (FP-5) (Paillère and García, 2003). This collaboration was extended up to 2006 and included not only CEA (France) but also FZK (Germany) and other institutions (Staedtke et al., 2005; García and Paillère, 2007). Among the specific developments, members of the group have extended existing Riemann Solvers such as AUSM-type to compressible two-phase mixtures and to low Mach number flows. They successfully applied them to transient two-phase (six-equation models) with non-hyperbolic systems that raise in nuclear safety and other fluid dynamic problems. In this case, the system provides complex eigenvalues in some parts of the solution yielding to ill-posed problems in finite volume formulation for multi-dimensional applications. Both solid and gas phases where resolved using a Eulerian approach. Examples of these problems are 3D shock tube tests, which are important for aerosol mobilization and dispersion, 2D boiling channel test (key in BWRs) or the problem of predicting the dispersion of two-phase (liquid–gas) flow in a convergent-divergent nozzle. This last problem is key as it includes strong mechanical and thermal non-equilibrium conditions typical of the fast depressurization of nuclear reactor systems during loss-of-coolant accident conditions (so called "blowdown" events). Furthermore, the presence of combustible dust particles in a hydrogen detonation sequence presents several challenges in physical modeling and numerical resolution. In particular, the source terms coupling the gas and solid phases generate a strong stiffness of the system of equations, so a splitting method that uses AUSM+ and Rusanov schemes and the linearization of source terms was developed (García-Cascales, 2014) and validated in order to achieve a numerical solution to the problem. The validation was performed through experimental data from a spherical bomb filled in with H2–O2–N2 mixtures in the absence and presence of solid particles (Velasco et al., 2016; García-Cascales et al., 2015), giving very promising results, despite the simplicity of the combustion model used at that time. These models can be used for the analysis of accident sequences with H2 combustion, both in fusion and fission reactors.

2.2. Combustion and fire safety

Between 2008 and 2014, the **UPCT** worked through specific research contracts financed by IRSN, in the development and validation of numerical codes for the 3D modelling of particle mobilization, combustion of two-phase mixtures, and detonation of hydrogen-air mixtures with CAST3M CFD code (García et al., 2014). In the last eight years, the research work in CFD modelling has focused on the collaboration with IRSN for the development of new models for turbulent hydrogen combustion to predict flame acceleration and deflagration to detonation transition with progress variable models and thickening flame models. These codes were developed to be used in OpenFOAM and can be combined with other available multi-physics libraries. In this context, UPCT has represented Spain in the ETSON-CFD-Benchmark organized by the European Technical Safety Organisation Network within the SAM-HY-CO net and sponsored by NUGENIA and MITHYGENE programs. This benchmark aims to identify the current level of accuracy of the available CFD tools in the area of hydrogen combustion simulation, under conditions that are representative of safety considerations in a Nuclear Power Plant, and testing CFD models' capacity to predict flame acceleration. Besides, additional efforts were focused on the development and validation of CFD models able to predict hydrogen flame dynamics of lean mixtures under isotropic turbulent fields in collaboration with CNRS at Orleans and IRSN at Fontenay-aux-Roses where different experiments were performed.

The **UC** has been actively collaborating with the CSN in the analysis, validation and application of CFD fire codes to enhance safety in NPP. Since 2014 both institutions have been working on the analysis in depth of the background of main fire models applied to nuclear power plants, in the development of a guide with the steps and input parameters necessaries to perform a simulation, in the creation of a software to easily create fire scenarios in nuclear power plants, in the development of simplified models to afford some specific fire related phenomena, as cable fire propagation in NPP (Lázaro et al., 2022b), in the definition of new methodologies to obtain the input parameters to improve FDS model prediction (Lázaro et al., 2023a; Lázaro et al., 2022a), in the applicability of FDS to model real NPP scenarios (Lázaro et al., 2018), in the validation of CFD codes through the implementation of large scale experimental tests, etc. A summary of the different projects in which both entities have participated is shown below.

- Collaborative project with the CSN entitled “Simulación de Incendios en Centrales Nucleares” (“Simulation of Nuclear Power Plant Fires”) from 2014 to 2018. The main objectives of this project were the definition of methodologies to obtain the input parameters to define material reactions in FDS model, the analysis of the applicability of FDS to model complex fire sources, like cabinets or cable trays, and the comparison of different methodologies to represent their behaviour in FDS, the simulation of real scenarios of nuclear power plants and the definition of a methodology to define fire scenarios in FDS and simulation and comparison of results versus the experimental results of the project OECD/NEA-PRISME (Propagation d'un incendie pour des scenarios multi.locaux elementaries) (NEA/CSNI/R(2017)14, 2018). Finally, a freeware was developed to facilitate the FDS computational modelling of nuclear power plant scenarios.
- Collaborative project with the CSN entitle “Metodologías avanzadas de análisis y simulación de incendios en centrales nucleares” (“Advanced methodologies for analysis and simulation of nuclear power plant fires”) from 2020 to 2024. Following the steps marked by the previous project, this project also adds the study of machine learning algorithms to improve the definition of the FDS input parameters and to decrease the computational cost. It also included the modelling of the detection and extinction systems, the development of a database and the improvement of the freeware to define FDS fire scenarios in nuclear power plants.
- Research project “NUCLEVS - Validación, calibración y aplicación de modelos de propagación de incendios en escenarios reales de Centrales Nucleares” (“NUCLEVS - Validation, calibration and application of fire models in real Nuclear Power Plant scenarios”). In this project, the validation of different computational fire models is analyzed. Based on this, an experimental test campaign will be performed to validate some phenomena like extinction due to lack of oxygen. Other phenomena like cable fire propagation will be validated by the use of literature available from experimental tests. Finally, it is proposed the development of a methodology applicable to real plant scenarios that facilitates Probabilistic Fire Safety Analysts to correctly define the maximum expected fire scenario.

These projects have allowed the participation of the UC jointly with the CSN in the common OECD PRISME 3 and FIRE Benchmark Exercise. The following three-step methodology for conducting this Benchmark Exercise was employed: (1) a calibration phase, (2) a blind simulation of a PRISME cable fire experiment, and (3) the real fire event simulation. The importance of this type of benchmark lies in the still need of validating fire computer models under certain fire related phenomena, as cable fire propagation (Plumecocq et al., 2023).

The application of CFD to predict fire propagation in NPP has been incremented since the publication of the NFPA 805 that allows the performance-based design in NPP (NFPA 805 Performance-Based Standard for Fire Protection for Light Water Reactor Electric Generating Plants, 2020). Nevertheless, the NFPA 805 indicates that the CFD has to be verified and validated for the specific phenomena explored in the study. For this reason, although fire CFD models, such as FDS, have been widely validated (NUREG-1824, 2016b), more works and assessments as those developed in the projects in which the UC and the CSN collaborate are required to extend its applicability and increase their reliability.

2.3. Nuclear spent casks

ENUSA has developed a strong research portfolio in the investigation of nuclear spent casks. Their main goal is to obtain a better understanding of the different phenomena and to study the capabilities for specific designs. The greatest efforts within the topic of spent fuel storage are specifically the dry storage systems. Due to the increasing need for medium-term spent fuel management, the realistic and accurate calculation of the peak cladding temperature during its dry storage is a key parameter. There are different tools to perform simulations, being one of the most advanced the use of CFD.

Since 2012, ENUSA has been participating in different projects for the thermal characterization of spent fuel casks using different tools (CFD and COBRA-SFS, that is a code specific for spent fuel package thermal analysis). Regarding the CFD codes that are the object of interest of this paper, in particular the following projects have been carried out. In 2012, a simulation of a ventilated dry storage cask was carried out under normal, off-normal and accident conditions and the results were compared with the experimental test performed by KAERI (Barrera et al., 2012). In 2017, a three-year project in collaboration with the UPM has been conducted to analyse the thermal behaviour of both the TN-24P spent fuel cask and the fuel inside it, and benchmarking against experimental measurements available (Benavides et al., 2018). In 2018, ENUSA collaborated with UPM to study the thermohydraulic response of a single BWR fuel assembly in the DCS (Dry Cask Simulator) experimental cask, obtaining results consistent with the experiments carried out in the Sandia National Laboratories (Benavides et al., 2019; 2020). Based on these studies, it has been possible to develop a validated methodology for the thermal calculation of spent nuclear fuel containers. Currently, ENUSA is working on a project in collaboration with the CSN to thermally characterize the HI-STORM100 container considering the PWR fuel elements in detail, without simplifying the geometry by using porous media and validated with the subchannel code COBRA-SFS (Esteban and Matías, 2022).

In this way, the main objective of these projects has been to verify that realistic calculations can be made using CFD code, reducing the uncertainties compared to conventional approximations that are not capable of observing certain phenomena such as the flow path between the fuel rods and the grids. Consequently, the management of spent fuel is improved by calculating the efficient heat dissipation that determines the temperature distribution in the cask/fuel.

Additional details concerning activities associated with spent fuel can be found in the parallel paper that will be featured in the same special issue (Feria et al., 2023), which also includes contributions from ENUSA and UPM focusing on CFX simulations in spent fuel containers.

2.4. Fuel assemblies

Related to the flow over fuel assemblies, different projects were carried out by **ENUSA**. This includes the participation in the phase 1 of the NESTOR-Round Robin benchmark (EPRI Technical Report, 2014). The objective of this benchmark was to assess CFD temperature, velocity and pressure loss predictions of the flow over a 5x5 fuel rod bundle with Simple Support Grid against experimental results.

In collaboration with **Westinghouse** and **UPM**, hydraulic forces were calculated to study fuel assembly distortion. ENUSA studied single and multiple fuel assembly spans to calculate lateral forces as a function of fuel rod bow and explore the effect of local hydraulic forces on fuel assembly distortion. Pressure drop over the grids was benchmarked against test results. The lateral hydraulic forces were then used in mechanical codes to assess the impact during operation (Petrarca et al., 2015; Corpa Masa et al., 2015). A characterization of the flow around the fuel assembly bottom nozzle was carried out to obtain a 3D velocity profile for the water downstream of it. Also, different bottom nozzle designs were studied to verify that changes in the flow distribution and fluid pressure drop due to each design has no safety impact (Corpa Masa et al., 2014).

In collaboration with UPM, two projects regarding fuel assembly integrity were carried out with computational codes. One was to develop a methodology to study GTRF. The methodology was based on the calculation with CFD codes of the forces subjected to turbulence-induced fluctuation that cause small amplitude vibrations in the rod. These forces are then used as inputs for a FEA code that calculate fuel rod motion (Matías et al., 2019). The other study was related to fuel assembly drop accident into the spent fuel pool. The impact velocity as a function of the drop height was calculated as a realistic input to calculate the mechanical damage produced by the accident. The objective of the projects related to fuel assembly is to have a better understanding of fuel assembly performance to ensure integrity during operation and handling. This allows to go to increased cycle length and burnup and more challenging operational scenarios (Corpa and Montero, 2014).

In the last years, ENUSA has also been developing activities related with radiological characterization robots and drones, for which CFD simulations were carried out during the design of these.

2.5. Containment

The **UPM** has participated in several projects related to CFD codes in plant application for containment analysis, especially hydrogen behavior during a severe accident. Since 1995, UPM has participated in CFD simulation activities in the FWP of the EURATOM and the European Commission (EC) and projects for CSN and OECD/NEA. A summary of the different projects in which the UPM has participated, along with the main objective of each one is shown below.

Containment Analysis with CFX (1995 – 2004):

- CEC-SCA-VOASM: 1997 – 1999: Validation of a simulation methodology for hydrogen mixing and catalytic recombination. Some steady states of Zx experiments in BMC Containment with PAR were simulated with a structured CFD code. These results were compared with similar simulations of other organizations and the experimental results. Finally, the results were applied to representative accidental conditions scaled to the experimental facility (Martín-Valdepeñas et al., 1999).
- CSN/UPM: 1995 – 2004: Several projects were done in collaboration with CSN related to hydrogen behavior within containment and application to Level 2 Probabilistic Safety Analysis. CFD plant applications were done during these projects for a restorative analysis in a Steam Generator room to a simplified full-scale PWR plant (Martín-Valdepeñas et al., 2005; Martín-Valdepeñas and Jiménez, 2003).
- CEC-EXPRO: 2001 – 2004: Experimental and numerical study of reactive flows in complex geometries with relevance to industrial safety for explosion protection. A methodology combining integral codes and a CFD code was developed during this project.

Containment analysis with GOTHIC (2013 - present):

- Iberdrola Engineering/UPM (2013–2017): several projects were done in collaboration with Iberdrola Engineering, including the PAR location and sizing for the Cofrentes Nuclear Power Plant containment building with a 3D GOTHIC model (Jimenez et al., 2015; Serrano et al., 2016; Díez Álvarez-Buylla et al., 2021) and the estimation of the hydrogen combustion risk in the Filtered Containment Venting System of Cofrentes NPP (Fernández-Cosials et al., 2018).
- CNAT/UPM (2013-): since 2013, Almaraz and Trillo NPPs have supported the UPM with a continuous line of research with GOTHIC from 2013. In those years, several 3D models have been created for both Almaraz NPP (Vázquez-Rodríguez et al., 2019) and Trillo NPP (Fernández-Cosials et al., 2019). Extensive work regarding Best Estimate Plus Uncertainty (BEPU) applied to a design basis accident for a PWR-W containment building was also done in the framework of this collaboration (Bocanegra and Jimenez, 2018).
- Ministry of Economy and Competitiveness/UPM (2016–2019): in the framework of the PYrolysis Gas Analysis and Safety project (ENE2015-67638R), it was possible to develop an AP1000 3D full containment model with GOTHIC (Estévez-Albuja et al., 2021a), validating the model both with experimental data from the Technical University of Munich (Estévez-Albuja et al., 2018) and from the North China Electric Power University (Estévez-Albuja et al., 2021b).
- EC-HORIZON2020/UPM (2020–2024): the UPM coordinates the AMHYCO European project (Herranz et al., 2022; Jiménez et al., 2022), in which several works related to 3D containment modelling are in progress (Serra et al., 2021), as well as PAR coupling with GOTHIC (Domínguez-Bugarín et al., 2022).
- Cardiff University/University of Liverpool (2020–2024): The UPM has worked in collaboration with the mentioned universities in helping to develop a GOTHIC model of a VVER-1000 nuclear power plant, (Kanik et al., 2024), (Kanik et al., 2022).

2.6. Other applications

The **UPV** has collaborated with the CSN de España in the validation of CFD codes through the implementation of benchmark activities featuring a variety of topical issues related to nuclear safety. Since 2008, UPV has participated in the CFD simulation activities organized by the WGAMA CFD Task Group, which is sponsored by the OECD, the NEA, and the CSNI. The main objectives pursued by these benchmarks are to develop BPGs for the use of CFD, define calculation strategies for predicting uncertainty, and establish guidelines for enhancing CFD-grade experiments for verification and validation purposes. Different organizations and entities worldwide are granted access to the measurements of a CFD-grade experiment and use them to validate their computational approaches. Moreover, WGAMA group activities involve assessing the state of the art and maintaining several reference documents, such as the aforementioned BPGs for the use of CFD in reactor safety (OECD/NEA/CSNI, Mahaffy, et al., 2014). A summary of the different benchmarks in which the UPV has participated, along with the main objective of each one is shown below.

- OECD/NEA-Vattenfall CFD Benchmark Exercise 2008–2011: Validation of a CFX model for the experiment at the Älvkarleby laboratory facilities on fluid mixing at different temperatures in a T-junction to predict the important parameters affecting high-cycle thermal fatigue (OECD/NEA/CSNI, Smith, et al., 2011).
- OECD/NEA-KAERI CFD Benchmark Exercise 2010–2012: Development of a model for the turbulence parameters' prediction downstream of a generic design of spacer grid in a rod-bundle geometry (MATiS-H experiment) (OECD/NEA/CSNI, Smith, et al., 2013).
- OECD/NEA-PSI CFD Benchmark Exercise 2012–2014: Validation of the buoyancy prediction capabilities of CFX for He stratification to address the erosion by a buoyant jet in one of the PSI PANDA vessels (Andreani et al., 2015).
- OECD/NEA-PSI CFD Benchmark Exercise 2014–2016: PCE UQ methodology development for CFD simulations through the PSI GEMIX database on the mixing of two fluids with different (OECD/NEA/CSNI, Fokken, et al., 2019).
- OECD/NEA-Texas A&M University Benchmark Exercise 2017–2019. Extension of PCE methodology for the normal uncertain variables within the frame of the Cold-Leg Mixing experiments at Texas A&M University about fluid mixing in presence of buoyancy effects (OECD/NEA/CSNI, Vaghetto, et al., 2022).
- OECD/NEA-OKBM Afrikantov Benchmark Exercise 2019–2021. Validation of a one-way coupled CFD-FEA model for the fluid–structure interaction during vortex shedding appearance in a channel with two bottom-fix cylinders.

So far, all the benchmarks organized by WGAMA CFD group correspond to single-phase applications. UPV has employed ANSYS commercial code, especially CFX, for this series of exercises focusing on the proper use of available models for each scenario. Since 2014, the different activities carried out have focused not only on obtaining predictions from CFD code, but also on extending the analysis to uncertainty quantification. Analyzing the uncertainty of the results is highly relevant if this tool is to be used in the future to make informed decisions that may affect public safety. Accurately calculating the uncertainty associated with simulations enables a greater degree of understanding of the studied phenomena and will allow for informed decision-making in nuclear technology in the coming years. UPV has mainly focused its efforts on developing and applying the Polynomial Chaos Expansion propagation method for uncertainty quantification in CFD calculations (Rivera et al., 2021).

In the framework of the projects started at the **UPM** in the 90 s—more information on the section dedicated to containment analysis—a multipurpose commercial CFD code was tailored and validated for hydrogen safety analyses. The most important items are listed below, with more information available in (Martín-Valdepeñas et al., 2007):

- Several condensation models with non-condensable gases were implemented into the commercial software using external functions coded in Fortran at the UPM.
- Hydrogen flame acceleration and deflagration to detonation transition criteria (Sigma and Lambda criteria) were implemented as online post-processing of the CFD code results.
- Several benchmark and validation exercises were done for different integral experiments: Zx-BMC, NUPEC and MISTRA.
- OECD/NEA-PSI CFD benchmark exercise (2014–2016): in the framework of the international benchmark exercise 3, validation exercises were made in the group for a helium stratification test made in PANDA within HYMERES project (Fernández-Cosials et al., 2016).
- CSN/UPM (2019–2023): in the framework of the GO-MERES project, several collaborations with PSI within HYMERES2 and PANDA projects from OECD/NEA took place. The main topics were BWR suppression pool test and PWR spray test (Vázquez-Rodríguez et al., 2023). In this project, plant application cases were done for PWR and BWR reactors, learning from the PANDA experimental test simulations with GOTHIC.

3. Research key outcomes

The long trajectory followed by the different Spanish research groups, described in the previous section, has led to the achievement of a series of major milestones. In particular, the different groups have contributed to development and validation work in the various fields of 3D codes. Their major contributions are described in the following subsections taking into account the different CFD research topics.

3.1. Code development

During the period 2003–2006, the **UPCT**'s research in collaboration with CEA Saclay (France) led to extend some Riemann Solvers and flux schemes classically used in supersonic flows to multidimensional, transient two-phase flows problems under compressible flow conditions. Specifically, AUSM schemes were extended for both two-fluid mixtures of water and air and phase change processes between water and steam and they were benchmarked with reference problems with satisfactory results (Garcia-Cascales and Paillère, 2003).

The implementation of international benchmarks in nuclear safety has enabled the scientific community to gather valuable information regarding the most suitable CFD methods for each scenario, based on the underlying physics of the phenomena. Potential issues have been identified where the proper utilization of CFD allows for a more detailed analysis, thereby enhancing the precision with which safety assessments are evaluated. Additionally, the Best-Practice Guidelines have been continuously updated, along with relevant documentation for uncertainty quantification (Bentaib et al., 2022).

3.2. Combustion and fire safety

The collaboration among **UPCT**, IRSN at Fontenay-aux-Roses and CNSR at Orleans (France) permitted testing of different turbulent combustion models coupled with LES for simulating H_2 combustion with spherical bomb experiments. Simulations and combustion experiments performed in a spherical bomb equipped with fans permitted to assess the effect of turbulence in the H_2 combustion sequences. Results showed that under high turbulent conditions LES models are more effective in predicting turbulent combustion characteristics than RANS models under "blind" conditions. In this context, an ATF model, also called thickening flame model (Colin et al., 2000) and a flame progress variable model were tested with LES and validated for predicting key combustion parameters under different H_2-air conditions. Results also showed that, for a fixed mesh, the ATF model was more robust than the flame progress variable model and provided a similar level of accuracy but with the advantage of providing a detailed description of the chemical composition of the flow, which is key in some sequences involving ignition, flame acceleration or quenching phenomena.

In the last years, the research group of Thermal and Energy System Modelling at UPCT has focused on the validation of turbulent combustion models able to predict flame acceleration in hydrogen-air mixtures. In this context, UPCT represented Spain in the ETSON Benchmark within the SAM-HY-CO project. UPCT showed that ATF turbulent combustion models coupled with detailed chemical kinetic schemes and LES were able to predict flame acceleration experiments of lean mixtures of H_2 in air performed in ENACEFF-2 facility at CNRS Orleans (France). The use of different sub-grid scale (SGS) turbulent models in LES (i.e. Smagorinsky-Lilly, WALE, k-equation model, dynamic k-equation model) did not significantly influence the results of this type of unsteady sequences. Besides, strategies based on Dynamic Adaptative Chemistry, In-situ Adaptive Tabulation and Adaptative Mesh Refinement were very effective to overcome the limitations due to the requirements of mesh resolution imposed by the use of LES and partially reduce the computational costs of the simulations. Other numerical strategies like the PSR model implemented in iLES (Berglund, 2010) and detailed chemistry models were also able to predict flame acceleration but required higher grid resolution. Specifically, this strategy was very effective to predict vortex-flame interaction and its contribution to flame acceleration. However, it was found that a minimum spatial resolution of 1/8 of the laminar flame thickness was required to predict correctly flame acceleration in the initial steps of the combustion sequence (Nicolas et al., 2021a). This increases the computational costs and limits the use of iLES to local regions in specific time lapses within scenarios such as the initial stages of flame growth and initial acceleration due to flame-structure interactions. Regarding numerical schemes, PISO, AUSMup and AUSM+ showed better prediction capacities than other more diffusive schemes like Rusanov's. AUSM was confirmed to be very efficient in transonic conditions, and its variations AUSM+, and AUSMup were also adequate for a wide range of Mach values.

All in all, the use of detailed chemistry models is key to predict not only flame acceleration but also other phenomena like deflagration to detonation transition or quenching (Fig. 1). The use of different chemical models tested (detailed with 27 equations, detailed with 21 equations or reduced with 12 equations) did not significantly influence the results as long as the species H, O, OH, H_2O_2 and HO_2 were considered in the scheme. Moreover, recently, H_2-CO-O_2 chemical kinetic models were also tested with the LES approach to simulate combustion experiments of H_2 and graphite in a spherical bomb (Nicolás-Pérez et al., 2021b). Results showed that the H_2-CO-O_2 combustion model of Yetter et al. (1991) that included C, CO, CO_2, HCO, H, O2, O, OH, H_2O, H_2O_2 and HO species coupled with LES was able to predict pressure evolution with time during the sequence with results in accordance with experiments.

The activities conducted by **UC** in collaboration with **CSN** in the different projects exposed in the research synthesis section can be divided into several topics connected to achieving the final goal of increasing fire safety in nuclear power plants through the use of CFD. The topics studied included thermal decomposition and combustion analyses of materials that could be present in a nuclear power plant. Furthermore, different methodologies and experimental tests have been developed to define different materials in the various fire scenarios

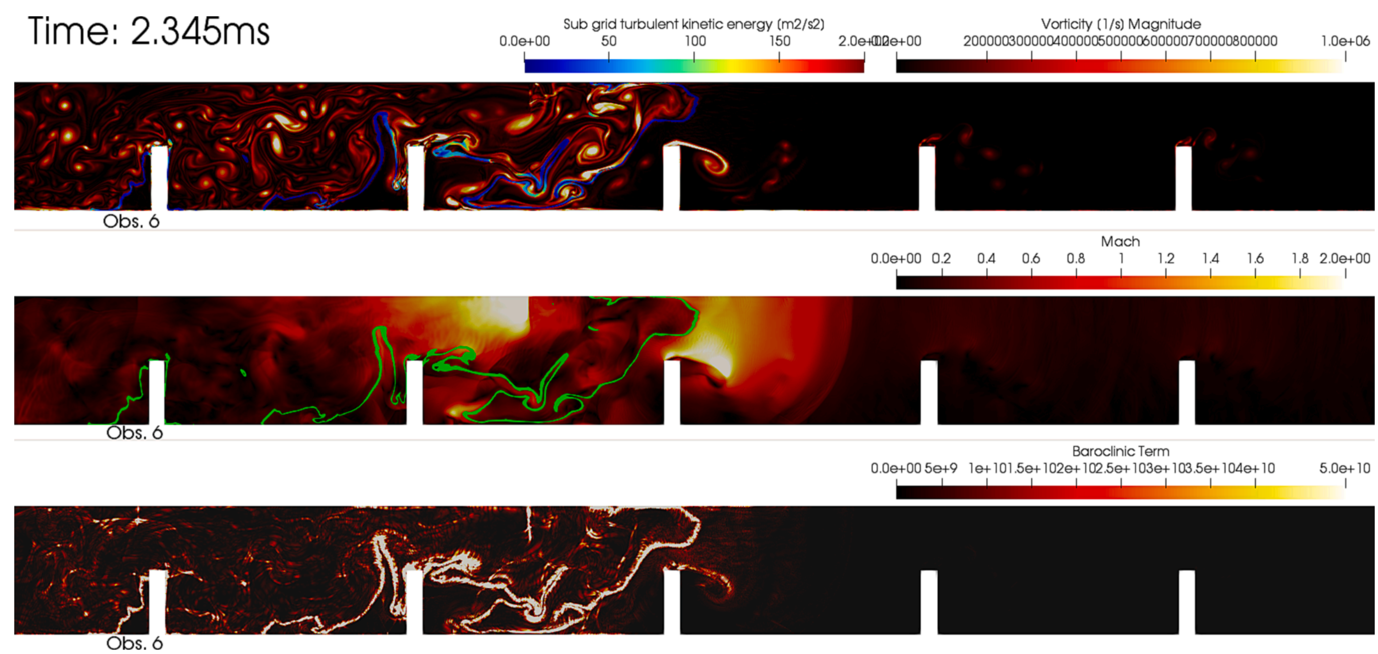


Fig. 1. Simulation of H_2 combustion in a channel with LES and Williams detailed chemisty scheme. The reaction flame front is identified by a green line. The figure shows the flame acceleration mechanism due to flame interaction with the obstacles. Both, the obstacles and the magnitude of the baroclinic term ($\nabla\varrho \times \nabla p$) induced by the flame, contribute to the production of vorticity what enhances mixing and flame acceleration. Numerical benchmark (Case B) (Nicolás-Pérez et al., 2021a,b). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

defined with CFD. Additionally, different real fire scenarios have been analysed with the CFD model FDS (McGrattan et al., 2023), examining the influence of input parameters and comparing the results with large-scale experimental tests. Moreover, participation in the benchmark organized under the support of the PRISME program has allowed for the evaluation of user effects during the modelling of cable tray fire propagation. In addition, a specific experimental test campaign has been conducted by UC-CSN to analyse cable fire propagation and improve data for validating computational models. This has also led to the definition of a specific model to address phenomena such as cable tray fire propagation. Finally, standards have been evaluated to enhance safety in nuclear power plants through the use of CFD.

According to the definition of the material's thermal behaviour in the CFD model FDS, it is necessary to conduct prior experimental characterization. To do so, thermal analysis apparatus, such as a simultaneous thermal analyser, can be utilized to study thermal decomposition reactions. Nevertheless, these techniques are very sensitive to the selected boundary conditions, which need to be carefully defined by the user based on the material and desired results. In this regard, UC-CSN has conducted important research on the influence of boundary conditions in the simultaneous thermal analysis on the thermal decomposition of thermoplastic polymers (Lázaro et al., 2019). Additionally, it has been analysed how the energy release by certain polymers in this apparatus can affect the results (Alonso et al., 2022). For complex components present in nuclear power plants, such as cables composed of multiple materials, it is common to perform bench-scale experimental tests, such as cone calorimeter tests, to analyse the entire cables and obtain the heat release rate per unit area, which can be directly used in FDS to define cable behaviour during combustion (Lázaro et al., 2023a).

Once the materials and components have been experimentally characterized, the data needs to be processed. Some material properties, like thermal conductivity, can be directly obtained from experiments, while other properties, such as kinetic parameters used to define reactions, require different methodologies. Throughout the projects, UC-CSN has developed new methodologies to obtain thermokinetic parameters for describing the thermal behaviour of materials in the CFD model. The methodology developed has specific characteristics, including a simple direct method defined in (Lázaro et al., 2021) for obtaining kinetic parameters for polymer thermal decomposition in a few seconds. More complex methodologies using artificial intelligence techniques, such as genetic algorithms, have been defined in (Alonso et al., 2019) and (Alonso et al., 2023). These methodologies use a CFD model of an experimental test, like cone calorimeter (Fig. 2a), to obtain the thermokinetic parameters that best fit the employed CFD model. This is important because, due to simplifications in some equations of the CFD models, directly using properties from experimental tests does not always yield the best CFD results. This is also why a study has been conducted on the influence of input parameter definition on decomposition prediction performed by CFD (Alonso and Alvear, 2020). The definition of cable combustion can be performed in FDS by directly imposing the heat release rate per unit area, but the incident heat flux on the cables can greatly affect this parameter, as evaluated by UC-CSN with the cone calorimeter tests (Lázaro et al., 2023b). UC-CSN propose a new methodology to better consider the effect of the incident heat flux on the heat release by the cables. Finally, it is also crucial to define the gases released during a fire in nuclear power plant simulations. UC-CSN has developed a methodology to estimate the FDS chemical reaction equation for modelling toxicity in fire scenarios (Lázaro et al., 2022a).

In addition, fire modelling in nuclear power plants involves predicting a large number of phenomena, whereas it is necessary to evaluate and validate the CFD model against real scenarios by comparing simulations with large-scale experimental tests (Fig. 2b). Some related achievements by UC-CSN include evaluating the influence of mesh size in real scenarios, as described in (Lázaro et al., 2016, 2017a,c, 2018; Lázaro et al., 2017b). The works performed on validating the species generated during a compartment fire (Lázaro et al., 2017b) and analysing the effect of ventilation on fire propagation in nuclear power plants (Lázaro et al., 2021) have also been significant. To improve the application of fire PRA, UC-CSN has evaluated the cable failure probability caused by a fire originating in a cabinet (Lázaro et al., 2020). All of these efforts have contributed to the definition of best practice guidelines for fire modelling in nuclear power plants.

With the goal of CFD validation and defining best practices for

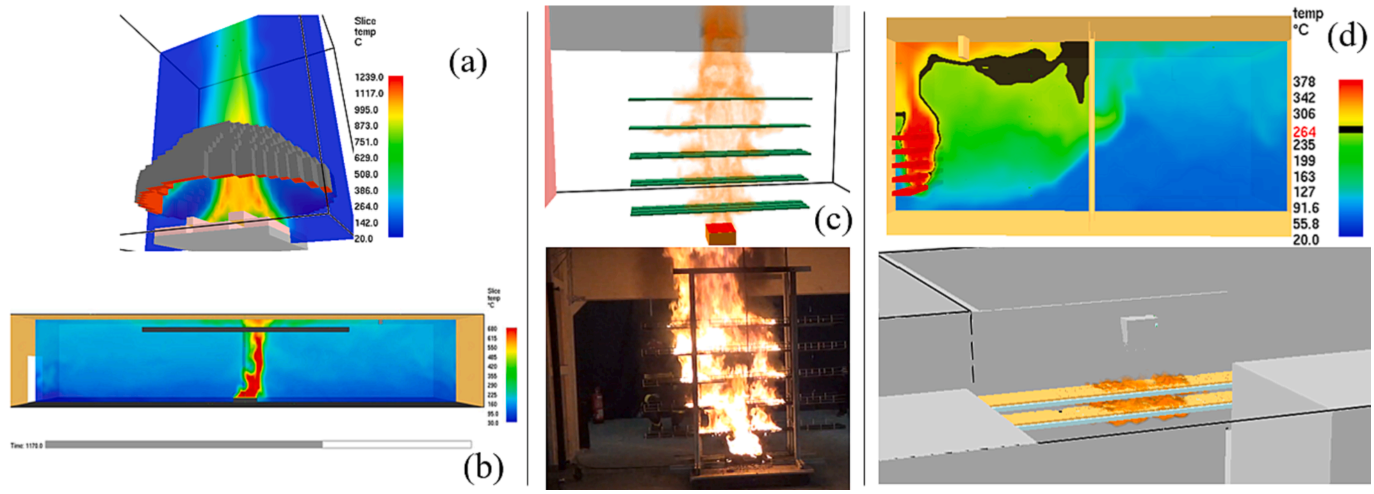


Fig. 2. Summary of some CFD fire safety results: (a) characterization and validation of thermal behaviour of typical components of NPP, (b) Modelling of real NPP fire scenarios, (c) Validation of CFD models by comparing with real scale experimental tests, and (d) Common OECD/NEA FIRE and PRISME Cable Benchmark Exercise.

simulations, the UC-CSN team has participated in the OECD PRISME 3 (Bascou et al., 2019) and FIRE Benchmark Exercise (Plumecocq et al., 2023) (Fig. 2d). During the different phases of this benchmark, UC-CSN has developed a modification of the FLASH-CAT model (NUR-EG/CR-7010, 2012) to predict fire propagation in cable trays and has subsequently used the results of the propagation and heat release by the cables as input in FDS to predict fire manifestations in the nuclear power plant (Lázaro et al., 2022a,b). This developed model has also been validated with large-scale experimental tests conducted in the Room Corner Test Apparatus by UC-CSN to analyse fire propagation in cable trays (Lázaro et al., 2022a,b) (Fig. 2c).

Another specific model being developed by UC-CSN to improve CFD application in NPPs is the neural network-based model described in (Lázaro et al., 2023). This model predicts tenability conditions during a fire in a nuclear power plant in real time by training it with validated fire computational models.

To provide users with a database that contains typical fire sources and material properties, as well as to facilitate the definition of CFD simulations, a tool called NuclearFire has been developed (NuclearFire 1.0). This tool is being improved for a second version, which will include a large database and more options for scenario definition.

The advances developed by UC-CSN also have a regulatory scope. To this end, analyses and comparisons of standards to enhance nuclear power plant safety have been carried out by the use of CFD. It allows performing detailed calculations in order to reduce the conservatism inherent in deterministic requirements. Additionally, in complex scenarios where this regulation may be difficult to satisfy, the use of CFD to support risk-informed regulation can be applied to demonstrate that fire damage to structures and systems important to safety does not affect their integrity.

3.3. Nuclear spent casks

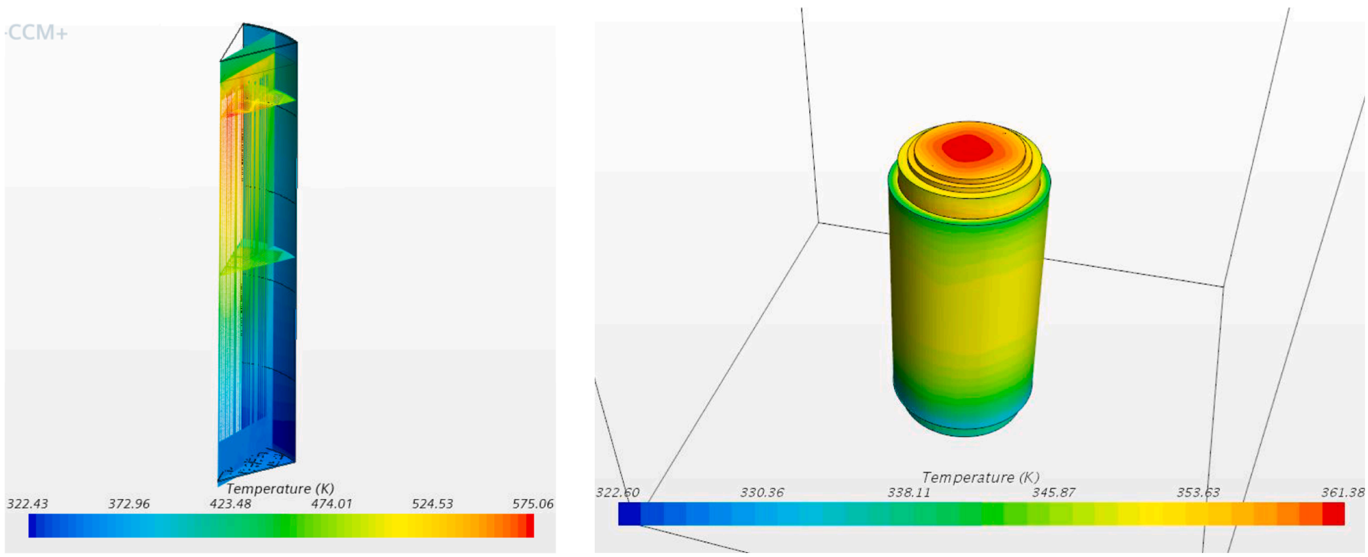
The advancement of CFD techniques in the nuclear industry over the years has made possible to obtain verified and validated CFD models for successful simulations and reliable results, as well as experience in dealing with specific thermal analysis problems. Within the expertise for CFD modelling, the solution algorithm must be defined, an appropriate turbulence model that gives reliable results for the characteristic flow of the problem must be chosen, and numerical parameters such as differentiation schemes, relaxation factors, convergence criteria, etc. must be correctly established.

In projects based on spent fuel containers carried out by **ENUSA**, for the thermal characterization of the cask/fuel through CFD codes, a two-step coupling methodology is followed. The first step consists of simulating the outside of the cask, modelling the external part of the container on the environment and its support slab; and the second step consists of simulating the inside of the cask that contains coolant gas surrounding the fuel elements, applying the heat transfer boundary conditions that are extracted from the first step. In this way, the precision of the calculations is improved employing numerical simulations with specific turbulence models, with respect to the use of empirical or semi-empirical correlations for the heat transfer mechanisms of the outer part of the cask (Benavides et al., 2018). This iterative two-phase methodology allows knowing the distribution of temperatures as well as the mechanisms of heat transmission inside the container. As a result, we can know one of the most important parameters which is the maximum rod temperature, and which must not exceed a specific value in accordance with current regulations.

This methodology has been correctly implemented with their respective sensitivity analysis of the mesh and of turbulence models, and validated through experimental results in TN-24P and DCS experimental cask. Also, for the DCS cask an approach of spacers in the fuel assembly modelled with porous media has been conducted. It has allowed it to be a reliable and useful methodology for its implementation in other containers such as HI-STORM 100. The modelling of the inside of the HI-STORM 100 with a high level of detail has resulted, despite its simplification in 1/8 of its cross section, in a computationally expensive model due to the large number of cells generated in the meshing of the fluid volume of helium (Esteban and Matías, 2022). The simulation, performed with a Realizable K-Epsilon Two Layer Buoyancy Driven turbulence model, has allowed to realistically predict the behavior of the fluid and the phenomena inside the canister with a very detailed geometry in addition to adequately capturing the heat transfer by the elements such as grids, nozzles and rods (Esteban and Matías, 2022) (Fig. 3a).

For the TN-24P cask, the turbulence model selected for the exterior cask simulations has been the Realizable K-Epsilon Shear Driven and the Realizable K-Epsilon Buoyancy Driven for the inner cask simulations due to the good agreement against experimental data obtained, and faster time to convergence (Benavides et al., 2019). Also, a study of the gaps between the canister and the inner cylinder has been carried out. The temperature results obtained on the outer surface can be seen on (Fig. 3b).

For the DCS container, the model used for the CFD simulations was the Realizable K-Epsilon. Several sensitivity studies have been



(a) (b)

Fig. 3. Temperature distribution of a) helium inside the canister in the radial and axial direction (HI-STORM 100), b) shell of the TN-24P cask.

performed under variety of heat loads and internal vessel pressures (Benavides et al., 2020). The case with the most accurate results is obtained, in addition to a better understanding of the different heat transfer mechanisms interactions under different conditions.

3.4. Fuel assemblies

Related to fuel assembly projects carried out by **ENUSA**, the main objective is to have a better understanding of fuel assembly performance to assure the integrity during operation and handling. This allows to go to increased cycle length and burnup and more challenging operational scenarios. The calculation of hydraulic forces in operating conditions using porous media and hydraulic resistance force in the FADA accident, were used as inputs to mechanical code to study the integrity of the fuel assembly in that situation. For these projects and others such as the study of different bottom nozzles designs, standard k-epsilon models were used, as the averaged values of forces and velocities are enough to characterize the flow. Other problems like GTRF (Fig. 4a), for which pressure or velocity fluctuations need to be properly characterized, have to used more complex models such as LES turbulence models.

One of the conclusions of all these projects is that simplifying geometries is a good way to model properly some problems, for example by replacing zones with less influence on the flow with porous media, applying symmetries or analysing only a part of the geometry.

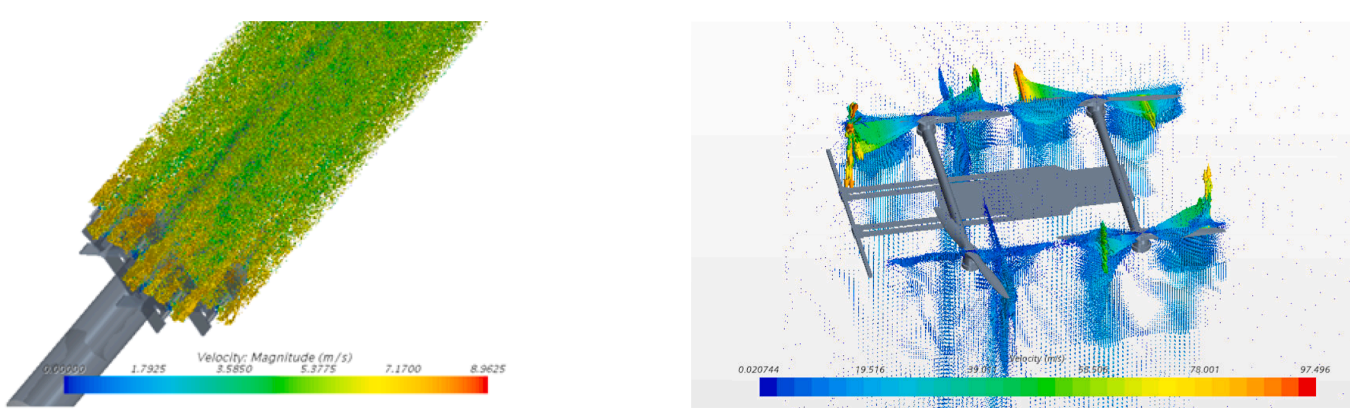
Also, CFD codes could be used to design other elements that are also relevant for the future of the nuclear fission energy. In the case of ENUSA, some simulations were done to help in the design of robots and drones for radiological characterization (Fig. 4b).

3.5. Containment

As results of the projects carried out by the **UPM** indicated in the Research Synthesis and extending their outcomes, a PhD thesis was developed (Martín-Valdepeñas et al., 2007) in this work CFX commercial CFD code was adapted for hydrogen containment analyses:

- Two examples of full plant applications were completed: a 3-loop large-dry PWR Westinghouse design and a 3-loop PWR KWU design. This analysis was done only for short temporal windows during the hydrogen release phase of the in-vessel accident for a limited number of sequences due to computational limitations.

The main outcomes after ten years of research modelling in 3D with GOTHIC are:



(a) (b)

Fig. 4. (a) Q-criterion isosurfaces around the rod fuel for GTRF analysis, and (b) Velocity vector around a drone.

- The continuous evolution of the 3D model development methodologies with GOTHIC has found an optimal balance between computational cost and thermal–hydraulic resolution of the models. The relative coarse-mesh approach used by GOTHIC allows addressing the long transients (several hours) of hypothetical accidents driven by phenomena with small characteristic scales (below the millimeter) within large computational domains (buildings 60 m in height and 40 m in diameter). Depending on the containment design, different strategies of geometrical simplification and mesh adaptation are needed, varying from a "Nesting Dolls" approach (Estévez-Albuja et al., 2021a; Jimenez et al., 2015) to an *a priori* adaptation of the geometry to the mesh, called Preventive Methodology (Arfinengo-del-Carpio et al., 2021), as shown in Fig. 5.
- The code validation has proven its ability to reproduce the main drivers of the containment thermal hydraulics such as wall condensation with large concentrations of non-condensable gases, buoyancy-driven flows, conjugate heat transfer, etc. (Vázquez-Rodríguez et al., 2022). Furthermore, under the correct set of hypotheses, it is also possible to replicate experiments on the main containment safety systems of PWR-W, such as the spray operation (Vázquez-Rodríguez et al., 2023) and the PAR actuation.
- From the 3D modelling work done previously in the research group (Bocanegra et al., 2016), it was also possible to evaluate the equipment qualification and instrumentation surveillance criteria for a PWR-W containment (Jimenez et al., 2017), developing a methodology for estimating the hydrogen combustion risk in a severe accident (Fernández-Cosials et al., 2017), an evaluation of the information on the hydrogen concentrations that may be available for the operators in the control room to use the FCVS as a hydrogen mitigation measure (Díez Álvarez-Buylla et al., 2021), and a detailed characterization of the 3D flow patterns within the containment of the AP1000 (Estévez-Albuja et al., 2021a).
- For the ex-vessel phase of a severe accident, further developments are needed regarding the mass and energy releases and the corium modelling.

The most recent research line is integrating all the information discussed above from some of the UPM in-house software whose development started in the 90s, such as PARUPM (Domínguez-Bugarín et al., 2022; Jimenez et al., 2007) and the sigma criterion for the hydrogen risk evaluation (Martín-Valdepeñas et al., 2007), to the *a priori* modification of the geometry and the implementation of the spray safety system. The combination of all the former research lines enables a comprehensive evaluation of the impact of different safety system actuation on the hydrogen risk in severe accident conditions. Fig. 6 shows the impact of the spray actuation on the hydrogen risk based on the sigma criterion.

The main outcome expected from this on-going work is to provide clear guidelines for severe accident management to minimize the risk of combustion inside the containment.

3.6. Other applications

The various activities conducted by **UPV** have predominantly focused on single-phase problems. Throughout the collaboration between UPV and CSN, multiple thematic areas have been covered, including thermal cycles and pressure thermal shock, the effects of spacer grids on turbulent parameter predictions, disruption of stratification layers through jets, UQ methodologies assessment, and calculations of buoyancy forces in different geometries. The research synthesis section provided an overview of each topic, offering additional details regarding the primary objectives and conclusions associated with each of them. Further information about geometry, mesh, models and data treatment employed by the UPV can be found in the respective references. Additionally, Fig. 7 provides a summary of qualitative results from the benchmarks conducted by the UPV, aiming to facilitate readability and comprehension for each activity.

- In relation to the OECD/NEA-Vattenfall CFD Benchmark Exercise 2008–2011, the main goal was to understand and predict the physics behind the T-Junction problem. One of the key findings highlighted the significant importance of accurately representing turbulence in achieving satisfactory performance across the various codes employed. It was strongly recommended to utilize LES models as opposed to SAS or RANS models. LES models demonstrated superior capabilities in capturing the turbulent flow characteristics, resulting in improved simulation accuracy. UPV-LES simulations demonstrated a good agreement on the velocity profiles and turbulent parameters employing a relatively small computational power (OECD/NEA/CSNI, Smith, et al., 2011).
- Moving on to the OECD/NEA-KAERI CFD Benchmark Exercise 2010–2012, the activities in this benchmark exercise primarily focused on obtaining turbulent parameters following a generic spacer-grid configuration in a rod-bundle structure (Fig. 7a). It was observed that incorporating second-order accurate discretization algorithms was crucial for obtaining reliable outcomes. The UPV employed a second-order discretization scheme for both time and space with a good agreement with the experimental data. Regarding the turbulence model, while RANS models performed well in calculating average velocity profiles, LES models offered superior predictive capabilities for the overall parameters studied. Nonetheless, computational cost again play a role for some participants as the UPV

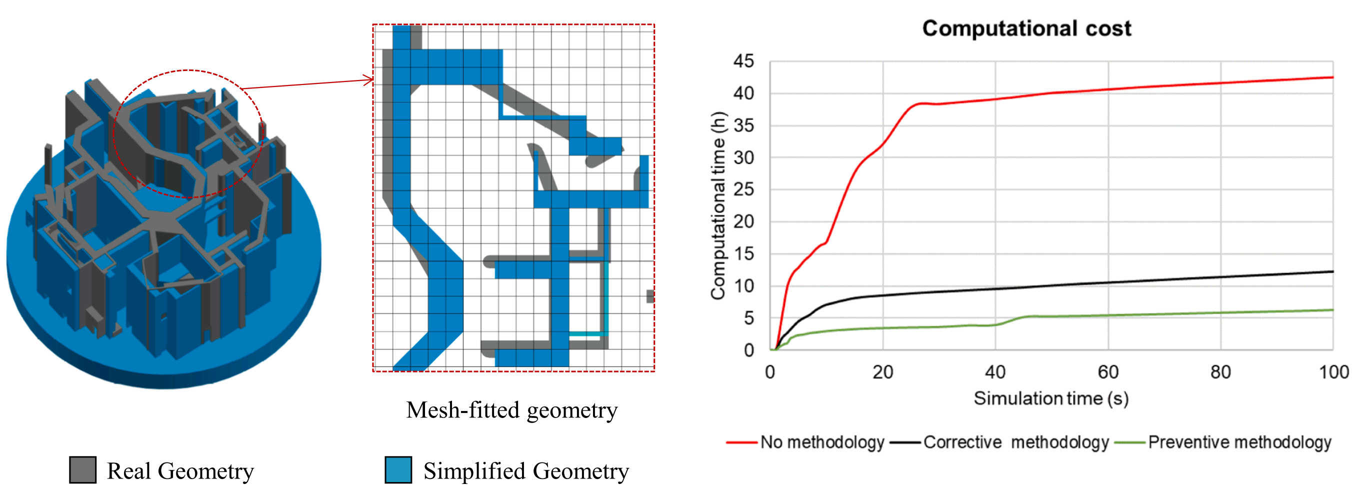


Fig. 5. Computational cost optimisation via an a priori adaptation of the geometry to the mesh.

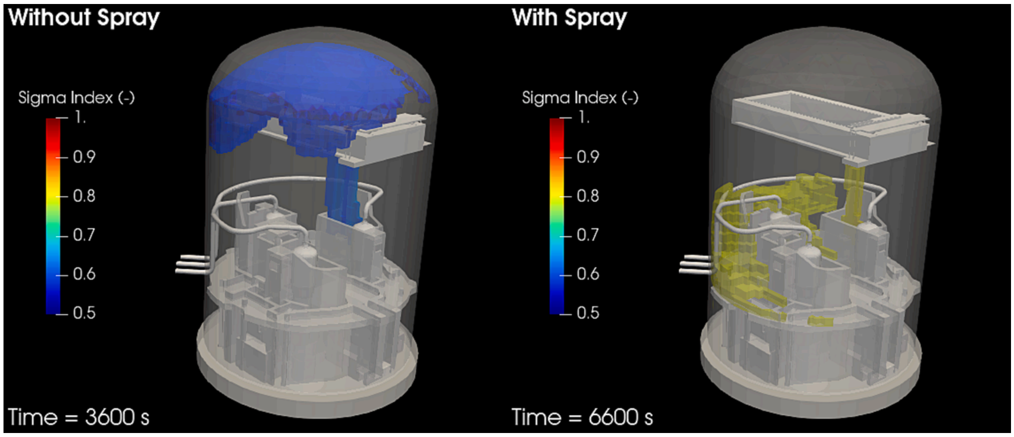


Fig. 6. Spray actuation on the hydrogen risk based on the sigma criterion.

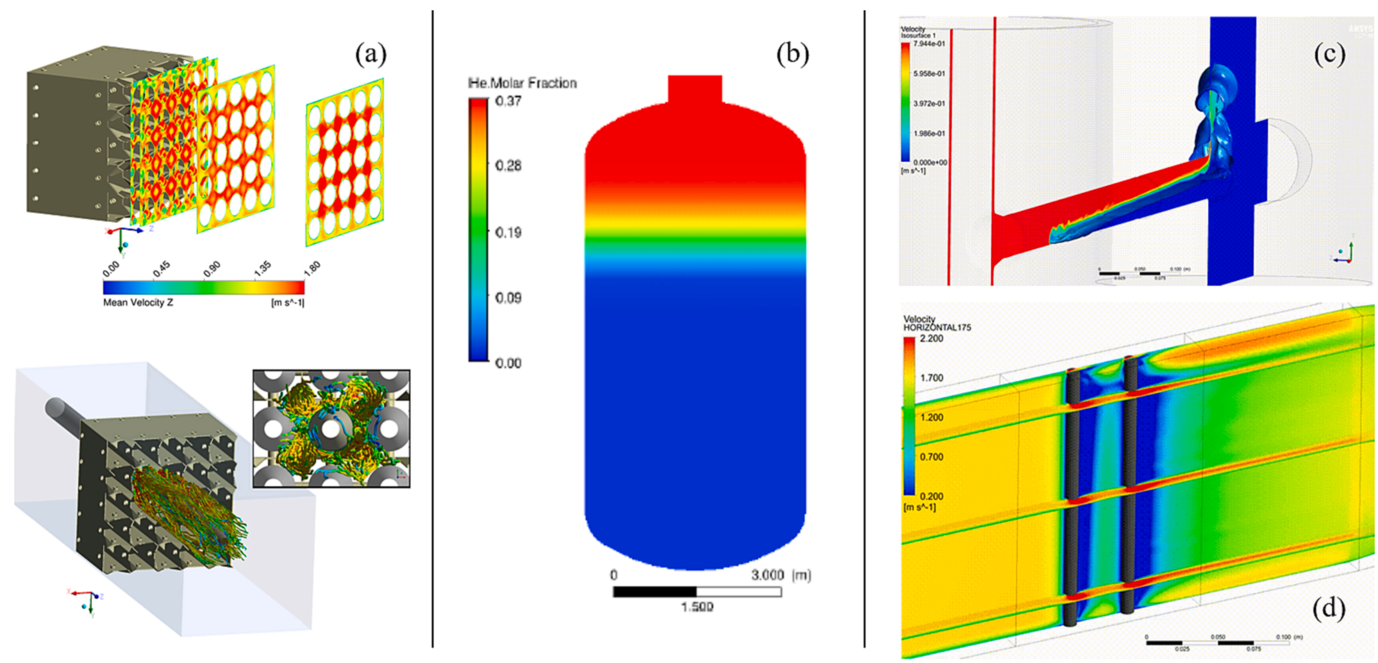


Fig. 7. Summary of different benchmarking results: (a) Velocity profile and streamlines for the OECD/NEA-KAERI CFD Benchmark Exercise 2010–2012, and (b) Helium molar fraction OECD/NEA-PSI CFD Benchmark Exercise 2012–2014, (c) Velocity isosurface for the OECD/NEA-Texas A&M University Benchmark Exercise 2017–2019, (d) Velocity contours for the OECD/NEA-OKBM Afrikantov Benchmark Exercise 2019–2021.

which were limited to RANS or hybrid models (OECD/NEA/CSNI, Smith, et al., 2013).

- In the OECD/NEA-PSI CFD Benchmark Exercise 2012–2014, the focus shifted to containment calculations using CFD. This exercise provided insights into the dynamics of transient events within the containment structure (Fig. 7b). As expected, user's choice of models emerged as a critical factor in accurately capturing the transients and ensuring the correct representation of the system behavior. Surprisingly, the selection of the turbulence model did not demonstrate a direct correlation with the correct prediction of transients. In fact, simulations employing LES models failed to meet expectations due to unfulfilled mesh requirements (Andreani et al., 2015).
- The most significant conclusions drawn from the OECD/NEA-PSI CFD GEMIX Benchmark Exercise 2014–2016 primarily focused on the development of uncertainty quantification methodologies in CFD codes. Traditional methods such as Wilks-type approaches are often computationally prohibitive in CFD simulations. In contrast, both metamodeling techniques (propagation) and extrapolation methods (comparing uncertainty in open and blind tests) achieved good results, even with a relatively small number of simulations. UPV started developing the PCE method with satisfactory results when using uncertain variables with uniform probability density functions (OECD/NEA/CSNI, Fokken, et al., 2019).
- The OECD/NEA-Texas A&M University Benchmark Exercise 2017–2019 was designed with a more complex geometry to push the boundaries further in single-phase applications with buoyancy effects and the quantification of uncertainty in CFD models (Fig. 7c). In fact, the activity involved conducting simulations for approximately 42 s (real time), leading to a significant increase in computational cost. The results once again highlighted the importance of utilizing LES models to solve problems where the turbulent component heavily influences the fluid behavior. Regarding uncertainty quantification, UPV continued developing the PCE method, extending its use to uncertain variables with a normal probability density function (Rivera et al., 2021).

- The most recently completed activity corresponds to the OECD/NEA-OKBM Afrikantov Benchmark Exercise 2019–2021, and its results are not publicly available. The focus of this activity was to validate different approaches for calculating fluid-induced vibrations in a tube bundle (Fig. 7d). Preliminarily, it can be mentioned that the choice of LES turbulence model and the level of detail in resolving vortices were crucial for accurately predicting the experiment as well as the coupling method between CFD and mechanical code. The one-way coupling approach applied by the UPV delivered good results for the cases where vortex shedding and the natural vibration frequency of the rods were not synchronized.

4. Challenges and expected developments

4.1. Identified challenges and general roadmap

As has emerged in the course of the present review, over the recent decades there has been a notable increase in the use of CFD models for the prediction of flow and transport phenomena within nuclear safety issues. This shift towards 3D CFD methodologies can be attributed to the recognition that numerous safety–critical phenomena within these systems, such as boron dilution, pressurized thermal shocks, main steam line breaks (with inherent flow asymmetry), containment atmosphere mixing and stratification, and hydrogen combustion processes, inherently exhibit three-dimensional characteristics. The incorporation of CFD methodologies into formal NS studies represents a complex task characterized by several significant challenges. One prominent challenge arises from the absence of well-established and universally accepted methodologies. For instance, in cases requiring coupling with other physics and thermal hydraulics at different scales, a common strategy should be adopted by the community in order to enhance its capabilities. In addition, the high-requirements expected in safety studies within the nuclear field arise the need for UQ analysis with solid methodologies, proven for different CFD studies in the field. UQ methodologies, though powerful, often lack definitive proof of applicability due to the substantial computational demands and associated costs they entail. According to the NEA/CSNI/R(2016)4 report (Bestion et al., 2016), UQ includes two distinct contributors: stochastic uncertainty, stemming from factors like the propagation of measurement uncertainties in boundary conditions, leading to a scatter around the 'real' value; and epistemic uncertainty, resulting from gaps in knowledge such as unknown boundary conditions, model geometry, or assumptions in physical modeling. Epistemic uncertainty cannot be quantified through statistical evaluations of parametric studies and frequently introduces biases into analysis results. While methodologies for UQ have been developed or adapted from system-scale analyses, their widespread adoption remains limited and a greater effort should be made by the CFD community, including Spain and Portugal.

Access to pertinent information constitutes another substantial challenge within the field of CFD in NS studies. According to the OECD/Nuclear Energy Agency WGAMA CFD Task Group ongoing studies, this challenge manifests in two dimensions: firstly, for researchers employing CFD, it involves access to comprehensive databases housing experimental results, including "CFD-grade" or Direct Numerical Simulation (DNS) data, crucial for code validation. Secondly, for decision-makers and project managers, it entails access to impartial, non-commercial information concerning CFD's capabilities, potential benefits, and inherent limitations, enabling informed decision-making processes. The CFD community involved in nuclear safety studies should continue pushing in this direction, joining efforts together to spread both their needs from other researchers and the capabilities of current CFD codes.

The human factor aspect of CFD implementation in the nuclear safety framework presents one of the most complex challenges. The constitution of a proficient "CFD team" that possesses expertise in both CFD methodologies and deep knowledge of nuclear safety within a research team or a company is itself a challenging task. Moreover, fostering efficient collaboration between this CFD team and other teams engaged in different aspects of physics and thermal hydraulics across varying scales poses an additional challenge. In accordance with numerous benchmarking activities aimed at CFD model validation, it becomes evident that discrepancies not only persist among results obtained from different computational codes but also in the CFD user decisions (Rein et al., 2009). Consequently, there exists a need to establish standardized methodologies that systematically demonstrate their consistency. Within the field of CFD, extensive efforts have been undertaken by the scientific community to formulate best-practice guidelines, with the primary objective of empowering researchers and engineers with a well-established framework to mitigate the aforementioned issues (OECD/NEA/CSNI, Mahaffy, et al., 2015). However, it is necessary to acknowledge that these actions have not provided a clear solution, primarily due to the inherent variability of scenarios encountered. Additionally, in fields like fire safety, the different fire related phenomena can impose different length and time scales for the computational model resolutions, being the extensive range and incompatibility of scales is an unavoidable complexity of explicit fire modelling (Torero et al., 2013). Although fire models like FDS are widely validated, there is still the necessity to validate it for specific purposed in order to improve the predictions.

Regulatory authorities, aware of the role played by CFD in the domain of nuclear safety studies, have shown keen interest in its applications while concurrently expressing concerns regarding the reliability and trustworthiness of the results generated through this methodology. During the recent *9th Computational Fluid Dynamics for Nuclear Reactor Safety* conference hosted in 2023 by Texas A&M University in College Station, the United States NRC has raised its pursuit of a "minimum standards" approach tailored specifically for single-phase flows. This initiative aims to facilitate the acceptance and integration of CFD-based validation studies within the regulatory framework for nuclear applications. The Spanish nuclear regulatory authority, CSN, has also shown interest in this initiative and further engagements are expected to happen in the next years. CSN has recently received topical reports for licensing methodologies in which some of the thermo-hydraulics issues are supported with CFD simulations. The need to establish this kind of framework to evaluate such studies is there. In the meantime, a case-by-case approach should be used from the regulatory perspective.

Cost considerations are also another main challenge in the utilization of CFD for NS studies. The computational cost associated with CFD calculations remains a substantial limiting factor, although advancements in computing power, continue to mitigate this challenge. Furthermore, the cost associated with geometry design and mesh generation prior to initiating CFD simulations also needs to be taken into account. This cost can vary depending on the chosen meshing technique and can be especially expensive for very highly refined meshes. While automatic meshing tools offer rapid solutions, the construction of fully conformal hexahedral meshes, in some instances, remains one of the most time-consuming phases of a study. The CFD research community is actively engaged in advancing techniques adapted for high-performance computing systems. However, experts in nuclear safety CFD must need to make deliberate efforts to integrate these promising new solutions into the framework outlined within this paper. A noteworthy example of such innovation is the ALYA code developed by the BSC for the MareNostrum Supercomputer. The ALYA code's team is developing a high-performance computational tool explicitly designed for massively parallel supercomputing architectures. Exploring potential collaborations between the nuclear safety CFD community and the BSC holds the promise of substantial enhancements in simulation performance.

In broad terms, to address the various challenges posed to CFD codes, it is expected that the scientific communities in Spain and Portugal will explore possible approaches. Promoting knowledge sharing, exemplified by the continuous and commendable efforts collaborating with working groups such as the WGAMA CFD task group and international workshops like CFD4NRS, constitutes an effective strategy for advancing the application of CFD in the context of NS analyses. An stride towards enhancing the reliability and consistency of CFD models within the NS field involves the promotion of benchmarking exercises. In Spain and Portugal, the collaboration in these tasks will be continued and nuclear engineering groups are encouraged to join the activities.

Another notable avenue for progress lies in the establishment of databanks covering safety-related configurations. Such repositories would facilitate the identification and accessibility of both experimental data and numerical solutions. Some research groups in Europe, such as the Thermo-Fluid Dynamics and System Analysis' group at the Institute of Energy and Climate Research at Forschungszentrum Jülich GmbH in Germany is fostering this activity through international associations (Kelm et al., 2021). The UPV has committed to support the initiative, but a bigger effort needs to be made by the community. In addition to the potential benefits of such database, there is potential value in exploring the adaptability of existing ones, originally constructed for the development and validation of system-scale analyses, to meet the specific requirements of CFD applications in the nuclear safety domain.

The ongoing efforts to enhance and commercialize novel SMR designs, including III and IV generation reactors, can find a formidable ally in the CFD. The versatile potential of CFD simulations can play a key role in advancing these unique SMR designs, offering a robust tool for their optimization and validation. Examples of the use of CFD in the context of water-cooled SMR designs have been documented in the existing body of literature, with a notable expansion in such studies in recent years. These investigations have even explored highly detailed resolutions, simulating the entire geometry of the reactor for steady-state simulations, as exemplified by the work of (Böttcher and Sanchez-Espinoza, 2023). In the domain of liquid metal-cooled SMRs, significant advances were established by Roelofs et al. (2019), laying a robust foundation for CFD studies. It is noteworthy, however, that current CFD research in this domain predominantly affects single-phase flows, despite the CFD potential for two-phase flow investigations in the context of liquid metal applications. Furthermore, the application of CFD with alternative coolants, distinct from water, is currently at a relatively early stage of development and lacks comprehensive studies including both CFD-grade experimental measurements and CFD validation. Regrettably, the research status of future SMRs technology within Spain and Portugal remains somewhat limited. Nonetheless, a promising trajectory is emerging, as collaborative initiatives with other European organizations in this sphere begin to take shape. For instance, promising collaborative efforts with PANDA facility and UPM are currently under development, setting the stage for forthcoming CFD investigations in the context of system testing for SMRs, as detailed in the work of Paladino et al. (2023).

4.2. *Future lines in Spain and Portugal*

This last section includes the different future activities expected for the following years within the organization in Spain and Portugal researching on CFD for NS. The main areas of future research for **UPCT** are focus on the application of turbulent combustion models to H_2-CO mixture employing RANS approaches. Reduced-order H_2-CO will be validated through reference databases, including experiments with flame acceleration. As a last step, the future research lines will focus on the application this type of models to PWR containment scenarios (OPENHYCOMB project with the CSN).

Within the following years, **UC** and CSN will jointly collaborate in the development of specific CFD models to improve prediction of various fire phenomenon that have not been completely validated yet as cable trays fire propagation, or combustion under vitiated atmospheres, and will increase the validation of the existing CFD models by the comparison to the large-scale experimental tests to be performed in the UC installations, and in international programs like Fire Risk Assessment through Innovative Research (FAIR) Project. Additionally, artificial intelligence-based methods will be developed to reduce CFD computational cost, allowing real time simulations to be used in emergency management at nuclear facilities.

The main effort that **ENUSA** expect to do in the coming years on CFD for NS is to continue working on the thermal characterization of the different container Spent Nuclear Containers designs that will be used in the Spanish ISFSI, applying the previously acquired knowledge regarding models and detailed geometry. Additionally, ENUSA will seek opportunities to perform thermal and CFD calculations in SMRs.

At **UPM**, the 3D GOTHIC model development methodologies have proven to be ready for technical-scale applications. The priority in future years will be to use these consolidated methodologies to produce an extensive database of containment sequences simulated with 3D resolution. The detailed implementation of the most relevant containment safety systems for Spanish nuclear power plants is being consolidated in ongoing projects: fan coolers (INTERCON3D Project with the CSN), spray safety system (GOMERES-2 Project with the CSN), and PARs (GOMERES-2 and EC-HORIZON AMHYCO Project). The 3D GOTHIC Models will be used to continue investigating design basis accident and in-vessel severe accident sequences, and also to advance on the state-of-the-art by producing the first 3D investigations of the ex-vessel phase of severe accidents. The UPM is expected to come with a methodology to study SMRs containments during transients using GOTHIC and commercial CFD software in the coming years. Additionally, more research on the different types of VVER reactor containments will continue in pair with their future build up. Finally, the use of GOTHIC and CFD to assess micro-reactors safety will be a part of the future studies.

UPV will continue developing methods for efficient UQ in CFD, specifically tackling the extension of PCE for all types of uncertain variables and the development of reduced polynomials order techniques such as sparse-grids. The coupling between CFD with FEA codes will also be explored for certain relevant scenarios in nuclear safety such as pressure thermal shock. Finally, as part of the future portfolio, comparatives between CFD commercial codes and new open sources codes with HPC capabilities will be done in collaboration with the BSC.

CSN, Spanish regulator, will continue supporting and collaborating with the Spanish organizations in the different activities for CFD within the NS framework. The main goal of CSN is applying the lessons learned, for instance throughout WGAMA benchmark participations or projects with UC, UPCT, UPM and UPV, to the evaluation of some utilities submittals about licensing methods modifications that make use of CFD calculations as hypothesis justification within methodologies.

5. Conclusions

The use of CFD models has become increasingly important in the field of nuclear reactor safety studies. This shift is primarily attributed to the rise in computational capacity together with enhancements in experimental methodologies, accumulated experience, and the refinement of complementary tools, including meshing and post-processing. In this context, CFD is well-suited to analyze various safety–critical aspects of nuclear reactors, such as cooling systems, combustion processes, and containment structures, which inherently possess three-dimensional characteristics. Traditional one-dimensional codes often require conservative approximations to account for these complexities. In contrast, 3D CFD approaches provide the precision and spatial resolution needed for accurate predictions across a wide range of scenarios in nuclear safety. The global efforts dedicated to verifying and validating these models are crucial, as they ensure that CFD tools can consistently deliver reliable and, when necessary, conservative results for specific flow configurations. In Spain, significant advancements have been made in the field of CFD for nuclear safety research, particularly in the context of code development and validation, combustion studies, nuclear spent-cask simulations, fuel assembly analyses, and containment investigations.

Regarding CFD code development, UPCT have done research, collaborating with international partners to refine numerical CFD codes. In the domain of combustion and fire safety research, UPCT and the UC have actively cooperated with the Spanish regulator, CSN, to apply CFD fire codes in nuclear power plants. Their projects include various subareas such as fire modeling methodologies, software development for fire scenario creation, and validation of CFD codes through large-scale experimental tests. Furthermore, ENUSA has dedicated significant resources to researching nuclear spent casks, focusing on dry storage systems. Through CFD modelling, they aim to accurately calculate, among other parameters, the peak cladding temperature during dry storage, a critical parameter for spent fuel management. Collaborations with research institutions like UPM have resulted in validated methodologies for thermal calculations of spent nuclear fuel containers. In terms of fuel assembly studies, ENUSA has participated in benchmark exercises to assess CFD predictions of temperature, velocity, and pressure loss over fuel rod bundles. These studies involve the analysis of hydraulic forces, fuel assembly distortion, pressure drop over grids, and fuel assembly integrity, contributing to the understanding and improvement of fuel assembly performance and safety. UPM has done extensive research in containment analysis using CFD-like tools, particularly GOTHIC. Projects span different topics, such as hydrogen behavior during severe accidents and combustion risk assessment in filtered containment venting systems. These initiatives have led to the development of 3D containment models, validation through experimental data, and ongoing collaborations under European projects like AMHYCO. UPV has focus on benchmarking activities within the WGAMA CFD Task Group tackling a wide variety of topics for nuclear safety such as grid spacers, buoyancy effects, uncertainty quantification stratification and fluid–structure interaction.

Several significant challenges were identified in the incorporation of CFD methodologies into formal nuclear safety studies. One key challenge is the lack of universally accepted methodologies, especially when coupling CFD with other physics and thermal hydraulics at different scales. Addressing this issue requires a common strategy adopted by the community to enhance the capabilities of CFD. Uncertainty quantification also poses challenges, as it demands solid methodologies proven for different CFD studies but involves substantial computational demands and costs. Access to databases with experimental results and impartial information about CFD capabilities is essential for researchers and decision-makers. As a result of the CFD features, regulatory authorities are showing keen interest in CFD applications but also express concerns about the reliability of results. The addition of CFD calculation for licensing purposes would be a cornerstone for CFD's continued development. To address all these challenges, the scientific community in Spain and Portugal will prioritize knowledge sharing and collaboration between both research institutions and regulators. Cooperative efforts with working groups and participation in benchmarking exercises will help advance CFD applications in nuclear safety studies and improve the reliability and consistency of CFD models.

CRediT authorship contribution statement

Y. Rivera: Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing. **A. Escrivá:** Data curation, Funding acquisition, Investigation, Resources, Software, Validation, Visualization, Writing – original draft. **C. Berna:** Data curation, Investigation, Resources, Software, Validation, Visualization, Writing – original draft. **E. Vela:** Data curation, Funding acquisition, Investigation, Resources, Software, Validation, Visualization, Writing – original draft. **J.M. Martín-Valdepeñas:** Data curation, Funding acquisition, Investigation, Resources, Software, Validation, Visualization, Writing – original draft. **G. Jiménez:** Data curation, Funding acquisition, Investigation, Resources, Software, Validation, Visualization, Writing – original draft. **C. Vázquez-Rodríguez:** Data curation, Investigation, Resources, Software, Validation, Visualization, Writing – original draft. **K. Fernández-Cosials:** Data curation, Investigation, Resources, Software, Validation, Visualization, Writing – original draft. **F.J.S. Velasco:** Data curation, Investigation, Resources, Software, Validation, Visualization, Writing – original draft. **R.A. Otón:** Data curation, Investigation, Resources, Software, Validation, Visualization, Writing – original draft. **I. Esteban:** Data curation, Investigation, Resources, Software, Validation, Visualization, Writing – original draft. **R. Matías:** Data curation, Investigation, Resources, Software, Validation, Visualization, Writing – original draft. **D. Lázaro:** Data curation, Investigation, Resources, Software, Validation, Visualization, Writing – original draft. **M. Lázaro:** Data curation, Investigation, Resources, Software, Validation, Visualization, Writing – original draft. **E. Morgado:** Data curation, Funding acquisition, Investigation, Resources, Software, Validation, Visualization, Writing – original draft. **J. Benavides:** Data curation, Investigation, Resources, Software, Validation, Visualization, Writing – original draft.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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