Nuclear Safety
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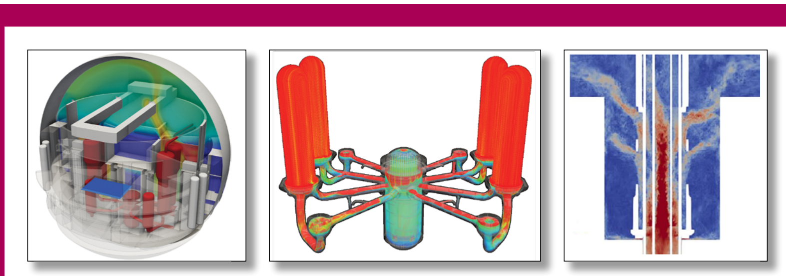
CSNI Technical Opinion Paper No. 20

Use of Computational Fluid Dynamics for Nuclear Safety



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Nuclear Safety

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Use of Computational Fluid Dynamics for Nuclear Safety

NEA No. 7615

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Cover photos: CFD calculation results for containment (Stephan Kelm, FZJ); Primary circuit (Nicolas Mérigoux, EDF); Control rod guide housing (Sofiane Benhamadouche, EDF).

Foreword

This Technical Opinion Paper (TOP) studies the emerging use of computational fluid dynamics (CFD) as an additional tool for the evaluation of safety cases implying thermal hydraulics. CFD allows a finer description of the phenomena compared to the present system-scale tools. This appears promising but also raises new questions in the assessment of safety studies and its use is currently still limited to a relatively small number of applications. The development of CFD is a fast-evolving and relatively recent activity in the context of nuclear safety. The Computational Fluid Dynamics Task Group (CFDTG), which is part of the Nuclear Energy Agency (NEA) Committee for the Safety of Nuclear Installations (CSNI) Working Group on the Analysis and Management of Accidents (WGAMA), has been continuously conducting collaborative work in this field since an explanatory meeting in 2002. Its most recent activity, started in 2019 and entitled "The CFD for Nuclear Reactor Safety Phase 5 – Toward an Enlarged Use", aims more specifically at providing the nuclear safety community with a clear view of:

- the current use and capabilities of CFD within safety demonstrations; and
- the main challenges hindering a broader use of CFD in nuclear safety studies, together with a discussion of possible ways of overcoming these.

This report was approved by the CSNI in May 2022 and prepared for publication by the NEA Secretariat.

Acknowledgements

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List of abbreviations and acronyms

ASN	Autorité de Sûreté Nucléaire (Nuclear safety authority, France)
BPG	Best practice guidelines
CAD	Computer-aided design
CAE	Computer-aided engineering
CFD	Computational fluid dynamics
CFDTG	Computational Fluid Dynamics Task Group (NEA)
CL	Cold Leg
CMFD	Computational multiphase fluid dynamics
CRUD	Chalk River Unidentified Deposits
CSAU	Code scaling, applicability, and uncertainty
CSNI	Committee on the Safety of Nuclear Installations (NEA)
DC	Downcomer
DDT	Deflagration to detonation transition
DIAS	Dynamic-Implicit-Additional-Source
DNB	Departure from nucleate boiling
DNS	Direct numerical simulation
D&V	Development and validation
ECC	Emergency core cooling
GPU	Graphics processing unit
HPC	High performance computing
HZDR	Helmholtz-Zentrum Dresden-Rossendorf
IAEA	International Atomic Energy Agency
IRSN	Institut de radioprotection et de sûreté nucléaire (Institute for radiological protection and nuclear safety, France)
IRWST	In-containment refuelling water storage tank
KKG	Kernkraftwerk Gösgen (Gösgen Nuclear Power Plant, Switzerland)
LES	Large eddy simulation
LOCA	Loss-of-coolant accident
LWR	Light water reactor
NRC	Nuclear Regulatory Commission (United States)
NRS	Nuclear reactor safety
ONCORE	Open-source Nuclear Codes for Reactor Analysis

PIRT	Phenomena Identification and Ranking Table
PTS	Pressurised thermal shock
PWR	Pressurised water reactor
R&D	Research and development
RANS	Reynolds-Averaged Navier-Stokes
RCP	Reactor coolant pump
ROM	Reduced-order models
RPV	Reactor pressure vessel
RTE	Radiative transport equation
SBO	Station blackout
SG	Steam generator
SOA	State-of-the-art
TOP	Technical Opinion Paper
TSO	Technical safety organisations
UPTF	Upper Plenum Test Facility
UQ	Uncertainty quantification
V&V	Verification and validation
WGAMA	Working Group on Analysis and Management of Accidents (NEA)

Executive summary

Three-dimensional computational fluid dynamics (CFD) applications are increasingly used to evaluate nuclear reactor safety (NRS) cases implying thermo-fluid dynamics. CFD provides greater phenomenological detail compared to established tools but also raises questions regarding the valuation and integration of CFD-based safety studies, which remain limited to a relatively small number of applications. For this reason and given the fact that the development of CFD is a fast-evolving and relatively recent activity in nuclear safety, the Computational Fluid Dynamics Task Group (CFDTG), which is part of the Working Group on the Analysis and Management of Accidents (WGAMA) of the Nuclear Energy Agency (NEA) Committee for the Safety of Nuclear Installations (CSNI), conducts collaborative work in this field that was initiated by an explanatory meeting in 2002. The present Technical Opinion Paper (TOP) was developed in the context of the Committee's recent activity, entitled "The CFD for Nuclear Reactor Safety Phase 5 – Towards an Enlarged Use". It seeks to provide a clear picture of the use and capabilities of CFD as well as of the main challenges hindering greater use of CFD in nuclear safety studies. This is complemented by a discussion of the possible ways of overcoming these challenges.

The writing of this TOP has been driven by several expert meetings and an analysis of a dedicated survey on the current use of CFD in NRS across a range of stakeholders (safety authorities, technical safety organisations, industry and academic institutions). The report first analyses the motivations for using CFD applications and the corresponding requirements for the qualification of the methods. It then examines the state of the art of current capabilities and ongoing activities. The report finds that the added value of CFD applications compared to established methods is its fundamental scalability and the increased level of insight, and thus the enhanced understanding and reliability of evaluations of physical phenomenology. CFD has a wide range of applications but high requirements for validation data and often a high computational cost. It is evolving rapidly and many of its applications are oriented towards nuclear energy. Development concerns single-phase as well as multiphase configurations and can also consider coupling with multiple physics (conjugate heat transfer, structural mechanics, neutronics) or multiple scales (physical to system scale). On this basis, the TOP focuses on the (slow) integration and actual use of CFD in NRS studies, where it has been accepted in a relatively small number of cases so far. This is partially related to the high level of requirements associated with safety studies. Three illustrative examples are examined: the analysis of heterogeneous boron dilution, a pressurised thermal shock situation and dry cask concepts.

While CFD capabilities are continuously improving as tools and methods are developed, several challenges have been identified to further extending the use of CFD in NRS. They concern the lack of established methodologies (e.g. uncertainty quantification), the availability of and access to an experimental database for code development and validation, and insufficient knowledge of CFD capabilities and/or limits outside of the expert community. An analysis of how to overcome these challenges and increase the use of CFD in NRS studies identified potential collaboration and led to the recommendation of the following priority activities:

- Building a library of links for data related to CFD for NRS, including links to validation databases and to fundamental documents (e.g. best practice guidelines [BPGs] and state-of-the-art reports).
- Enhancing reliability and credibility through blind CFD-model benchmarking, extended towards application-oriented comparative studies.
- Updating and promoting existing reference documents (such as BPGs and synthetic reports on CFD activities).

- Supporting future work on the development of uncertainty quantification methodologies for CFD. Collecting and summarising existing work and organising exercises of applications.
- Providing help to newcomers to CFD in the form of a few short primers on themes such as “CFD for decision makers”, “CFD for system code users” or “system codes for CFD users”.

This publication is organised in two parts. In Chapter 1, CFD is first presented from a general point of view, after which some specificities regarding its use in safety demonstrations are explored. This chapter also includes a short summary of the most striking recent evolutions of this tool as well as illustrative examples of the assessment of safety demonstration based on its use. In Chapter 2, the focus is on the apparently most problematic current limitations of the CFD method for a more generalised application in safety studies, with a discussion of possible solutions.

Chapter 1. The current use of CFD for nuclear safety

1.1. Main motivation for the use of CFD in safety studies

Computational fluid dynamics (CFD) has evolved from being a research method to a fundamental step in the design process (computer-aided design [CAD]/computer-aided engineering [CAE]) in many engineering disciplines (such as chemical engineering, automotive, turbomachinery, external aerodynamics, environmental or fire safety engineering), which in turn is driving CFD development. In parallel, computer capacities have grown by orders of magnitude. Today cloud computing capabilities and open-source CAE tools (e.g. OpenFOAMTrioCFD or SALOME Platform[1]) allow everyone to adopt the CFD method in principle.

In the context of nuclear safety, simulation tools are applied to safety demonstrations (to provide argumentation and evidence in the licensing process), safety justifications (to document risk assessments and implemented safety measures), safety assessments (to identify potential hazards) and safety systems and procedure designs. Such analysis is conducted primarily on the basis of 1D system codes or subchannel codes (e.g. SUBCHANFLOW [1], ASTEC [2], MELCOR, CATHARE) or 3D nuclear field codes (e.g. GOTHIC). The coarse mesh 3D capabilities of system codes is restricted to cylindrical or Cartesian coarse meshes and their use in reactor analysis is growing for the simulation of 3D thermal-hydraulic phenomena inside the reactor pressure vessel (RPV) and core, steam generator or pressuriser; they are based on porous models of the flow domain and inner structures. 1D models of system codes are well validated against a large number of experiments relevant for each reactor design and contain a significant amount of physical models, which are either based on similarity mechanics or empirical correlations. A thermal-hydraulic system code model is principally built as a network of control volumes which may be coupled with solid structures with or without energy sources.

In recent decades, the use of three-dimensional CFD models to predict flows and transport phenomena in nuclear reactor cooling systems and containments has increased. One of the main reasons for the increased use of the 3D CFD method is that a number of safety-relevant phenomena (for example, boron dilution, pressurised thermal shocks, main steam line break [flow asymmetry], containment atmosphere mixing and stratification, or hydrogen combustion processes) are essentially 3D in nature. The application of one-dimensional thermal-hydraulic codes for such conditions is not fully valid due to their inherent model deficiencies, whereas CFD provides the required spatial resolution and better accuracy. It may notably help evaluate the conservatism of the one-dimensional approaches. In addition, CFD allows an explicit representation of the geometric aspects affecting the flow and heat transfer of nuclear power plant systems or components.

Simulations are subject to different errors, such as numerical errors, resulting from the selected schemes and solution methods or modelling errors, caused by a simplification of the physical phenomenology. Besides, previous assessments of system code predictions, such as benchmarks, identified the “user effect” as a major source of the difference between simulation results, leading to potential additional uncertainty, which could be related to a large extent to the chosen nodalisation (discretisation in control volumes and definition of flow paths between them) and user dependent model parameters. Generally, these errors may add up or balance each other.

For CFD, a rigorous methodology, summarised in the best practice guidelines (BPG) [3], exists to minimise and quantify the numerical error associated with a simulation result, and specifically for mesh convergence studies. Furthermore, CFD has a reduced modelled and increased resolved

[1] Please refer to the Index of codes at the end of this publication.

part of the problem and is thus expected to be less sensitive to user effects. This can reduce conservatism and thus provide a more reliable quantification of the margins in the design.

The governing equations of CFD do not contain lengths or reference scales, meaning the CFD method can in principle be transferred between different applications and scales. However, the constants in the closure laws[2] still implicitly contain information on the scale of their validation experiments, which remains a not fully resolved issue for scaling. Nevertheless, CFD can serve as a carrier to scale up experimental results via validated models to plant applications. Specific caution must then be used to ensure that the validation process covers all scales involved in the experiments. Furthermore, CFD can help to investigate safety issues where a classical scaling approach may fail, such as multi-physics problems with a large count of characteristic dimensionless numbers or innovative reactor safety systems and concepts with no engineering correlations yet available. For existing engineering correlations, CFD can complement established analysis methods by confirming such correlations for the targeted applications.

Whenever experiments are too difficult or too expensive to be performed, no appropriate measurement techniques are available, or the experimental target is not accessible due to its size, geometry or conditions (high temperature, contamination or radiation), CFD can support and complement the experimental approach. Unsteady effects (e.g. thermal fatigue) can also be characterised by CFD simulations.

CFD naturally has a role in a multi-scale approach to the analysis of reactor thermal hydraulics. Figure 1.1 depicts the different temporal and spatial scales that need to be considered in model V&V (verification and validation) and in the application to safety studies on different scales. While the correlations in system codes are often derived from system-scale experiments to maintain the characteristic numbers (e.g. Ra) in the relevant range and ensure scalability, CFD can in principle cover the whole range of scales, even though in practice it focuses mainly on component or assembly-scale applications. Note that while CFD models are usually developed and validated at a specific physical scale, or micro-scale, where all relevant phenomena are resolved, their application can be transferred to component or even assembly analysis, which represents a limited section of the system and transient. For system-scale analysis, the transient duration often becomes the limiting factor, as it cannot be overcome by HPC (high performance computing) in a reasonable time frame. Such analysis is today conducted mostly by deriving porous (spatially homogenised) models from detailed component or assembly scaled analysis.

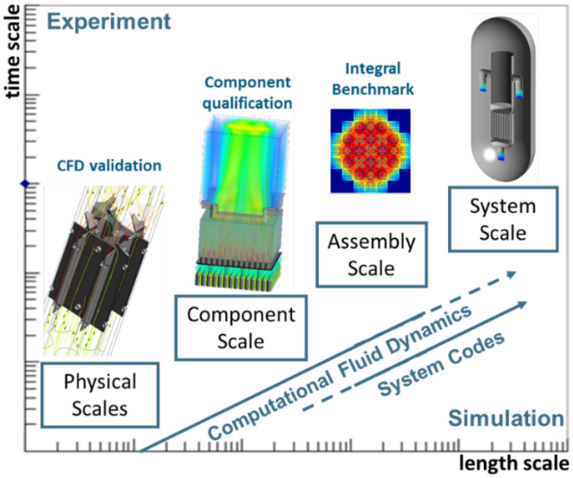


Figure 1.1: **Illustration of the multi-scale analysis of reactor thermal hydraulics [4]**

2. Strictly speaking, except for the case of direct numerical simulations (DNS) that does not use any closure law.

Multi-physics simulations are becoming more common, for e.g. to assess thermo-fluid dynamic feedback on neutron transport. CFD can provide the necessary input in a spatial resolution that corresponds to 3D neutron transport methods and thus allows for a more consistent coupling and representation of the physics.

In the last two decades, significant efforts have been made in the development and validation (D&V) of single- and multiphase CFD models around the world. Organised by the NEA WGAMA Computational Fluid Dynamics Task Group (CFDTG), a number of benchmarks (e.g. [5]), state-of-the-art reports (e.g. [6]), BPG and recommendations (e.g. [3]) were summarised to channel development efforts, maintain a high standard and recently, to further develop uncertainty quantification methods for CFD [7] as well as uncertainty reduction in CFD-validation experiments [8]. Visible progress has been achieved in the modelling and the quality and detail of validation experiments. This has been documented in dedicated journal papers, conferences and workshops, such as the NEA and IAEA co-sponsored Computational Fluid Dynamics for Nuclear Reactor Safety Applications (CFD4NRS) biannual workshop series (e.g. [9]). The possibility of systematically eliminating numerical errors [1] along with the more resolved physical phenomena and their visualisation as well as the potential to scale approaches and increase the number of references and documented applications suggest that the use of and trust in CFD predictions is likely to increase. Compared with the investments made in large experimental devices like thermal hydraulics loops, CFD is a very flexible and cheap tool to study the design of components. Nevertheless, CFD and analytical tools cannot replace experimental evidence, and an innovative design based only on calculations may include erroneous evaluations. This Technical Opinion Paper (TOP) will therefore also discuss the current limitations, maturity and challenges in the use and acceptance of CFD in nuclear safety.

1.2. Requirements for CFD to be applied in nuclear safety studies

Fully validated numerical CFD simulations combined with analysis of uncertainty quantification aim to be as valuable as experimental data, provided that all the physical phenomena are (i) being modelled without bias, thus minimising the number of assumptions and/or approximations, and (ii) resolved with corresponding space (and time, if transient data are concerned) resolution. This objective must be assessed through V&V and deviation from it must be quantified (uncertainty quantification, or UQ) in the context of a given application. This may require large computation resources[3] and is currently not achievable for large-scale problems.

The following have been identified as potential uses of CFD for nuclear safety:

- Independent of the safety assessment process:
  - CFD is already used to support the design process [10];
  - CFD can be used to support the validation of larger scale studies;
  - CFD can be used in addition to experiments to increase knowledge about a specific phenomenon;
  - CFD can be used to support design of experiments by simulation-driven designs;
  - CFD can be used to complement an experimental database.
- Within safety studies:
  - CFD can be used in a safety assessment study to provide additional support, such as to:
    - contribute to criteria justification/choice;
    - justify a hypothesis within a methodology;
    - evaluate margins.
  - CFD can be used for the safety demonstration to show that criteria are fulfilled, making it the main evaluation tool in an assessment.

3. CFD use with all relevant time and space scales resolved is called direct numerical simulation (DNS). In other cases, which cover all the application cases, the use of CFD requires closure models, i.e. for turbulence in single phase flows and also for interfacial structure and transfers in two-phase flows.

The qualification of a CFD tool is mandatory for each specific application. Hence, CFD simulations must fulfil a high level of reliability when used in the assessment process of a specific safe case, i.e. to assess safety-relevant phenomena. The verification against a reference solution and validation against experimental data (V&V) is a central part of the CFD qualification process that allows identifying possible sources of errors in the computational result. Several assessment principles have been defined worldwide ([11–15]) and characterise the procedure for V&V for nuclear safety transients and accident analysis in a rather general way. Some of them have been updated recently, leading to some evolution in both the studies and the regulatory processes. Some specificities of the application of these requirements for CFD tools are discussed below.

Figure 1.2 shows an idealised diagram illustrating the steps in the development of CFD tools for use in safety analyses. For maturity-level improvement (and therefore reliability), the text on the left-hand side of the arrows identifies the type of development actions required. They are discussed hereinafter.

First, the maturity-level steps correspond to a motivation for the detailed 3D analysis of the flow and the CFD model capability for this purpose. This allows the identification of gaps in understanding of the corresponding physical processes involved, which motivates the potential development of both experimental work and models.

V&V+UQ must be studied for each given application, identifying quantities of interest, related dominant physical phenomena and associated influential parameters in their evaluation. Notably, an iterative PIRT (Phenomena Identification and Ranking Table, [16, 17]) exercise is required to identify dominant phenomena at the corresponding CFD scale of analysis. Comparing CFD predictions with experimental data implies that experiments provide appropriate data at the relevant accuracy (localised measurements and flow features). It may lead to some challenges for the instrumentation and the design of the experimental device, but also requires a specific process in the way experiments are conducted. Several studies and guidelines are concerned with this aspect, and referred to as "CFD-grade experiments", [8,18,19].

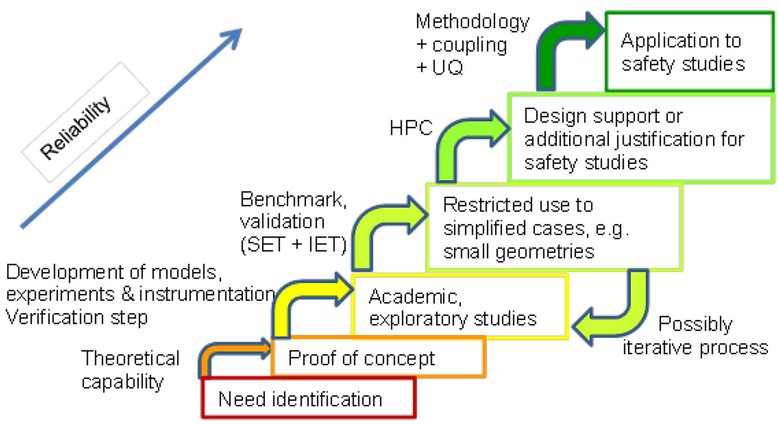


Figure 1.2: **Schematic diagram of progressive improvement of reliability**

With both experimental data and models being available, the first process is the implementation of the models into the CFD tools. Then, the verification process is meant mostly to check that the model implementation and coding is done correctly by testing each model individually against some functionality tests and by comparing with some exact solutions – sometimes analytical – of idealised problems. The validation process against separate and integral effect tests (SET and IET) mainly consists in comparing predicted and measured data, identifying the origins of discrepancy. The V&V+UQ process for CFD codes consists of the following steps: (i) the choice for models of the physical phenomena (uncertainty source is associated to both the model formulation and/or to the model parameters); (ii) the numerical model of the physical domain (geometry representation and space discretisation or meshing) and of the fluid properties;

and finally (iii) the numerical parameters for the solving procedure (accuracy, time step, stabilisation), see [20]. The specificity of CFD in the evaluation process of uncertainties has been addressed already in several papers, see [21] for a UK regulatory perspective, or [22] for the adaptation of the VV&UQ in the US regulatory process to turbulent single-phase flows with CFD. The review proposed by the CFDTG in 2016 [7] indicated that all the UQ methods reviewed had either a low or very low degree of maturity for CFD application at that time.

Most application cases of CFD require large computational domains due to the required fine nodalisation to catch the effect of geometrical singularities, e.g. the need to resolve wall boundary layers and their potential unsteady transient computations with a high cost of computation. Moreover, parametric studies imply a potentially large number of computations. Performing such numerical analyses requires good numerical performance and stability in the solver as well as the availability of large computational resources (a large number of processors and, in the case of commercial software, code licences). The cost of HPC may significantly hinder the use of CFD. However, nowadays, on-demand cloud-based computing as well as open-source CFD software may help to overcome this and to support a wider use of CFD in nuclear safety, as is the case in other industries. Still, HPC needs may limit the number of independent evaluations which can be realistically required in regulatory processes for nuclear safety.

Qualification of a numerical tool over the validation database domain must be transposed to the application domain: the uncertainty levels deduced from comparative studies with respect to the experimental database only partially reflect the UQ to the safety study. This includes the scalability issue: while the governing equations of CFD do not contain explicit length scales and are therefore not concerned by scalability, this is not the case for the closure models (e.g. turbulence model or interfacial transfers). This also includes the validity range of the models; in fact the models are being possibly used for the application out of the explored domain of the database. This may impact (i) the justification of some fittings or parameter choices but also (ii) the uncertainty of the result. UQ for CFD needs the above-mentioned scalability step. Although several UQ methods are issued from system-scale analyses, their adaptation to the CFD case is still extremely limited.

Predicting the accuracy of the numerical tools used for safety demonstrations is only a part of the assessment process. The purpose of a CFD computation is to provide a realistic evaluation of a given situation, although for safety cases a conservative evaluation is usually needed. CFD can possibly be conservative (e.g. by using penalised initial or boundary conditions) but it is not sufficient: having UQ methods associated to CFD methodology is mandatory to determine the conservative value of figures of merit. In addition, the introduction of CFD in nuclear safety study methodologies has some specificities when it is coupled with or used alongside other tools resolving other physics, part of a RPV or circuit, or another specific phase of an accident sequence. This may occur when CFD is coupled with system-scale studies that define either initial or boundary conditions, e.g. [23]. This is also the case when the safety analysis implies some coupling with other physics (conjugate heat transfer, neutron kinetics or structural mechanics).

The analysis of an accident situation within a CFD-scale study also implies some specific issues or challenges. From a general point of view, increasing the details resolved by a method requires increasing the amount of information to be provided accordingly. The boundary and initial conditions must be specified at the corresponding refined scale. This potentially concerns the correct definition of some profiles at the inlet boundary conditions (both for the main variables of the governing equations and for some input variables of the models) or of the fields throughout the whole domain for initial conditions. This is also the case for coupled studies. Since geometrical details are considered, it must be checked that the choice for their description (like wall roughness for example) does not impact the results. Moreover, the geometric parameters of the scenario of the situation have to be refined as well. For example, if any leak is considered, the degrees of freedom within a CFD study are larger than for a system-scale study; its position (abscissa along the tube, orientation with respect to gravity, etc…) and its shape can impact the results. For all the aspects mentioned above, there could be choices leading to certain penalisation of the result. Nevertheless, if no clear principle can be applied for penalising those aspects, an additional uncertainty quantification study and/or a set of sensitivity studies to those additional parameters is required.

Moreover, for any analytical tool (both CFD and system codes) the whole process of V&V and UQ has to be sustained by a consistent quality management, as outlined in [24]. This relies on a strict application of established guidelines by CFD analysts through a quality assurance process. Many recommendations for CFD analysts, for example, have been formalised by the CFDTG [3] and discussed in the literature [25,26].

1.3. Recent evolution of the use of CFD in the field of nuclear safety

The field of CFD has considerably evolved over the past decades, driven by the rapid development of available computational power, numerical methods and validated physical modelling implemented in the simulation software. As previously stated, CFD has become a key design tool in many industrial sectors (aeronautics, astronautics, turbomachinery, car and ship design, medicine, etc.) and is also widely used in various fields of environmental science (atmospheric flow modelling, oceanography, etc.). Focusing on the nuclear sector, if we start the analysis at the beginning of the 21st century, there are some clear indicators of the rise in the use of CFD – one of them being the number of published papers over this period, which has multiplied by a factor of roughly 10 (see Figure 1.3):

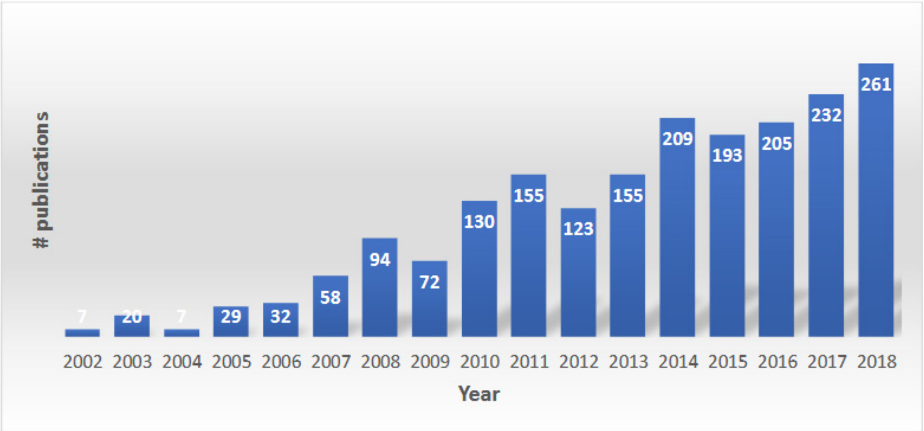


Figure 1.3: Number of publications concerning CFD in the journals *Nuclear Engineering and Design* and *Annals of Nuclear Energy* [18]

As mentioned earlier, one of the main motivations for the development of CFD in the nuclear sector, particularly in nuclear safety, is the better description of multi-dimensional, mixed convection, detailed physical phenomena that take place in a nuclear power plant (core, RPV, circuits, components, etc.) at different spatial scales and are of great importance for the design optimisation and safety assessment. However, gaining insights into the local structure of the flows – especially highly turbulent ones – depends on the availability of sufficient computational power. Therefore, the huge increase in computational power available to CFD users (whether in workstations or in supercomputers) and the development of robust numerical algorithms for parallel computing are among the reasons behind the increased use of CFD. Gordon Moore's observation of 1965 that the number of transistors on an integrated circuit (equivalent to the computing power) will double every two years is still valid today, as illustrated in Figure 1.4. This is further complemented by the increasing use of graphics processing units (GPU).

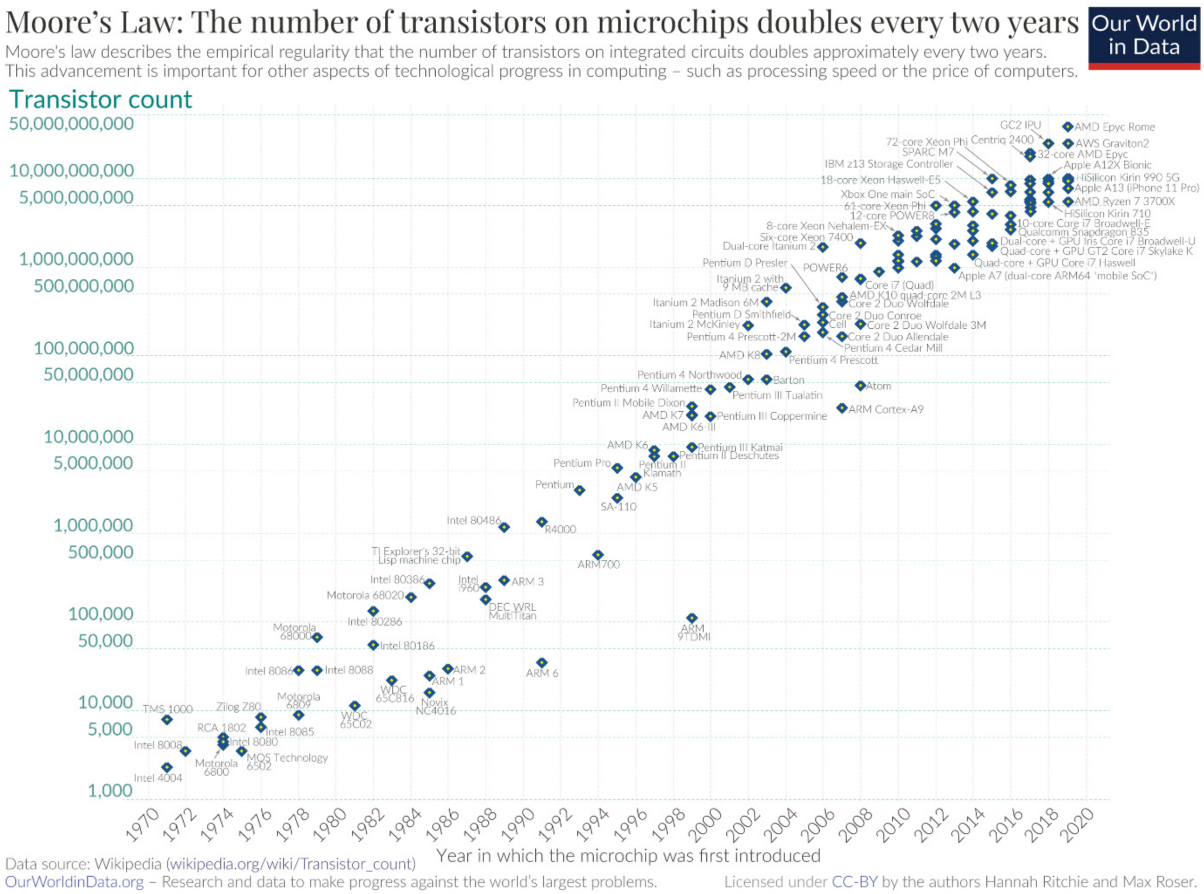


Figure 1.4: **Logarithmic graph showing how transistor counts in microchips almost double every two years from 1970 to 2020; Moore's Law**

This evolution in hardware has been coupled with an evolution in the capacity of various CFD software programs to take advantage of this power, especially through the development of parallelisation algorithms. These kinds of algorithms have recently made it possible to perform billion-cell calculations of nuclear applications, see [28], hence making it possible to probe very fine details of flow structures or to simulate the detailed mechanisms of bubble formation [27]. However, since such calculations demand access to petascale supercomputers, they are still out of reach for most teams working to apply CFD-based methods to nuclear safety and licensing. The same holds true for reviewers from safety authorities or independent safety organisations.

1.3.1. *Evolution of physical modelling*

The main developments in physical modelling implemented in CFD simulation software are considered below; first for single-phase flows and then for multiphase flows, for which a considerably larger number of models are required.

Numerical simulation of single-phase flows has drawn considerable attention over the past decades. One of the most important evolutions in the physical modelling of this kind of flow is the treatment of turbulence (details about the most established methods to model turbulence can be found in classical textbooks – see for instance [28]). In recent years, progress has been made at different levels. The classical RANS (Reynolds-Averaged Navier-Stokes) turbulence models still constitute the most widely used class of models for industrial applications: second-order turbulence models (applied both for the dynamic and thermal turbulent fluxes) have been developed and implemented in CFD software [29]. Taking advantage of the rise in computational power, LES (large eddy simulation) methods are increasingly used to simulate industrial applications [30]. So-called hybrid methods, which try to combine the advantages of the RANS and LES methods, are already used widely, with new methods still under development [31].

Due to its crucial importance in a number of nuclear thermal-hydraulic applications, multiphase flow modelling development has been the main interest of several research teams worldwide in recent decades (see [32] for a summary of these applications). The French joint R&D initiative NEPTUNE started in 2001 [33] (gathering the four main actors of the French nuclear industry: EDF, CEA, FRAMATOME and IRSN) and has notably triggered the development of the Neptune_cfd solver, currently used in France to tackle several applications in the field of nuclear safety. In the United States, the US/DOE CASL project explores the capacities of CFD solvers to simulate complex multiphase applications, such as the departure from nucleate boiling (DNB) in fuel assemblies. Recently, significant progress has been made in the modelling of flow-regime transitions, i.e. the capacity to simulate the transition between different two-phase flow topologies, for instance bubbly flows to slug flows. Examples of such methods include the GENTOP (GENeralised TwO-Phase flow) concept [34] being developed at the Zentrum Dresden-Rossendorf (HZDR) in Germany, and the GLIM (Generalised Large Interface Model) approach implemented in the Neptune_cfd software [35]. Both approaches belong to the multi-fluid Eulerian methods.

Other approaches developed to describe the (dispersed) two-phases flows are the particle-tracking (Lagrangian) methods based on the coupling between a continuous carrier flow simulated by a classical RANS approach, and a particulate field simulated by a large number of particles. This method can be applied in particular to simulate sprays in containment [36]. Other applications include aerosol dispersion and deposition (in containment or in the atmosphere), and the transport of debris by a water flow.

In support of the validation of the CFD tools for nuclear safety applications, several benchmark exercises have been organised in the scientific community, e.g. [37], including by the CFD Task Group of the WGAMA. Those benchmarks are:

1. OECD/NEA-Vattenfall T-Junction Benchmark Exercise (high-cycle thermal fatigue) [38]
2. OECD/NEA-KAERI Rod Bundle CFD Benchmark Exercise (turbulent mixing downstream of a spacer grid) [5]
3. OECD/NEA-PSI CFD Benchmark Exercise (jet erosion of a stratified atmosphere based on PANDA) [39]
4. OECD/NEA CFD Benchmark with Uncertainty Quantification (turbulent mixing based on GEMIX) [40]
5. OECD/NEA Cold Leg Mixing Benchmark with Uncertainty Quantification [95]
6. OECD/NEA Fluid-Structure Interaction benchmark exercise [96]

1.3.2. ***Multi-physics and multi-scale analysis***

In recent years, a significant effort was made to integrate classical, fine-scale CFD calculation (resolving flow structures of about 1 mm) into a larger simulation framework to better approximate real-life applications. This kind of approach comprises the coupling of a CFD model – thus solving the flows – with dedicated numerical tools aimed at modelling other physics, the most classical one being structural and fracture mechanics (although the temperature field in the solid due to conjugate heat transfer may be treated within the CFD model), which is important in thermal shock studies. Other aspects of the management of solid structures in (potentially multiphase) flows include flow-induced vibration, for instance in the study of the behaviour of steam generator tubes. To gain more precise insight into the core behaviour, CFD codes have recently been coupled to neutronics codes [41,42] and advanced chemistry codes [43] to predict crud deposition on fuel rods.

As mentioned in the introduction, specialised simulation software acting at the scale of a component (for example, the core or steam generators) or a whole nuclear reactor have long been used in safety analysis. While they can often simulate a whole industrial transient at the real scale, they cannot simulate very local details of the flow and resort to correlations. To combine the benefits of CFD approaches and component/system-scale approaches, several research teams have sought to develop and validate numerical methodologies coupling CFD and system-scale codes [23, 44–49]. Different strategies have been developed with respect to this type of coupling, which can be achieved either through boundary conditions (the CFD code is then used to model a component in which three-dimensional phenomena can play a key role, while the parts of the circuit which can be modelled by 1-D components are treated by the system-scale code – see for instance Figure.1. 5), or by overlapping two domains – the CFD approach being then considered as a "zoom" in on a specific part of a thermal-hydraulic circuit that is fully modelled by the system code.

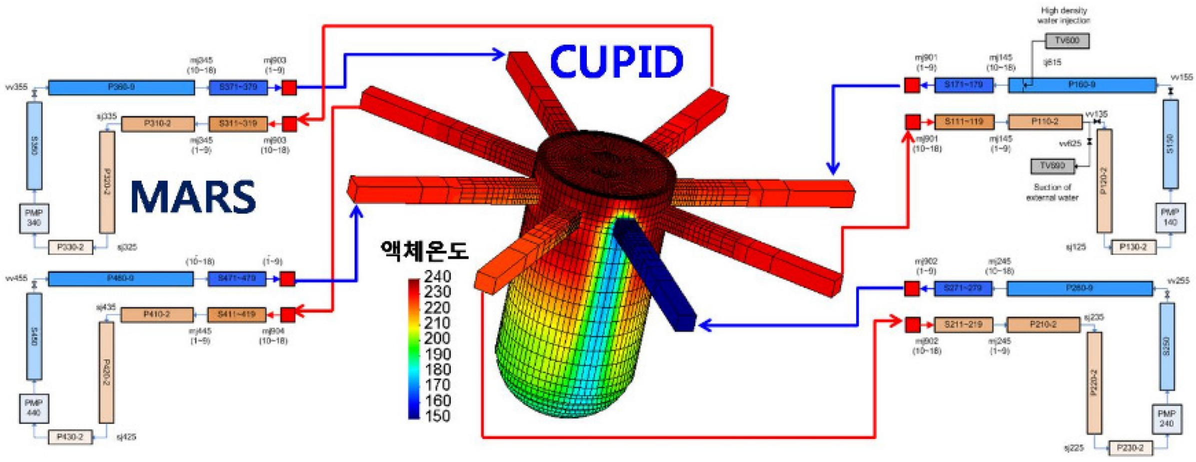


Figure 1.5: **Illustrative diagram of the MARS/CUPID coupling [44]**

In addition, multi-scale coupling between CFD and subchannel codes are also under development [50] using advanced coupling approaches. Related to this topic, it is worth mentioning the recent development of a "coarse-grained CFD-scale" approach in the context of nuclear applications. This consists of developing a methodology based on a CFD code [51] with a classical existing strategy that resorts to adding porosity and head loss terms in the equations (with the proper correlations) to model fine geometric details[4]. Some studies based on this methodology appear promising to model components such as spent fuel pools [52] or steam generators [53].

*1.3.2. **Open-source CFD codes***

Open-source software is typically distributed under the GNU Public License, which implies that whoever obtains a copy of the software must also receive its source code along with the right to modify and further redistribute it. This "viral" licensing makes collaborative open-source software development a catalyst in several ways:

- It makes it possible to link the experience of a broad community of contributors so that the software benefits from continuous development in other fields of science.
- Active open-source projects feature modern state-of-the-art programming paradigms, like object-oriented programming, that promote the transparency of the code and thus maintainability and re-usability.

4. Here, small scales of geometry are therefore not explicitly represented while the approach is still considered as being CFD.

Today, many modern scientific libraries and cutting-edge HPC-capable algorithms are also released as open source. They can be linked relatively easily, both from a licensing perspective as well as from a programming point of view, to construct a new application, which again must be released under the same base licence. Remarkable examples are the OpenFOAM (Open Field Operation and Manipulation) CFD toolbox, developed originally at Imperial College in the 1990s, or (for single-phase flows) Code_Saturne [54], developed by EDF. These two are today the main open-source CFD codes and are increasingly applied in nuclear research. They were used to address a number of nuclear safety issues, e.g. [55–61]. Another example is the single-phase TrioCFD code, which is under development at CEA-Saclay and NEK5000Among others, TrioCFD [62,63], has been used and validated for the analysis of heterogeneous boron dilution [64,65], the flow in fuel assemblies [66,67], the single-phase pressurised thermal shock on the reactor pressure vessel [68,69], containment flows [70] and thermal striping [71,72]. TrioCFD is able to support large meshes (billions of degrees of freedom) and can also now be used on GPUs. Furthermore, the direct source code access allows – in principle – a direct and thorough review of the method and may thus support acceptance of results during a licensing process.

Nevertheless, open-source software still has drawbacks, such as limited quality control and documentation as well as fragmented developments and limited support. These drawbacks can be mitigated to some extent by using version control systems (e.g. git or subversion), bug trackers or forums/wikis. These tools promote a collective contribution to documentation, tutorials and V&V and support interactions among users and developers. Operating system-level virtualisation in the form of containers facilitates distribution and use of applications. For these reasons, the "Open-source Nuclear Codes for Reactor Analysis (ONCORE)" initiative has been recently launched under the aegis of the IAEA [73].

1.4. Applications for which the use of CFD is under development

Over the past decade, significant progress has been made in the general capability of CFD tools to describe a wide variety of flows occurring in nuclear applications.

- Some single-phase flow applications can be considered as sufficiently mature to be treated by means of CFD calculations in the framework of the safety demonstration. This treatment requires a robust qualification procedure. Typically, this includes sufficient and shared knowledge of the physics at stake and sufficient confidence in the models implemented in the CFD tool, which itself results from a solid V&V activity coupled with a robust methodology (which can rely on sufficiently fast simulations). Examples of this kind will be detailed in the following section.
- Still, for a large number of applications, some of the items mentioned above would be missing, thus triggering research and development activities of a potentially different nature. For instance, if the physics of the application appears complex (for instance in the case of two-phase flows with phase change, or reactive flows), a dedicated experimental programme can be carried out and used as validation for the evolution of the physical modelling implemented in the simulation tools. Examples for such a strategy are the TOPFLOW-PTS programme, dedicated to the pressurised thermal shock application, or the NEA THAI, SETH and HYMERES programmes dedicated to the hydrogen risk assessment.

Because of their industrial interest and complexity, several applications involving two-phase flows are the subjects of a significant volume of R&D effort (boiling crisis analysis, gas transport in hydraulic pipes, pressurised thermal shock, etc.). Among these, the modelling of the behaviour of **spent fuel pools in accident situations** [97] has drawn the interest of several research teams. The main thermal-hydraulic phenomena that need to be modelled include:

- Two-phase natural convection flow with formation of thermal plumes;
- Low-pressure nucleate boiling;
- Free surface with heat and mass transfer;
- Effect of pressure on the formation and growth of bubbles;
- Critical heat flux (CHF);

- Fuel cladding oxidation; and
- H_2 production.

A whole category of CFD development is related to **next-generation nuclear reactors**. Among those, liquid metal-cooled reactor thermal hydraulics have recently been the main topic of a collaborative European project that includes a large collection of CFD studies – the main findings of which have been summarised in a textbook [74]. In recent years, passive systems in various small modular reactor (SMR) concepts have also been the subject of numerical studies that incorporate the use of CFD, e.g. [75], as their application is beyond the validity of the established system codes and their experimental validation. For integrated SMRs, the presence of components like helical heat exchangers and pumps inside the RPV increases the complexity of the 3D-flow that is characterised by mixed convection flow. This kind of flow can be simulated with CFD or coupled CFD/system thermal-hydraulic codes, as done for example in the H2020 McSAFER project, [76].

Another active field of development is the **containment safety analysis**, which alone encompasses a wide range of activities, including:

- Modelling of the pressurisation (depending strongly on local wall condensation rates, other buoyancy-driven heat and mass transfer processes and thermal radiation of surfaces and gases).
- Assessment of containment atmosphere mixing and the formation of flammable mixtures.
- Evaluation of the impact of spray operation on pressure and flammability.
- Numerical analysis of loads due to deflagration and the possibility of flame acceleration and deflagration to detonation transition (DDT).
- Numerical studies of the effectiveness of passive safety systems (e.g. passive autocatalytic recombiners, containment condensers).
- Phenomena related to filtered containment venting, e.g. aerosol resuspension, sump boiling.

Classically, these issues are addressed for multiple scenarios by means of system codes and partially 3D field codes/coarse mesh CFD codes (cell size ~1 m^3) such as GOTHIC [77] or GASFLOW [78]. But increasingly refined CFD methods are being developed (e.g. [79]) and employed and they will be integrated into the methodology [80] in the upcoming European AMHYCO project.

Containment safety analysis includes hydrogen combustion loads. Such a CFD combustion study is presented in more detail below as an illustrative example of plant application. H_2 is released to the containment in large quantities due to core oxidation during a loss-of-coolant accident (LOCA) and a possible subsequent molten-core-concrete-interaction (MCCI) during a severe accident. While the containment atmosphere is globally steam inertised for the initial phase of the LOCA transient, flammable conditions may be reached locally with the initially available atmospheric oxygen, where steam condenses and H_2 can accumulate. Safety measures aim first at avoiding such locally flammable mixtures, and at least preventing flame acceleration to mitigate pressure loads on the containment structures and safety-relevant equipment.

In [58], a small break (SB)-LOCA and a station blackout (SBO) in a Korean APR1400 were analysed with the aim of investigating the possibility of flame acceleration and DDT. Both scenarios represent a fundamentally different accident phenomenology and transient evolution regarding the release location, gas-mixture composition evolution and the position of potentially flammable clouds:

- In the SB-LOCA, H_2 is released via the break location and after vessel failure from the reactor cavity and accumulates in the steam generator compartments and in the free dome area above.
- During the SBO, the reactor cooling system is depressurised by bleeding steam (and H_2) into the in-containment refuelling water storage tank (IRWST). While the steam condenses, a H_2-rich atmosphere is formed, which may leak into the dry containment atmosphere.

Method

Providing an initial state for combustion analysis with CFD is still challenging, as all relevant phenomena, safety measures and technical systems have to be represented in a large and geometrically complex domain (here ~90 000 m³) and possibly analysed for long transient durations. For these reasons, the authors implement a different approach: the initial fields are mapped from MAAP5 system code analyses onto the CFD mesh. In contrast to previous approaches, the entire combustion process is computed within a single solver framework and does not require the use of empirical transition criteria. The solver utilises the k-ω SST turbulence model in combination with a hybrid combustion model accounting for effects of turbulence as well as chemical kinetics on a mesh with ~9 Mio cells and a mean edge length of ~22 cm, which is considerably finer than those used in previous studies, but still under-resolved.

Results and relevance for safety assessment

The simulation results revealed that for both the small break loss-of-coolant accident (SBLOCA) and SBO with an activated three-way valve, weak thermal ignition could not be triggered, as the mixture is beyond the flammability limit. For the realistic case of an SBO with a deactivated three-way valve, the mixture is ignited in the IRWST. There is a slow complete combustion in the IRWST and a partial burnout in the annular compartments is observed. For the given initial conditions, no combustion occurs in the upper part of the containment in this scenario (illustrated in Figure.1. 6).

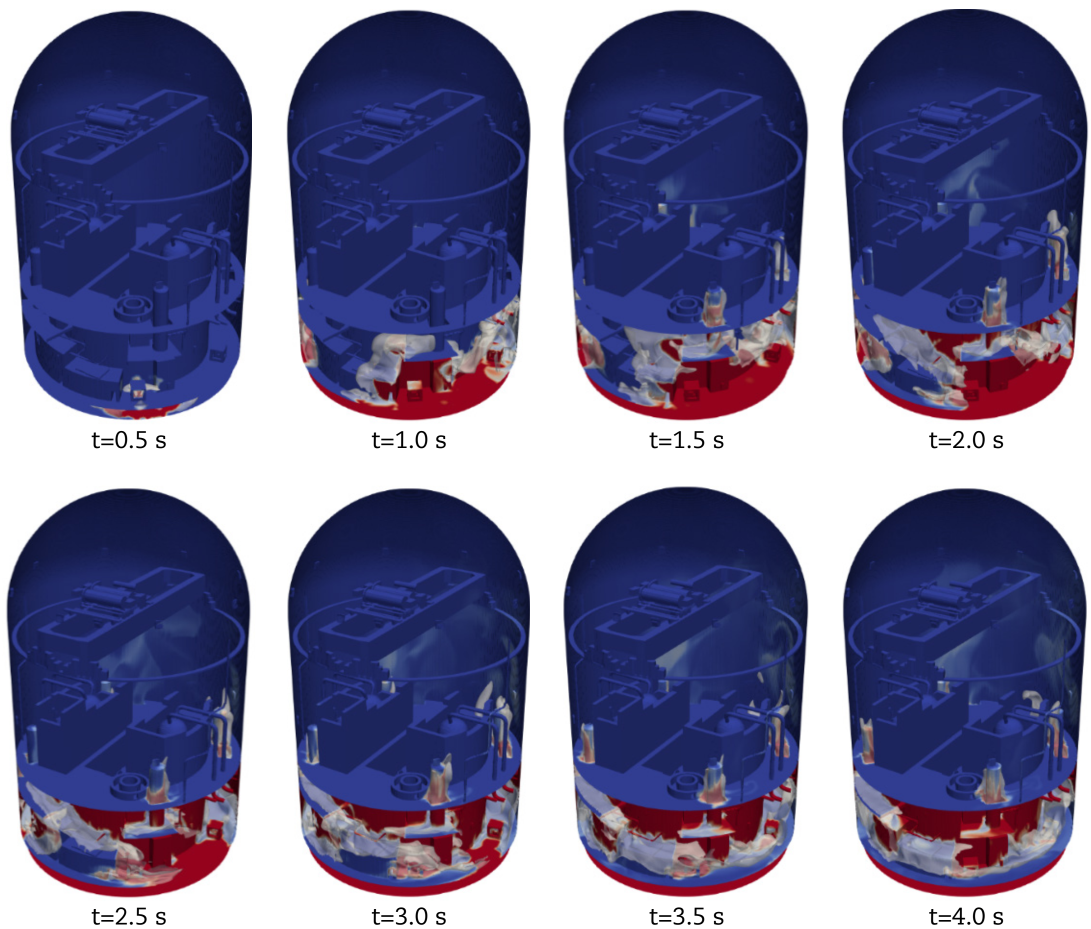


Figure 1.6: **Flame contour for a realistic deflagration process inside the containment**

In addition, two generic cases based on artificial initial mixtures were used to demonstrate the predictive capabilities of analyses of the global behaviours of a fast deflagration and a detonation propagating via the venting stacks and the gaps surrounding the safety injection tanks in the whole containment. This work demonstrated that 3D under-resolved CFD methods can be applied to analyse and estimate the risk of flame acceleration and even DDT on containment scale. Detailed information on the flame propagation and acceleration in the complex containment geometry was obtained without the need to provide combustion regime transition criteria. However, 3D initialisation, obtained by CFD, is still necessary to make use of the full potential of 3D combustion analysis.

1.5. Examples of CFD applications for safety assessment studies

This section presents three examples of CFD in studies for nuclear safety. The examples deal with heterogeneous boron dilution, dry cask application and pressurised thermal shock.

Example 1 – Heterogeneous boron dilution – Use of CFD to study the mixing of a boron-depleted volume of water in French PWRs

A heterogeneous boron dilution accident scenario may occur when a volume of "clear" water, i.e. water at a zero or low boron concentration, accumulates somewhere in the primary circuit of a pressurised water reactor (PWR) – typically in a crossover leg – and is later moved in the direction of the RPV and the core. A risk of criticality may exist when this volume of clear water enters the core.

Two classes of heterogeneous boron dilution scenarios have been studied for French PWRs:

- External heterogeneous boron dilution – in this scenario, the volume of clear water is injected into the primary circuit from another connected circuit and is later sent to the RPV when a reactor coolant pump (RCP) is started.
- Inherent heterogeneous boron dilution (which means the dilution is "inherent" to an accident scenario, like a LOCA) – in this scenario, the clear water is produced in the steam generators (SG) when the primary circuit is operating in reflux-condenser mode: the vapour produced in the core, with almost no boron, is condensed in the SGs and the core residual power is thus evacuated by the SGs to the secondary side. This condensed vapour accumulates in the form of clear water between the outlet of the SGs and the RCP and may be transported to the RPV if natural circulation is re-established in the primary circuit at a later stage of the scenario.

Methodologies used to study heterogeneous boron dilution in France until the early 2000s relied on the mixing hypothesis, which requires rigorous justification. For instance, one approach could suppose that a boron-depleted volume of water is transported as a whole, without any mixing at all, from the crossover leg where it was initially accumulated to the RPV lower plenum and is then perfectly mixed with the borated water present in this plenum.

The use of CFD calculations was introduced as part of new methodologies in the late 2000s, [81] to improve the evaluation of the mixing of a boron-depleted volume of water with the borated water present in the loops, in the RPV and, for certain scenarios like inherent boron dilution, with the borated emergency core cooling system water.

This raised significant questions on:

- The validation of the CFD codes used for the two types of boron dilution studies, and the representativeness of the separate effect test and integral effect test cases that were used.
- The variability of CFD calculation outputs (the minimum boron concentration and the boron concentration map at core entrance, which are the main variables of interest) when the initial and boundary conditions of the scenario vary. The necessity of sensitivity studies was underlined [82], especially to assess whether a cliff edge effect could occur.
- For inherent boron dilution studies, a first step consists in several LOCA simulations with a system code to identify penalising conditions (break size). The second step is a CFD

simulation that represents the transport of a volume of boron-depleted water towards the RPV at the restart of natural circulation. Results from the system code step for the penalising break size (only) are used as input data for the CFD step. The fact that this break size was penalising for the overall scenario had to be justified [83].

The evolution in the application of methodologies using CFD for heterogeneous dilution scenarios was clearly an important step towards the understanding of the physics involved in the heterogeneous boron dilution scenarios.

For instance, in inherent boron dilution, the volume of clear water is at a high (saturation) temperature, whereas the water present in the RPV when natural circulation restarts is much colder, and buoyancy effects in the downcomer thus play a dominant role. In this scenario, CFD studies showed that the (hot) boron-depleted water first accumulates in the upper parts of the downcomer, above layers of colder water. When this (partially mixed) boron-depleted water is finally pushed past the bottom of the downcomer, it does not enter the core homogeneously through the lower plenum, but rather tends to rise at the periphery of the core, still under the effect of buoyancy forces.

For external heterogeneous boron dilution scenarios, the physics is quite different: the volume of boron-depleted water is moved when a primary pump is started, which implies that convective effects are dominant, and buoyancy effects (for a cold volume of clear water in this case) are of lesser importance, although not completely negligible. In this case too, CFD calculations show that the boron-depleted water reaches the entrance of the core in a very inhomogeneous way.

The introduction of CFD in safety studies for heterogeneous boron dilution scenarios in France led to long and intensive discussions between the utility (EDF) and the Technical Safety Organisation (IRSN) of the French Safety Authority (ASN).

These discussions notably concerned the following points:

- As uncertainty quantification studies have not been performed yet for these two safety cases, sufficient margins are necessary in the comparison with the safety criteria.
- Concerning inherent boron dilution, EDF performed additional CFD simulations with clearly bounding hypotheses for initial and boundary conditions (to account for uncertainties associated with the scenarios).
- Concerning external heterogeneous boron dilution scenarios, the lack of validation and the large variability of results forced EDF to finally present a different solution (equipment and operating rule modifications) for certain French PWRs (900 MWe plants), because of the low margins in the CFD study results. For 1 450 MWe plants, EDF proposed up-to-date CFD studies that showed higher margins. These studies now need to be assessed by the IRSN.

CFD has therefore become a central part of the safety demonstration for heterogeneous boron dilution scenarios for French PWRs, largely used for the evaluation of margins. The quantification of uncertainties remains one important field where progress can still be made.

Example 2 – Use of CFD for dry cask applications in the United States

Dry casks are used for the transfer, transport and storage of spent nuclear fuel in the United States. Designs of spent nuclear fuel dry casks are submitted to US Nuclear Regulatory Commission (NRC) for certification. Upon receiving such a design, the NRC performs a thermal review as part of the technical review: the cask and fuel temperatures must remain within allowable limits that are defined for normal, abnormal or accident conditions.

In recent years, applications have increasingly used thermal-hydraulic analyses relying on CFD codes to demonstrate the adequacy of the thermal design. Furthermore, applicants are increasingly looking to license casks for use with decay heats that lead to peak cladding temperatures (PCT) close to the allowable limit. However, the NRC notes that applicants seeking to assure that the temperature margin is adequate often fail to support such PCT predictions with an appropriate UQ analysis.

The NRC therefore began a significant programme of work focused on the thermal study of dry casks using CFD. This work notably included the writing of a BPG document and taking part in an experimental validation programme.

In 2013, the NRC produced a BPG document [84] for dry cask applications. This BPG provides guidelines on the validation of modelling approaches used for heat transfer and fluid flow in a dry cask; the objective is the reduction of modelling uncertainties. For instance, most applicants use the standard k-ε not the best choice for this kind of transitional flow, although it is often the default choice. The modelling of radiation heat transfer is also very important.

Furthermore, the BPG provides guidelines on application uncertainties, with a focus on pressure boundary conditions, which are crucial to the uncertainties that can be introduced in the thermal hydraulics simulation of a dry cask.

More recently, the NRC engaged in another programme to validate CFD codes for dry cask applications. Validation is based on data collected in a demonstration project at the North Anna Power Plant; this corresponded to a TH-32B cask loaded with a high-burnup fuel. Extensive temperature measurements were made throughout the cask. This resulted in the writing of a validation document [85] in 2019.

In this document, the NRC estimated that *"CFD using finite volume is one of the best and most valuable methods for the applicants to show compliance with regulations concerning dry cask storage systems thermal response"*.

Clearly, CFD has matured over the last few years as method to be applied in the thermal study of dry casks.

The NUREG/CR-7260 document [85] underlines that it is valuable to quantify the uncertainties in the simulation results as a function of the computational mesh and simulation inputs.

It also underlines the importance of performing "CFD-grade experiments". Strictly speaking, the TH-32B experiment was not "CFD-grade" (even though it was still valuable) because of its large validation uncertainties.

Example 3 – Pressurised thermal shock (PTS) – Use of CFD to explore margins in a two-phase PTS scenario

To ensure the integrity of an RPV throughout its life, its resistance to brittle failure needs to be assessed, taking into account all possible loading cases. One of the loading cases is a LOCA with cold-leg (CL) injection of emergency core cooling (ECC) water at hot conditions. During this loading case, considerable loads known as PTS result from the temperature gradient between cold injected water running downwards along the inner RPV wall and hot-water inventory in combination with high operational pressure in the RPV.

CFD has been used in the evaluation of PTS in the nuclear power plant Gösgen-Däniken (KKG), which is a German-type three-loop PWR. The simulation work briefly described here was presented at the CFD4NRS-7 conference in Shanghai and subsequently published [86].

The accident progression was at first calculated with the thermal-hydraulic system code S-RELAP5, which simulated the injection of cold ECC water into one CL and partial mixing with the hot coolant in the CL and the downcomer (DC) of the RPV. Due to this cold water injection, strong thermal gradients are generated in the RPV wall in addition to the changes in pressure. The most critical regions in the RPV during such PTS sequences are the most irradiated regions in the DC wall below the CL in the vicinity of the first weld of the first ring of the RPV. Because no thermal mixing with the hot RPV inventory can occur in the CL when the water level is low, free-surface condensation of steam on the water stripe (see Figure 1.7) is the most important mechanism to heat up the injected water during its flow from the injection location through the CL and the DC into the RPV water.

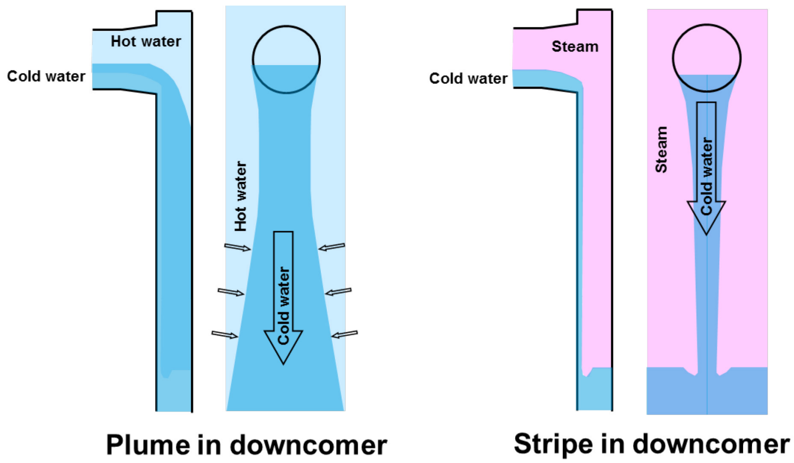


Figure 1.7: **Schematics of plumes and stripes in the downcomer [87]**

System-level codes like S-RELAP5 fail to predict the complex three-dimensional flow phenomena resulting from the ECC injection. However, they are used to define and derive boundary conditions for subsequent analysis steps. To generate temperature profiles and heat-transfer coefficients for the subsequent fracture mechanics analysis, various methodologies can be followed (see Figure 1.8).

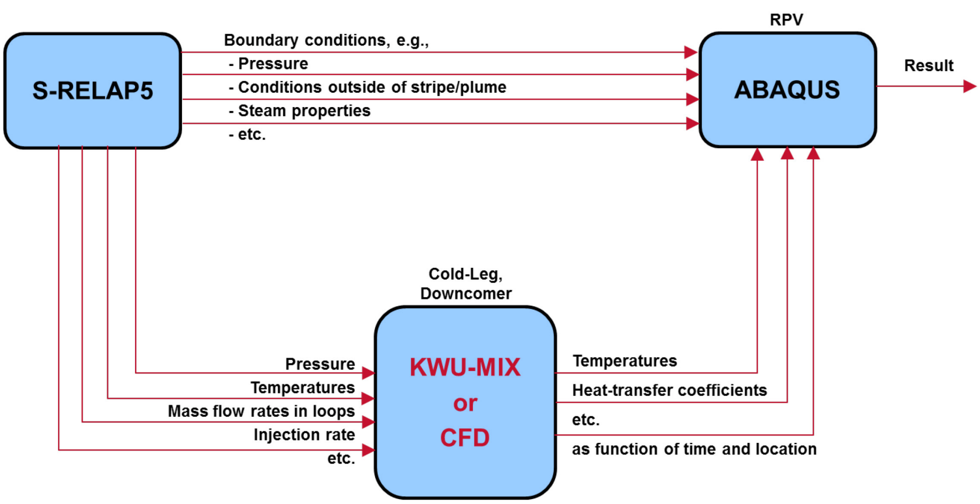
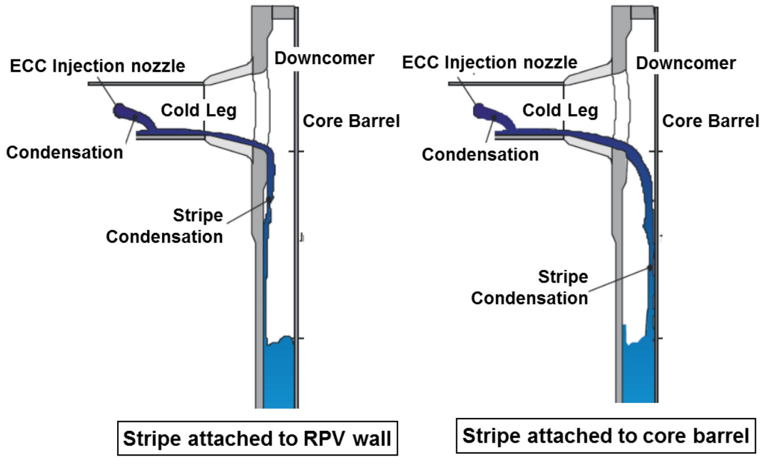


Figure 1.8: **Workflow at Framatome GmbH for PTS analyses: Chain of S-RELAP5, KWU MIX or CFD, and ABAQUS calculations [87]**

One methodology is the calculation of these data by analytical fluid-mixing codes verified with experiments, such as KWU MIX. Alternatively, CFD tools can be used after suitable validation. Whereas in KWU MIX conservative analytical models to quantify the mixing and the free-surface condensation in the CL and the DC are used, CFD can take into account detailed geometry and resolve more realistically the formation, development and behaviour of a cold-water plume and stripe. One advantage of CFD is the possibility to show the attachment of plumes and stripes to the inner wall of the RPV or detachment towards the core barrel. Without attached plumes or stripes (see Figure 1.9), the load on the RPV is significantly reduced, and for PTS only the thick structure of the RPV is of primary interest. Thus, the unsteady two-phase CFD simulation of a PTS-relevant transient with a low water level focuses on the DC in a full-scale reactor geometry.



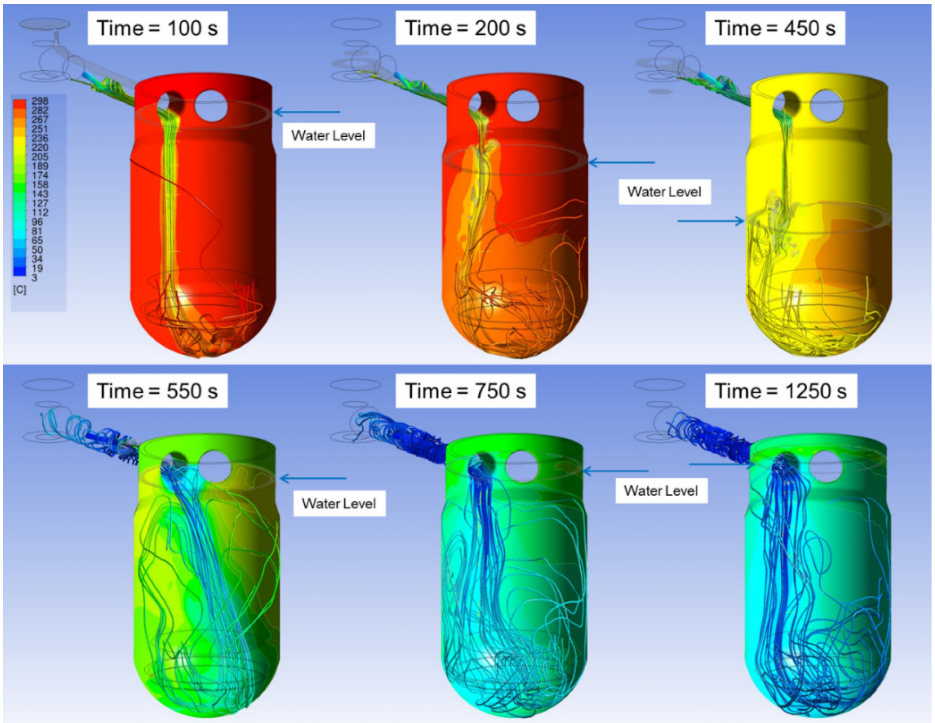
Note: The figure is based on a picture taken from [87].

Figure 1.9: **Schematics of a water stripe attached to the RPV wall (left) and detached from it (right)**

The two approaches, using either KWU MIX or a CFD code, which in this case was ANSYS CFX, were conducted for the same postulated LOCA transient of KKG. For both approaches, a series of different loading cases leading to PTS was first assessed using the system code RELAP5 to derive global parameters such as pressure and mass flow rates. These parameters then served as input data to KWU MIX which, due to the short calculation time, was used to derive the temperature profile and heat-transfer coefficients for each of the cases. The results from the system and mixing analyses were used as input in fracture-mechanics analyses in order to determine the limiting transient with respect to thermal loadings on the RPV's core weld among these loading cases. This limiting transient was finally recalculated with ANSYS CFX to reduce the conservatisms inherent in the analytical approach with KWU MIX.

A free-surface condensation model was implemented in ANSYS CFX to allow simulating the two-phase time period of the transient when the water level is below the CL nozzle. The implemented condensation model is based on the surface-renewal theory as described by Hughes and Duffey [88]. The exchange process at a liquid/gas interface is controlled by the turbulence in the liquid. This is based on the observation that on a calm water surface the water on top becomes saturated. To validate the free-surface condensation and the maximum mass flow rate for the stripe of liquid water before detachment from the RPV wall, experimental data from the TRAM C2 Run6b experiment at the full-scale Upper Plenum Test Facility (UPTF) were used [89]. To minimise the influence of different meshes, the validation simulations were performed using a mesh resolution similar to the target application at KKG. The threshold mass flow rate for attachment of a water stripe in the DC was checked and adjusted with the drag coefficient. It must be noted that this threshold mass flow rate for attachment is a function of the nozzle geometry, particularly of the radius of the lower edge, where the stripe of cold water turns into the downcomer. Thus, it is important to mention that the nozzle geometry of the cold leg used for ECC injection in this specific UPTF experiment has a similar radius as the CL nozzle in KKG. Without this similarity, more validation efforts would have been required to show the validity of the adjusted drag coefficient to match the threshold mass flow rate for different radii of the CL nozzle.

The validated setup was finally used to perform the simulation of the KKG PTS transient. Figure 1.10 shows fluid temperatures at the RPV wall from the CFD calculation with a condensation model at different time points of the transient. The water level is moving according to the blue line in Figure 1.11.



Note: streamlines started from ECC inlet coloured with fluid temperature and water level at different time points [87].

Figure 1.10: **Fluid temperatures at the inner RPV wall**

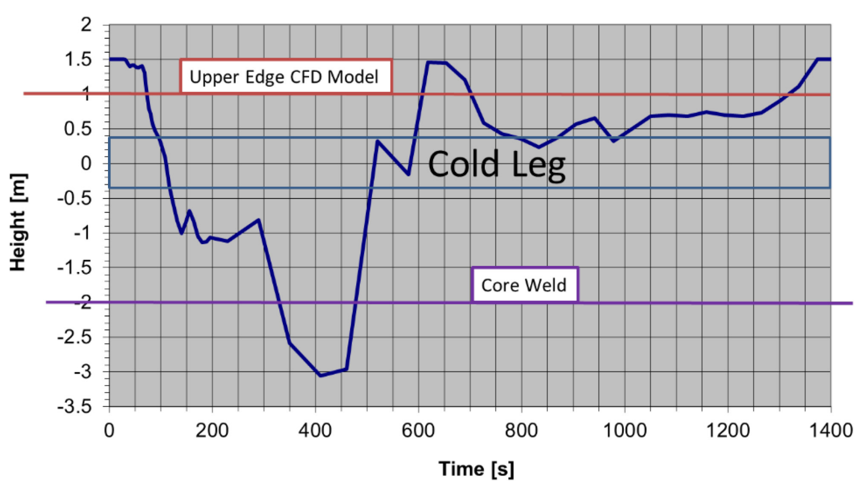


Figure 1.11: **Temporal evolution of the water level in the downcomer [87]**

The comparison of CFD and KWU MIX analyses of the limiting transient for the core weld, obtained from the selection process with KWU MIX, shows that the inherent conservatism in the standard KWU MIX approach leads to higher thermal loading than the chosen CFD approach and demonstrates the benefit of a CFD tool to quantify potential margins.

Chapter 2. Towards an expanded use of CFD

In this chapter, some of the reasons for the limited use of CFD in nuclear safety studies are identified and analysed to establish recommendations to be potentially endorsed by the NEA Computational Fluid Dynamics Task Group (CFDTG).

A survey was launched in 2019 on the status of CFD in safety studies. Although a majority (79%) of people over 82 respondents considered CFD to be mature, its use remains rather limited. Those respondents incoming from research institutions, industry, technical support organisations and regulator agencies who saw CFD as still immature cited three main reasons, as illustrated in Figure 2.1.

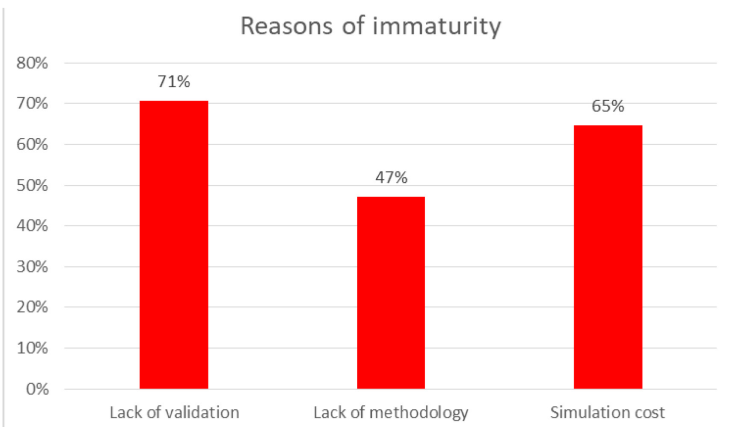


Figure 2.1: **Ranking of the main reasons of immaturity from the 2019 CFDTG survey**

These reasons are considered in the following discussion, with a focus on the "Need for CFD tool improvement", including validation (Section 2.1.1), and the "Need to further develop and implement methodology" (Section 2.1.2). In the survey, "Human-related factors" (Section 2.1.3) resulting from different perception of the capabilities of CFD were also identified.

"Simulation costs" are not further discussed as they are relative to the problem solution and depend, for example, on the availability of high performance computing (HPC) resources, which vary strongly between countries and within academia and industry. Furthermore, this Technical Opinion Paper (TOP) aims to highlight the capabilities and limitations of CFD in nuclear reactor safety (NRS) applications. Furthermore, this TOP's analysis of the capabilities and limitations of CFD in NRS applications finds that the higher simulation costs of CFD are justified.

2.1. Obstacles to an increased use of CFD

2.1.1. *Need for CFD tool improvement*

A significant challenge to the broader use of CFD tools in the nuclear safety field is the global issue of verification and validation (V&V) to demonstrate the accuracy of a simulation's results. This includes the question of how it can be demonstrated that the models (both numerical and physical) implemented in the CFD software can yield reliable (and/or conservative) results for given flow configurations for given variables of interest. This validation step is classically performed by comparing numerical results to experimental data: as CFD tools resolve local structures (~1 mm in size) of the flow, the most useful validation experiments are equipped with fine-grained instrumentation to make sure the numerical models are able to capture the relevant physics. Special care should also be given to initial and boundary conditions. Meeting these requirements is a difficult task and has led to the development of the concept of "CFD-grade" experiments, [19]. General observations that arise are then:

- The awareness of the existence of these experiments by numerical analysts. To the authors' knowledge, no shared and regularly updated framework exists that lists potentially interesting experiments and their characteristics. Thorough literature surveys through scientific journals and conference proceedings therefore become mandatory and must be repeated by numerical analysts worldwide.
- The accessibility and conditions for the use of data from these experiments:
  - Datasets can be stored on computers of individual scientists who may have changed activities when the experiments are planned to be exploited by numerical analysts.
  - Datasets may be protected by non-disclosure agreements.
  - Datasets may use non-standard formats.

Data is scattered over a large number of databases, for example:

- Databases for general validation purposes:
  - Classic Collection Database (http://cfd.mace.manchester.ac.uk/ercoftac/doku.php)
  - Turbulence Modeling Resource (https://turbmodels.larc.nasa.gov/)
  - Validation on cases from NASA Turbulence Modeling Resource and other academic cases (http://elsa.onera.fr/TMR-0001/index.html)
- Direct numerical simulation (DNS) data:
  - Johns Hopkins Turbulence Database (http://turbulence.pha.jhu.edu/)
  - Database of Wall-Bounded Turbulent Flows (https://torroja.dmt.upm.es/turbdata/index)
  - Databases on turbulent flows (https://thtlab.jp/)
  - Turbulence data (https://turbulence.oden.utexas.edu/)
- Application-oriented validation experimental databases (limited access):
  - International Experimental Thermal HYdraulics Systems database (www.oecd-nea.org/tiethysweb)
  - CSNI Code Validation Matrix (www.oecd-nea.org/jcms/pl_25369/csni-code-validation-matrix)
  - Containment Code Validation Matrix (www.oecd-nea.org/jcms/pl_19413)
  - Integral Experiments Data, Databases, Benchmarks and Safety Joint Projects (www.oecd-nea.org/jcms/pl_72332)
  - Storage of Thermal REactor Safety Analysis Data (https://stresa.jrc.ec.europa.eu/)

Legacy data are still an irreplaceable resource for application-oriented validation for existing reactors (e.g. HDR, BMC, ROCOM, PKL experiments). However, their availability and documentation are still largely limited.

Besides the validation of a given set of models within a specific CFD code, questions can be raised concerning the genericity of a model's options, closure laws and the setup of the computation with the CFD approach for a given application. In other words, using the same set of choices with different codes should provide the same result (but does not always do so). This was highlighted, for example, in a benchmark conducted in the NEA HYMERES project on the erosion of a stratified layer by a vertical jet in presence of a flow obstruction [90]. The experimental setup was close to an existing benchmark case [91] and a certain validation experience was expected. Furthermore, the blind benchmark involved two submissions: one "best-estimate" result and one result obtained with a predefined "common model" that covered various aspects of the simulation (geometry, turbulence modelling, initial and boundary conditions, some fluid and flow properties, etc.). Unexpectedly, the spread in the results of the "common model" was large, indicating that besides the physical modelling, the adequacy of the mesh, wall treatment, numerical schemes and parameters, etc. can have a significant and partially compensating effect. The lack of systematic studies in most contributions underlined how difficult it is to implement a rigorous approach to guaranteeing mesh and time step independence in the analyses of transients requiring hundreds of hours of central processing unit (CPU) time. The benchmark also identified the need for continuous application-oriented coupled effect/integral effect test validation and a backward assessment against previous results.

Currently, a significant part of published CFD analyses uses commercial multipurpose CFD packages. These are used widely in many industries and feature a rigorous quality assurance of the source code, a user-friendly and fault-tolerant graphical user interface (GUI) and a comprehensive and documented validation database. However, this validation often targets flow conditions (e.g. external aerodynamics, gas turbines) that do not apply to nuclear safety. Consequently, the application of commercial codes also requires a thorough review of their modelling assumptions and validation basis. The assessment of the code for application to the expected flow conditions (e.g. natural circulation flows) remains the responsibility of the user.

A related point concerns the genericity of models with respect to a range of applications. This concerns more particularly multiphase flow computations, for which the number of closure laws is large and can be specific to the application and/or code.

Another aspect that is often associated to CFD, and which may hinder a more global use, is the fact that CFD calculations (and, more generally, industrial CFD studies that can include a number of CFD calculations to perform sensitivity analysis to various parameters) are generally computationally expensive; this is due to the amount of degrees of freedom (number of mesh cells and variables) inherent to CFD. Solving a transient flow in an industrial configuration with a RANS-class turbulence model on several hundred cores of a recent cluster typically takes days or even weeks, depending on the performance of the built-in algorithms of the software and hardware properties. There are then two bottlenecks:

- The availability of computational power – clusters dedicated to scientific calculations being costly (to acquire and to exploit). These machines are often shared between several institutes, and calculation hours are often difficult to obtain.
- The cost of the licence of the commercial products, often related to the number of cores. This can limit the size of the problem to be solved and/or the number of possible calculations.

It is also worth mentioning that the calculation period is preceded by a period dedicated to the construction of the calculation domain itself (creation of computer-aided design [CAD] from plans, meshes from CAD), which can be time-consuming, depending on the complexity of the geometries and the kind of meshing tool being used. For projects with severe time constraints, this pre-processing step can be a limiting factor. Finally, the post-processing step can also involve a non-negligible cost, depending on the complexity of the targeted data.

A final issue concerns the reliability of computational power: a "bug" in one core is sufficient to break down the full computation.

2.1.2. ***Need to further develop and implement methodology***

The methodology for nuclear safety studies including CFD computations appears to be lacking or to be at least incomplete in some cases. Indeed, the introduction of CFD computations within a safety study can induce some specific work that goes beyond the scope of the CFD study itself and is not covered by the previous methodology without CFD.

In addition to establishing the validity of using CFD for a specific case, the parameters of the CFD study must also be properly chosen and justified. Even if some guidelines have already been edited [3], covering many situations, they could be insufficiently known, applicable or updated. An example where guidance was missing and experience insufficiently documented is the modelling of gas radiation heat transfer, which has been identified to be of high relevance, for example, for heat and mass transfer in humid atmospheres [92]. Besides modelling the spectral properties of the gas mixture and surrounding structures, the user must also select an approach to solving the radiative transport equation (RTE). The latter is often accompanied with strict assumptions (e.g. optically thick media) or numerical methods to limit the additional computational cost (e.g. a reduced update frequency of the RTE, solution of the RTE on a coarser mesh and mapping of the source terms), which can affect the accuracy of the result significantly.

Another difficulty in the methodology is related to the justification of the accuracy of the CFD result, which has to be supported by an evaluation, the so-called uncertainty quantification. Several methods have been developed to derive this quantification more often for system-scale studies, but their application to CFD is still limited and so far concerns mostly benchmark studies, not industrial cases.

Whenever a CFD study is used to focus on a sub-part of a more general study (e.g. a sub-geometrical domain with respect to the domain of interest to be studied), a strong coupling of the CFD evaluation with other tools may be required. It could induce some complexity in the methodology to justify some choices made for this coupling or even to perform such coupled evaluations. Not so many coupled methods are available, and some are still in development. The coupling could be complex or partially inefficient (costly) without having full access to the sources of the codes. Indeed, more than the individual tools, the coupling must be verified and validated: both the coupling algorithm and the accuracy of the coupled evaluation. This is the case for both multi-scale and multi-physics studies.

Furthermore, for coupled multi-physics analyses, a well-balanced representation of the single physics is required to enable an efficient and representative analysis. For example, a highly accurate 3D simulation of a boiling flow may be of limited impact if the coupling with neutron physics feedback (void coefficient) is missing or simply provided on a coarser pin/subchannel level that cannot account for the detail provided by the CFD analysis. Another example is a detailed 3D analysis of a transient which focuses on a certain region of interest. Here, the system feedback must be carefully considered, for example by means of a coupling to established nuclear system codes, to ensure a representative assessment.

2.1.3. ***Human factors***

Human factors are a significant impediment to the broader use of CFD for NRS applications. Most people working in the field of nuclear safety analysis have been familiar with thermal hydraulics system codes for many years. Even people not directly working with simulation codes usually have a good idea of what system codes can or cannot predict. System codes were/are developed and maintained within the nuclear industry and thus often contain the specific expert knowledge of a company, national laboratory or technical safety organisations (TSO). Users are carefully trained in their usage as a part of the maintenance of competence. The codes have been used for decades in licensing processes and a certain understanding exists among authorities and applicants on how to conduct and document a design and safety analysis. In contrast, CFD codes mostly originate from academia (e.g. OpenFOAM) or commercial providers (e.g. ANSYS or Siemens), with only a few developed in the nuclear industry (e.g. EDF's SALOME platform). On the positive side, this makes it possible to directly involve cutting edge computational methods and models developed with significant manpower outside of the nuclear field. However, it also opens nuclear safety assessment to a broad variety of models, methods and tools that have neither been developed nor sufficiently validated for it. It opens the rather closed group of nuclear engineers to contributors from other industries and academia who have excellent knowledge of CFD but not on its specific application in nuclear engineering. Significant effort is still needed to build trust in CFD.

For people directly performing calculations, those who start to work with CFD codes in the field of nuclear reactor safety are often either confirmed CFD users (from academic or R&D company divisions) but newcomers to the field of NRS, or people with experience in NRS (from industry, regulators or TSOs) but newcomers to CFD. The first category of people, even if they are confirmed CFD users, may lack some "NRS culture" basics, notably when V&V is concerned. The second category of people are familiar with the "NRS culture" and may have a previous experience with system codes, but are not very aware of the specificities of CFD. Having the two categories of users in a single team can be positive if they can work together and learn from one another.

For people who are not directly involved in performing calculations, like project managers or decision makers, a lack of information concerning CFD may have different consequences:

- On the one hand, some people may be reluctant to have CFD used for a NRS application for which it has not been used before (out of conservatism or fear of the unknown).
- On the other hand, other people may have extremely high expectations concerning CFD, which they see as an almost "magical tool", even believing that a CFD simulation is a "perfect" representation of reality without the need for any physical modelling as is required for system codes. This may be the case with people who were informed about CFD through some sort of 'advertising for decision makers'. It can be cited from well-known fundamental literature on CFD [93]: "*..Industrial users of commercial CFD-codes should especially be careful, as the optimism of salesmen is legendary. Wonderful color pictures make a great impression but are of no value if they are not quantitatively correct. Results must be examined very critically before they are believed.*"

In the latter case, people are likely to get disappointed at some stage, which could then make them reluctant to use CFD again.

Due to a continuous rise in CFD applications, there still are many "first of its kind" applications of CFD in projects. Also, on the regulatory side, the acceptability of a CFD-based safety assessment is often questioned as there is no existing valuation standard. Consequently, applicants often stick to established methods. However, these methods might not be accurate enough to keep with the trend of the last 40 years to reduce margins to achieve financial savings. CFD can be a way to reduce conservatism in a plant's design and safety layout in the right places, but only if it is based on qualified CFD methods. The evolution of the US NRC best practice guidelines (BPG) for dry casks [25,84] shows that work in this direction is ongoing on the regulatory side, too.

2.1.4. ***Main remaining challenges for CFD***

To sum up, some of the main issues still hindering greater use of CFD in NRS studies are:

- The lack of qualified/accepted/established methodologies in certain cases. This notably concerns situations where coupling with other physics and/or thermal hydraulics at other scales is needed. For uncertainty quantification, even though methodologies have been developed or adapted from system scale, they are still not widely used and their applicability has to be stated.
- Access to information: for people using CFD in NRS studies, this concerns access to databases of experimental ("CFD-grade" or DNS) results of interest for code validation, or even simple awareness of the existence of such databases. For people like decision makers or project managers, this concerns access to independent (i.e. non-commercially biased) information on CFD, including its potential benefits and limitations, so that they can make the right decisions.
- Human factors: it can be a real challenge for a company or institute to build up a "CFD team" with knowledge of both CFD and the nuclear safety framework. Another challenge is then to have this "CFD team" work efficiently with teams dealing with other physics and/or with thermal hydraulics at different scales.
- Cost: the cost of CFD calculations can of course be a major limiting factor. Such costs result from engineering hours, licence fees in case of the use of commercial CFD software and hardware costs for the HPC environment. However, the preceding discussion may serve as a basis to justify these costs for studies that really profit from the use of CFD. The cost of the CAD and meshing steps, before running a CFD calculation, can also be a serious limiting factor, depending on the meshing technique being used. While using an automatic meshing tool can be quick and easy, building up a fully conformal hexahedral mesh can be the most time-consuming part of a study. Hardware costs are difficult to

overcome, except by simply waiting for more powerful calculators to become available (Moore's law is still valid).

2.2. Possible ways to overcome the challenges

Three types of solutions can be identified from the previous chapter and are discussed below: sharing knowledge, enhancing reliability and addressing human-related factors.

*2.2.1. **Knowledge sharing***

There are multiple ways promoting knowledge sharing and this document identifies a set of potential actions that make it possible to better include CFD in NRS studies.

Reference documents already exist (like BPG or synthetic reports on CFD activities) but still must be regularly updated and promoted for their information to be efficiently spread. This is a continuous effort to be made by the community and the NEA CFDTG in particular.

Most of the documents written by CFD specialists are meant for relatively advanced CFD users. Documents to better popularise the capabilities and limits of CFD could be useful, such as a synthetic document about CFD capabilities, successful applications and limits in the frame of NRS.

The development of the use of CFD could be better oriented towards NRS by spreading the knowledge of safety studies from the CFD community to other communities. This could be done through broadening the public of the CFD4NRS workshops by, for example, including dedicated sessions on NRS issues; inviting system code users to exchange on system-scale open issues to be addressed (for established and also new reactor concepts) and complemented by means of CFD; and inviting more TSO and regulators.

Guidance exists both for good practice in the use of CFD for an application and for the qualification of calculations in safety demonstrations. The current update of the BPG for CFD in NRS includes references to such qualification processes. A strong connection between best practices and qualification requirements could help clarify the assessment process of safety studies including CFD and could result in a recommended process for this purpose.

*2.2.2. **Enhancing reliability***

Enhancing reliability through reference data comparison

As pointed out above, limited access to reference data can be an issue for the needed validation of CFD. Building a databank for safety-related configurations would therefore be useful to better identify existing data. This databank could include both experiments and numerical solutions (e.g. DNS). There exists a large database built for the development and validation (D&V) of system-scale analysis. A possible activity is to identify among them those that could also be used for CFD. This work could also be an opportunity to revisit the data and some practical aspects (e.g. renewed documentation including data format description, availability). This activity could be carried out with a tight link between the system-scale and CFD communities.

There are several good examples of existing platforms to access data:

- the ercoftac database (http://cfd.mace.manchester.ac.uk/ercoftac/doku.php);
- the European projects for building databank as FAIR (findable, accessible, interoperable, reusable) data (https://cordis.europa.eu/project/id/831558) and the related CERN tool Zenodo (https://zenodo.org).

Given the large number of existing databanks, it seems more relevant to build a library of links for data related to CFD for NRS. The NEA website could host a dedicated (potentially community-based) page that would be the centralised entry point for CFD for NRS users. It would include:

- links to validation databases;

- links to BPGs;
- agenda and history of relevant conferences (NURETH, NUTHOS, CFD4NRS, etc.);
- selected publications.

Collaborative work in this area is of great interest and must be continuously promoted. From the NEA perspective, this concerns activities like international benchmarks, their connection with international workshops and conferences and their permanent link in the NEA databank.

Another example of potential collaborative activity in this area could be an application-oriented analysis of the required and existing data: such a review could result in a validation matrix identifying available data for particular nuclear safety applications and potentially defining needs for further activities [10].

Enhancing reliability through CFD-model benchmarking

The variety of CFD models for a given phenomenon to be described (e.g. turbulence or two-phase flows) most of the time is the result of separate efforts in the community to tackle an issue. There is a benefit in reducing or clarifying this diversity once the models are strong enough (through validation).

For two-phase flow, without being exhaustive, several initiatives can be noted:

- the work on the so-called baseline model by the HZDR team, [94];
- the benchmark project on the DEBORA experiment (convective subcooled boiling), which includes both a comparison with data and “a collective review of the pros and cons of the models offering a mutual effort towards the improvement of their weaknesses”.

This activity goes beyond the classical experimental vs numeric analysis of gaps since the comparison also concerns a priori also, for example, internal data that are predicted by models but not measured.

In many benchmark activities, the motivation is related to a given application, but the analysis is restricted to a comparison between experimental data and numerical results. The link between the results and the application target variables is not always sufficiently made and the conclusions drawn are then insufficient with respect to the application goal. In the future benchmark activities, it is recommended to add a more “application-oriented” comparative study. For example, participants should provide their evaluation of an elementary study derived from the application case. This elementary study has to be defined as being between the full-scale application case and a more simplified case. The link between a numerical simulation performance with respect to an experimental case and the potential scattering of participants’ results on this applied exercise is of interest. It is certainly useful for this analysis to define an “application-oriented” post-processing of the numerical simulation of the experiments that differs from the list of available experimental data.

Enhancing reliability through uncertainty quantification

There is a clear lack of proof of applicability for many of the uncertainty quantification methods, mainly due to the large number of computations they imply and the associated cost. Efforts to reduce the number of costly CFD simulations for UQ include using clever algorithms (e.g. deterministic sampling) or setting up reduced-order models (ROM) for specific applications. The latter approach includes the demonstration of the applicability and limitations of the developed ROM for the full-scale CFD application. Recent work, [22], has provided a promising alternative methodology to address model uncertainty on a more general way than a parametric variation of model parameters. There is a strong desire to bring such UQ methods to maturity so that they can be used “off-the-shelf”.

Furthermore, uncertainty always comprises two contributors:

- The aleatory or stochastic uncertainty arises, for example, from a propagation of measurement uncertainties of the boundary conditions into the results. It results in a scatter around the “real” value and can be quantified by a statistic evaluation of parametric analysis.

- In contrast, the epistemic uncertainty results from a lack of knowledge (e.g. model geometry, unknown boundary conditions and physical modelling assumptions). It cannot be quantified by a statistic evaluation of parametric studies and often leads to a bias in the analysis result.

To make progress in this area, it could be worth dedicating collaborative exercises on the topic to summarising and documenting experience and to deriving commonly accepted (maybe application-specific) UQ strategies and processes.

2.2.3. ***Human factors***

As outlined in part 3.1, engineers and especially decision makers need to avoid excesses of conservatism or enthusiasm when about to initiate a first-of-a-kind use of CFD for a problem. Conservatism is fundamentally a sound attitude when nuclear safety is concerned, as long as it does not lead to a “frozen” situation that blocks any progress. Excessive enthusiasm resulting from exaggerated expectations concerning the CFD method will often lead to disappointment.

Giving decision makers and project managers, among others, information on CFD, including its possibilities, cost and limitations, can be useful. This information may take the form of a document a few pages long, a “CFD for decision makers”, created by the community of nuclear safety and independent of commercial codes’ advertisement.

Within companies, CFD experts (or confirmed users) should also consider making introductory presentations on CFD for their colleagues, particularly for decision makers. This can be useful to avoid keeping CFD teams isolated within entities dealing with NRS. Close collaboration with teams dealing with thermal hydraulics at other scales (component, system, etc.) and/or with other physics (solid mechanics, neutronics, etc.) is essential to help CFD find its right place in NRS teams. One important role for CFD experts, or confirmed users, is to be able to tell their colleagues whether the use of CFD is the best option for a given problem or not.

- If the use of CFD can bring real benefits, they should tell colleagues who may not be aware of this fact (and who may thus fail to ask them). CFD experts should proactively talk to potentially concerned people.
- If the use of CFD would bring no real benefits compared to “simpler”, cheaper and faster approaches, the experts should be able to explain why, notably to decision makers who would otherwise tend to “rush” into the CFD approach.

For people directly involved in performing CFD calculations for NRS studies, having people with different backgrounds work together is usually a good idea: people with more experience in CFD will thus learn from people with more experience in NRS, and vice versa.

A short “CFD for system-scale code practitioners” document and a “system-scale codes for CFD practitioners” document could help bridge the gap between the two communities.

Open-source CFD code development in the nuclear sector may support acceptance of CFD solutions as they are completely “reviewable” and developed from nuclear R&D teams for nuclear applications. Of course, they can also help to reduce/avoid costs for commercial CFD software. Open-source licences imply easy access to existing models and solutions to reuse and adopt them. Furthermore, there is a growing and active community around less commercial open-source codes such as OpenFoam or Code_Saturne, which provide online training materials such as video tutorials, report bugs and support further development and maintenance of the projects. In this context, the Open-source Nuclear Codes for Reactor Analysis (ONCORE) initiative [73] has been recently launched as an IAEA-facilitated international collaboration framework for the development and application of open-source multi-physics simulation tools to support research, education and training for the analysis of advanced nuclear power reactors.

2.2.4. *Synthesis*

Problems	
CFD improvement and validation	(1) Limited availability/awareness of appropriate "CFD-grade" data or at least well documented validation data. (2) Limited access to legacy experimental data for application-oriented validation. (3) Limited genericity: Broad range of closure models. Using the same set of choices with different codes does not necessarily provide the same result. (4) Commercial CFD code development aims at "multipurpose" tools, while application-oriented extension and validation remains sole duty and effort of the user.
Method development	(5) CFD is not yet a widely established/accepted element of a safety study. (6) CFD is not a method developed within the nuclear industry but is adopted from other fields → thorough qualification and integration into NRS is necessary. (7) Partly missing guidelines (e.g. with regard to specific physics). (8) Partly missing approaches (e.g. UQ) to justify results' significance. (9) Multi-physics or system-scale coupling approaches are necessary to enable a representative CFD study, but are often still under development.
Human-related factors	(10) Acceptance of established methods has grown, but there is lacking knowledge or a wrong perception of the capabilities/limitations of CFD codes. (11) CFD experts often have limited experience in nuclear engineering and lack "NRS culture" (in particular on V&V, leading to conservatism). (12) A CFD team is often a separate group of experts in a company or involved as external contractors with limited view of non-CFD-applications. (13) CFD applications are mostly first-of-a-kind, so there is limited experience on CFD in NRS among industry, authorities, and TSOs.
Cost	(14) Comparably high cost compared to established methods in both computing time and pre- and post-processing. (15) Availability of computing power and licences.
Solutions to:	
(1, 2, 13)	Create and maintain a centralised entry point for CFD for NRS users providing links to validation databases, BPGs, selected publications.
(2, 3, 4)	Create "CFD4NRS validation matrix" (connection to NEA data bank).
(5, 6, 7)	Continuous updating of SOA/BPG documents.
(3, 4, 9)	Extend benchmarking activities by code-to-code comparisons and even towards application-oriented comparative studies focusing on the prediction of safety criteria.
(3)	Definition of "baseline" models with known capabilities and limitations.
(8) (8)	Collect and summarise experience with the application of UQ to CFD in NRS. Support future work on UQ methods for CFD.
(4, 5, 6, 12)	Write white paper to inform decision makers and beginners about CFD capabilities and limitations with respect to NRS applications, independent from commercial code advertisement.
(10, 11, 14)	Enable/motivate CFD experts/confirmed users to decide whether the use of CFD is the best option for a given NRS problem.
(4, 6, 15)	Follow NRS-related open-source projects.
(9, 10, 11, 12, 13)	Improve participation of system code users, TSOs and regulators in CFD4NRS workshops.

Given the points examined above, the following priority actions could be taken to extend the use of CFD in NRS studies:

- Building a library of links for data related to CFD for NRS, including links to validation databases and to fundamental documents (BPG, etc.).
- Enhancing reliability through CFD-model benchmarking and extending application-oriented comparative studies.
- Updating and promoting reference documents that already exist (such as BPGs and synthetic reports on CFD activities).
- Supporting future work on the development of UQ methodologies for CFD. Collecting and summarising existing work.
- Providing help to organisations that are new to CFD in the form of a few short, simple documents such as "CFD for decision-makers", "CFD for system code users", and "System codes for CFD users".

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CSNI Technical Opinion Paper No. 20

Applications using computational fluid dynamics (CFD) are gaining interest as complementary methods to evaluate nuclear reactor safety (NRS) cases implying thermo-fluid dynamics. CFD resolves a higher level of phenomenological detail compared to the established system-scale tools. While this appears promising, it also raises new questions in the valuation and integration of CFD-based safety studies, which are still limited to a relatively small number of applications. For this reason, and given that the development of CFD is a fast-evolving and relatively recent activity in nuclear safety, the CFD Task Group (CFDTG), which is part of the Working Group on Analysis and Management of Accidents of the NEA's Committee for the Safety of Nuclear Installations, has been conducting collaborative work in this field since 2002. This Technical Opinion Paper aims to provide the nuclear safety community with a clear picture of the current uses and capabilities of CFD. It also outlines the main challenges hindering greater use of CFD in nuclear safety studies and discusses ways to overcome them.

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