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SUMMARY REVIEW ON THE APPLICATION OF COMPUTATIONAL FLUID DYNAMICS IN NUCLEAR POWER PLANT DESIGN

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The Agency's Statute was approved on 23 October 1956 by the Conference on the Statute of the IAEA held at United Nations Headquarters, New York; it entered into force on 29 July 1957. The Headquarters of the Agency are situated in Vienna. Its principal objective is "to accelerate and enlarge the contribution of atomic energy to peace, health and prosperity throughout the world''.

IAEA NUCLEAR ENERGY SERIES No. NR-T-1.20

SUMMARY REVIEW ON THE APPLICATION OF COMPUTATIONAL FLUID DYNAMICS IN NUCLEAR POWER PLANT DESIGN

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FOREWORD

The IAEA's statutory role is to "seek to accelerate and enlarge the contribution of atomic energy to peace, health and prosperity throughout the world". Among other functions, the IAEA is authorized to "foster the exchange of scientific and technical information on peaceful uses of atomic energy". One way this is achieved is through a range of technical publications including the IAEA Nuclear Energy Series.

The IAEA Nuclear Energy Series comprises publications designed to further the use of nuclear technologies in support of sustainable development, to advance nuclear science and technology, catalyse innovation and build capacity to support the existing and expanded use of nuclear power and nuclear science applications. The publications include information covering all policy, technological and management aspects of the definition and implementation of activities involving the peaceful use of nuclear technology.

The IAEA safety standards establish fundamental principles, requirements and recommendations to ensure nuclear safety and serve as a global reference for protecting people and the environment from harmful effects of ionizing radiation.

When IAEA Nuclear Energy Series publications address safety, it is ensured that the IAEA safety standards are referred to as the current boundary conditions for the application of nuclear technology.

This publication presents the results of the coordinated research project (CRP) entitled Application of Computational Fluid Dynamics Codes for the Design of Advanced Water Cooled Reactors, which addresses the application of computational fluid dynamics (CFD) computer codes to the process of optimizing the design of water cooled nuclear power plants and their components. Building on past initiatives in which CFD codes have been applied to a wide range of situations in nuclear reactor technology, the 15 CRP participants from 11 Member States aimed to develop a systematic framework for the consistent application of CFD codes and to establish a common understanding of the capabilities of CFD codes and their level of qualification.

The results of this CRP are expected to be of interest to a broad range of Member States, including those currently operating or embarking on nuclear power programme. As of March 2022, there were 441 nuclear power plants in operation around the world, with a further 51 under construction, bringing the total operating experience to slightly over 19 000 reactor years. Advanced nuclear power plants that increasingly use CFD codes in their design are being offered by various vendors.

This publication presents examples of CFD applications in nuclear power plants component and system design from Member States participating in the CRP. The publication focuses on CFD aided modelling in technology development and design, and thus complements existing publications that concentrate largely on the use of CFD codes for nuclear safety analyses. Issues and interests common to both efforts, lessons learned and application guidelines derived from validation against relevant scaled experiments are also described to aid in the correct and practicable application of these tools.

The IAEA expresses its appreciation for the contributions of several Member States. It is particularly grateful to the participants of the CRP for their contributions to the publication. The IAEA officer responsible for this publication was M. Krause of the Division of Nuclear Power.

CONTENTS

1. INTRODUCTION

1.1. BACKGROUND

The growth in computer hardware over the last 30 years, accompanied by the development of stable and efficient numerical algorithms, has created opportunities for the use of computational methods, greatly reducing the earlier reliance on experimental testing in the design and development of multiple industrial systems. The rise of computational fluid dynamics is part of this advancement. However, during a period of low growth in the nuclear power industry (starting in the mid-1980s), the primary driving force for the development of CFD technology has been in the non-nuclear area, such as in the aerospace, automotive, marine, turbomachinery, chemical and process industries and, to a lesser extent, in the environmental and biomedical fields. In the power generation area, the principal applications have again been non-nuclear: combustion dynamics for fossil fuel burning and gas turbines, vanes for wind turbines, etc.

A resurgence of interest in nuclear technology between 2005 and 2011, the much heralded ‘nuclear renaissance’, was interrupted directly by the accident on 11 March 2011 at the Fukushima Daiichi nuclear power plant in Japan, and indirectly by the low cost of alternative energy production methods, especially gas turbines, and renewable sources such as solar and wind power. Nevertheless, many countries are still actively pursuing NPP construction policies as part of their future energy mix.

The IAEA has long been aware that there will be increasing interest in the use of CFD codes and, in particular, in their verification, validation and uncertainty quantification. As a result, it has collaborated with the OECD Nuclear Energy Agency (OECD/NEA) in sponsoring the initial exploratory effort to document the progress of CFD as a simulation tool in the field of nuclear reactor safety, and advance it by proposing numerical benchmarking exercises and organizing international workshops. These jointly sponsored activities remain ongoing. This coordinated research project) seeks to fill a gap in the original initiative, recognizing the growing use of CFD tools for reactor design purposes, while maintaining the existing synergy with the OECD/NEA by continuing efforts in the area of reactor safety.

In recognition of the increased use of CFD in the design of advanced water cooled reactors, a publication on the subject was requested from the IAEA in 2010 by the technical working groups on advanced technologies for light water reactors (LWRs) and heavy water reactors (HWRs). In addition, these two technical working groups also suggested the preparation of a CRP on the Application of CFD Codes for the Design of Advanced Water Cooled Reactors, to be initiated in 2012.

As a first step in the establishment of this CRP, a Technical Meeting was convened in Vienna in December 2010 which served to showcase current efforts in the field. A number of major reactor vendors were represented, as well as CFD researchers from academia and national institutes. There was a consensus that this subject be formalized in terms of a fully developed CRP, and that an IAEA publication on the subject be published. Sixteen organizations from 11 Member States participated in the CRP: Algeria, Canada, China, France, Germany, India, Italy, Republic of Korea, Russian Federation, Switzerland and the United States of America (USA).

1.2. OBJECTIVE

This CRP addresses the application of CFD computer codes to the process of optimizing the design of water cooled NPPs, though it is not limited to this reactor type. Building on past initiatives in which CFD codes have been applied to a wide range of situations in nuclear reactor technology, this CRP aims to define a framework for the consistent application of CFD codes for NPP design purposes, and to establish a common understanding of the capabilities of CFD codes and their level of qualification.

The primary objective of this publication is to determine to what extent CFD has become a part of the NPP design process over the past ten years, how it is expected to develop over the coming years, and how CFD will continue to contribute to the assessment base of the technology. The role of the IAEA is to report on the current status of CFD in NPP design and sponsor international CFD benchmarking exercises in areas of relevance to design engineers. One of the benchmark activities is based on rod bundle tests [1], relating directly to design optimization of a fuel assembly spacer grid, while the other benchmark [2] applies to safety considerations. Selected results have also been summarized in a recent conference paper [3].

1.3. SCOPE

This publication summarizes the current capabilities and applications of CFD codes, and their present qualification level, with respect to NPP design requirements. It is not intended to be comprehensive, focusing instead on international experience in the practical applications of these tools in designing NPP components and systems. The guidance in this publication is based on inputs provided by international nuclear industry experts directly involved in NPP design issues, CFD application, and in related experimentation and validation brought to light during the CRP.

1.4. STRUCTURE

Section 2 contrasts CFD codes and their use with traditional lumped parameter system codes, while Section 3 gives a wide-ranging survey of CFD applications in NPP component and system designs from Member States considered, within the context of this CRP, to have capabilities in the nuclear power area. It describes the design issues and physical phenomena currently being addressed, the benefits to be derived from using CFD tools in the analyses, their limitations, and the need for further improvements.

Section 4 focuses on the status of CFD code verification and validation procedures for those applications for which CFD tools are either already being used, or planned to be used, in the near future for NPP design purposes. In the latter case, attention is given to the outstanding technology gaps, be these in terms of limitations of the current capabilities of the codes, or the availability of ‘CFD-grade’ experimental data to provide the requisite validation database needed to support the numerical predictions. Section 5 investigates the near-term future with respect to the use of CFD.

Section 6 provides current best practice guidance, Section 7 gives some examples of existing experiments suitable for CFD code validation, and Section 8 attempts to define high level minimum CFD code user requirements, including summaries of the available training courses.

Section 9 provides insights into CFD code uncertainties, including a very recent development in CFD applications to nuclear technology, while Section 10 provides an overview of remaining technology gaps on a variety of important topics of current research interest.

Finally, Section 11 summarizes the general intent of the publication, and overall findings from related activities conducted within the context of the CRP.

2. ROLES OF SYSTEM CODES AND COMPUTATIONAL FLUID DYNAMICS IN THE NUCLEAR POWER PLANT DESIGN PROCESS

The growth of computer hardware over the last 30 years also saw the development of very reliable thermal hydraulic codes to examine system behaviour under a variety of transient conditions. These numerical tools are invaluable to the design engineer in determining the global response characteristics of the primary system to a variety of non-steady incidents affecting the plant, under both normal and abnormal operating conditions. Codes such as RELAP-5, TRACE and CATHARE, for example, have been used in the thermal hydraulic analyses of primary circuit transients. Other programmes, such as GOTHIC and GASFLOW, are widely used for containment analyses, especially for the buildup of hydrogen following a severe accident, and MAAP and MELCOR for assessing the risks of vessel penetration arising from such events. These codes are now well regarded among reactor vendors and their regulatory authorities in supplying evidence of the robustness of the plant to certain foreseen and unforeseen operating incidents.

Traditional approaches to plant safety using system codes have been successful due to the very large database of phasic exchange and wall heat transfer correlations that have been built into them. These correlations have been established from essentially 1-D separate effects experiments (initiated by events at the Three Mile Island accident in 1979) and their range of validity has been well scrutinized. Thus, although 1-D formulations may restrict the application of system codes in simulations in which there are 3-D geometrical complexities, and the associated 3-D motion of the coolant fluid, the physical models are now well-established and reliable, provided they are used within their specified ranges of validity. In addition, mock-up tests are invariably conducted with 3-D effects in mind. The trend has therefore been to continue with such approaches, but to respect their geometrical limitations.

The application of CFD methods to nuclear reactor design is less well developed than for other industries, but the technology is advancing, principally directed at those situations in which 3-D flow conditions prevail, which of course are already a feature of NPP operation. The data storage and CPU issues associated with a description of 3-D fluid flow, as opposed to the essentially 1-D description embodied in the system codes, throws up new challenges, and progress of necessity has been constricted by the time scales associated with the advances in computer hardware and the efficiency of the numerical algorithms being used to ensure processing of the information in acceptable times. In addition, knowledge of the exchanges of mass, momentum and energy between phases for multiphase 3-D flows is very limited, and it is not acceptable for those formulated for the 1-D situations underpinning the system codes to be applied in 3-D situations (though this is often done for want of a better option).

Nonetheless, CFD is now a well established, state of the art technology used for design purposes in many branches of industrial engineering simply because it is cheaper and faster than performing a multitude of special-effect tests specifically aimed to guide the design thinking. CFD offers a more efficient route to a prototype design by: (i) rapidly dispensing with poor, or limited, design options prior to testing; and (ii) providing optimization data concerning flow parameters before the construction phase, whether at an integral or component testing stage. Hence CFD is now used routinely in many industrial design processes.

In 2002, a joint IAEA OECD/NEA Technical Meeting provided a broad overview of the use of CFD codes for safety analysis of nuclear reactor systems [4]. Since then, considerable effort has been devoted to assembling the available information on the use of CFD in the field of nuclear reactor safety (NRS) [5]. Another study, still continuing and overseen by the OECD/NEA, has resulted in the publication of three publications on different aspects of the subject. Typical application areas here are heterogeneous mixing and heat transfer in complex geometries, buoyancy induced natural and mixed convection, etc., with specific reference to NRS accident scenarios such as pressurized thermal shock (PTS), boron dilution, hydrogen buildup in containments, thermal fatigue and thermal striping issues.

From a regulatory perspective, a common approach to dealing with practical licensing issues is to employ very simplified modelling, coupled with conservatism to cover the unknown factors. In this way, acceptable safety margins can be ensured. The advantage of this approach is that many sensitivity studies can be carried out to determine how plant parameters have to be modified in order for the predictions to remain conservative. Sophisticated statistical methods, such as Latin Hypercube Sampling, have placed this practice on a firm mathematical basis. However, a key issue is then to determine the degree of conservatism needed to cover the lack of physics embodied in the simplified models. Information here can be obtained from mock-up experiments, but considerable care is then necessary in extrapolating results to full scale. Moreover, the experiments themselves contain simplifications, and judging the conservatism involved in introducing the simplifications is itself quite difficult. The only way to ultimately ensure conservatism is to increase the margins, but this often places unwelcome constraints on plant efficiency, and hence the unit cost of the electricity it produces.

The trend has been to gradually replace conservatism by a best-estimate methodology, coupled with an uncertainty evaluation. This process has already taken place in the context of the system analysis codes with the development of second generation codes in the 1970s based on the two fluid approach as a means of replacing the conservatism of simplified two phase flow models. The use of CFD codes in licensing may be viewed similarly in regard to the multidimensionality of some of the safety analyses that need to be performed, always with the aim of reducing the conservatism associated with using over-simplified or inappropriate analysis tools. But reducing conservatism is not the only benefit of CFD approaches. The technology can also be used to better understand important physical phenomena, and by this means to justify, or challenge, the 'historical' conservative assumptions built into the state of the art tools.

The use of CFD in licensing practices is not yet common, but the number of licensee submissions involving CFD is growing steadily. To gain acceptance, such investigations need to be underpinned by a comprehensive validation programme to demonstrate the capability of the technology to produce reliable results. Nonetheless, an increase in the use of CFD for the design of Gen III+ (and beyond) reactors will ensure that CFD will continue to expand into the regulatory domain.

3. ACTIVITIES INVOLVING COMPUTATIONAL FLUID DYNAMICS IN SUPPORT OF NUCLEAR POWER PLANT DESIGN

3.1. REACTOR DESIGNERS

3.1.1. Westinghouse

CFD has been used at Westinghouse since at least the mid-1990s. The applications described here primarily focus on the application of CFD to pressurized water reactors (PWRs), though Westinghouse has applied CFD in many other areas, with boiling water reactors (BWRs) as well as NPPs in general. The first CFD models of PWR fuel assemblies consisted of relatively simple two-subchannel models and have since expanded to much larger models, encompassing entire fuel assemblies or even full vessel models. Most of the current CFD analyses are performed using three commercial codes: STAR-CCM+, ANSYS-FLUENT and ANSYS-CFX[1]. Westinghouse has several clusters dedicated to CFD, with 192–256 cores each, as well as numerous large memory workstations used for pre- and post-processing. Current CFD application areas for PWR fuel at Westinghouse include the following.

3.1.1.1. Core inlet flow and upper core/outlet plenum flow

CFD simulations have been performed to predict the flow distribution to the fuel assemblies [4, 6] or various reactors, and to design the flow skirt for AP1000 PWR reactor vessel internals. These analyses have also been used to provide detailed flow distributions to core subchannel flow models for the US Department of Energy funded CASL (Consortium for the Advanced Simulation of Light-Water Reactors) programme.

[1] The same codes are used by Framatome. StarCD is also used with legacy methods, but less than before.

In addition, CFD has also been used to study the flow distribution in the AP1000® upper core and outlet plenum [7]. These studies were used to examine the effects of differences between the AP1000®, which has two hot legs, and earlier reactor designs, which typically have three hot legs.

3.1.1.2. Full vessel modelling

Recently, CFD models of the full reactor vessel (downcomer, inlet plenum, core and outlet plenum) have been built and analysed for a variety of purposes [8, 9]. Many of these analyses have been performed as part of the CASL programme [10]. These have included coupled analyses of neutronics and thermal hydraulics [11] and studies of fibrous debris blockage [12].

3.1.1.3. Nuclear fuels

CFD has been used to predict single phase pressure drop and heat transfer for new mixing vane grid designs, as well as for pressure drop of top and bottom nozzles and other fuel assembly components. In addition to its use for new designs, an important application of CFD has been the assessment of changes to existing designs on pressure drop and heat transfer.

Westinghouse has been an active participant in the Electric Power Research Institute NESTOR round robin benchmark since its initiation in 2009 [13, 14]. The goal of the NESTOR project has been to assess the ability of state of the art CFD to predict single phase flow and heat transfer in fuel assemblies, especially related to assessments for crud induced power shift and crud induced localized corrosion. Additionally, NESTOR has been developing best practice guidelines for performing such CFD simulations. Westinghouse has participated in the NESTOR programme by performing CFD simulations, and through attendance at meetings to assess and document results and to define best practices.

A CFD methodology for the modelling of boiling and the prediction of critical heat flux (CHF) in fuel assemblies has been under way in Westinghouse for several years [15, 16]. This is a very challenging area for CFD, so the current licensed practice for CHF modelling is still the use of subchannel codes, such as VIPRE. However, subchannel codes lack the capability to capture differences between mixing grid designs, so CFD prediction of CHF has found some limited use in the context of studies of new designs. Westinghouse is also working closely with the CASL programme to develop and test new boiling and CHF models for application to nuclear fuel assemblies, including accident tolerant fuel.

Flow induced vibration is another challenging area for CFD. At Westinghouse, there have been some applications of CFD to predict time dependent forcing functions (surface pressures) for flow induced vibrations of grid straps, vanes and fuel rods using large eddy simulation (LES) [17]. There has also been development of methodologies for coupled fluid structure interactions, but these are currently at relatively early stages [18].

3.2. UTILITIES

3.2.1. Électricité de France

CFD has been in use for a long time at Électricité de France (EDF) using, in particular, the in-house CFD Code Saturne [19, 20], developed by the R&D branch of that organization. The CFD activity concerns both safety assessments of the EDF reactor fleet, as well as some design issues. In this latter context, work includes improvements to present Gen II reactors and studies of future projects.

3.2.1.1. Reactor flow–boron behaviour

The reactor itself is the primary focus of present CFD activities. Boron distribution at core inlet during asymmetric startup is an ongoing concern. In combination with scale model experiments, which provide validation data, CFD is used to calculate the behaviour of boron free water slugs arriving from the cold legs according to various incident scenarios. The objective here is to obtain a reliable core inlet map for boron concentration for a given scenario to predict the subsequent neutronics behaviour within the core region.

3.2.1.2. Pressurized thermal shock

Numerical simulations undertaken on this topic involve several degrees of complexity. The goals here are: to be able to predict temperatures on the walls of the reactor pressure vessel (RPV) and to estimate the associated heat transfer coefficient. Calculations of conjugate heat transfer in the vessel wall itself are of primary importance, especially for ageing plants, since they correlate directly to the thermo-mechanical loading of the vessel. CFD is also used to evaluate alternate design strategies for emergency core cooling (ECC) injection such as, for example, direct vessel injection [21].

3.2.1.3. Core inlet flow

The use of CFD allows the behaviour of the coolant in the lower plenum at full power to be assessed, and in particular the impact of the flow diffuser on the flow rate heterogeneity and associated pressure drops. Moreover, for accident transient studies, CFD is used to determine the thermal field at core inlet (thermal mixing in the vessel); both nominal conditions and some specific transients are being investigated.

3.2.1.4. Temperature heterogeneities in hot legs

The average hot leg temperature is of considerable importance for reactor monitoring and safety. Calculations of the temperature distribution in the different hot legs are being performed using CFD to fully understand the turbulent fluid structures involved, and to improve the uncertainty evaluations of the estimates of the actual average loop temperature [22].

3.2.1.5. In-vessel retention systems

In the case of severe accidents, knowledge of the thermal hydraulic behaviour during cavity reflooding is aided by the use of CFD.

3.2.1.6. Pipe flow

CFD applications in this area are mainly to determine pressure drops in bends (for flow rate measurement purposes) and for thermal mixing in T-junctions as an aid to assessing their susceptibility to high cycle thermal fatigue [23, 24].

3.2.1.7. Containment studies

This item is investigated in the context of severe accidents. The phenomena simulated using CFD are the mixing of the different gas components (steam, air, hydrogen), stratification effects, and condensation on cold surfaces. The objective of the work is to demonstrate that the composition of the gas in relation to the hydrogen combustion hazard can be reliably predicted, and to determine the pressure field. Optimum recombiner location and the design of inner condenser systems are both items for which CFD is useful.

3.2.1.8. Fuel

CFD is employed in the design of fuel assemblies to estimate the pressure losses in the different components of the fuel assemblies. CHF calculations are performed but remain in an exploratory form only [25].

3.2.1.9. Storage pools

These devices are studied regarding their global behaviour — i.e. the general cooling characteristics of spent fuel stored in racks — and the operational design of the local pumping system. This requires primarily single phase flow modelling (stratification, temperature field and head loss assessments), but two phase models also need to be developed in circumstances in which there is loss of a cooling circuit, which may induce pool boiling leading to a cavitation hazard during pump restart [26].

3.2.1.10. Cooling towers

The heat sink performance of the cooling tower(s) is of fundamental importance to the total thermal efficiency of the plant. Here, CFD is used to optimize the cooling tower design, with a focus on non-homogeneous fill distribution within the cooling tower, new designs for the air inlets and for the estimation of cross-wind effects [27].

3.3. CODE DEVELOPERS OF COMPUTATIONAL FLUID DYNAMICS

3.3.1. Électricité de France

EDF is a utility, as well as a code developer (Saturne and Neptune). Its activities are described in Section 3.2.1.

3.3.2. French Alternative Energies and Atomic Energy Commission

In the framework of the advanced sodium technological reactor for industrial demonstration (ASTRID) project [28] for Gen IV sodium cooled fast reactors (SFRs), extensive R&D efforts are under way at the French Alternative Energies and Atomic Energy Commission (CEA) to improve and better validate the available SFR thermal hydraulic codes with the objective of performing more predictive calculations for safety assessment, and to evaluate margins for reactor safety demonstration [29]. These efforts include the development and validation of:

- *SFR:* Specific models in CATHARE, the current reference system thermal hydraulic code for French LWR safety studies;
- *TrioMC:* A subchannel code specific to SFR core thermal hydraulics;
- *TrioCFD:* A general purpose CFD code based on a unique staggered mesh approach.

These three codes are described below in more detail. Necessary SFR specific code modifications and model developments are described and selected validation tests are reported.

3.3.2.1. CATHARE

CATHARE is the reference system scale thermal hydraulic code for French PWR safety studies. Developed by CEA, Framatome, EDF and the Institut de radioprotection et de sûreté nucléaire since 1979, the code solves a two phase, six equation model on a network of 0-D, 1-D and 3-D meshes using a staggered discretization (i.e. velocities are defined at mid-faces between mesh cells) with a fully implicit (0-D/1-D) or semi-implicit (3-D) time discretization scheme. The code also includes a point kinetics model to predict the evolution of neutronics power during a given transient.

In order to adapt CATHARE for SFR applications such as ASTRID, the following code developments have been undertaken [30]: sodium physical properties and correlations are included, additional feedback parameters added to the code's neutronics model, and SFR mechanical and electromagnetic pump models also added. Simultaneously, a validation base was constructed to cover these developments, ranging from analytical subassembly experiments, such as GR19 [31], SIENA and SENSAS [32], to the analysis of reactor tests on the RAPSODIE, PHÉNIX [33, 34], SUPERPHÉNIX and MONJU reactors.

3.3.2.2. TrioMC

The development of TrioMC began at the CEA in 2009. The initial aim was to provide a fast-running code to compute the maximum cladding temperature in fuel assemblies, and to predict and optimize the flow zone map of SFR cores. To avoid the cost of specific geometry resolved CFD, the subchannel scale approach was a natural choice for this code. Correlations are used at this scale to account for the influence of the wire wrappers on bundle pressure drop, and for the mixing between subchannels. In order to avoid duplication, TrioMC shares common functions with the TrioCFD code, also developed by CEA. Currently, these common functions have been open sourced as a general thermal hydraulic platform called TRUST.

The validation database for TrioMC has been progressively extended in a stepwise manner. In addition to six subassembly experiments in forced, mixed and natural convection, the GR19 [31] and ECONA experiments have been used to validate two phase flow predictions under forced and natural convection conditions.

3.3.2.3. TrioCFD

In 1993, the CEA initiated the development of Trio_U, a parallelized, general purpose CFD code with an object oriented software architecture. The code includes numerical algorithms for solving single phase flows using a staggered discretization on either structured parallelepipeds or unstructured tetrahedral meshes. Turbulence can be represented using either Reynolds averaged Navier–Stokes (RANS) or LES approaches. A front tracking capability is also available, which allows liquid–gas interfaces to be explicitly described. In 2015, those parts of the Trio_U functions library common to other code developments, such as TrioMC, were integrated into the open source platform TRUST. Trio_U was then renamed TrioCFD.

Efforts to extend the validation database of TrioCFD to sodium applications began in 2006 [35]:

- Modelling of wire wrapped fuel assemblies was validated against the PLANDTL-37J [35] and Lafay experiments [36].
- Predictions of jet and stratification behaviour were validated at the analytical scale using data from the CORMORAN [34] and SUPERCAVNA experiments [37], at an intermediate scale on the PLANDTL-DHX [34] experiment, and on an integral scale on the MONJU [38] and PHÉNIX [32] reactors.
- Prediction of thermal striping phenomena using LES have been validated using the PLAJEST experiment in the framework of a benchmark with the Japan Atomic Energy Agency and Argonne National Laboratory [39].
- Predictions of free surface behaviour were tested using data from the BANGA experiment and applied to the hot pool of ASTRID [40].

Data from the PLATEAU facility [41] for large scale water mock-ups will be used to further validate TrioCFD. This facility houses the current MICAS experiment, a 1/6 model of the ASTRID hot pool.

3.3.2.4. Coupling strategy via ICoCo

In order to calculate thermal hydraulic issues at very different scales, a common coupling interface, called ICoCo, has been implemented into CATHARE, TrioMC and TrioCFD. This interface allows each code to be used as a library via C++ function calls. This allows an external programme to perform and control a coupled calculation by:

- Setting the value of the code's next time step, solving for this time step, and either advancing the simulation or resetting the code to its previous state;
- Receiving internal data from the codes and/or modifying data with external values.

Two strategies have been pursued at the CEA to implement such coupled calculations:

- Initially, application specific supervisor programmes were written for each simulation case. This method was successful, but has led to unwelcome user effects.
- Since 2015, CEA has developed a new coupling tool called MATHYS, which is based on the TRUST platform. This tool provides a generic, single–phase coupling algorithm to ensure that both validation studies and reactor applications utilize the same algorithm.

3.4. RESEARCH ORGANIZATIONS

3.4.1. French Alternative Energies and Atomic Energy Commission

Launched in 2006, the ASTRID project (Advanced Sodium Technology Reactor for Industrial Demonstration) [28] aims to design and construct a Gen IV, 600 MW(e) SFR in France. In 2016, the project entered its basic design phase.

Compared with the previous French SFRs, PHÉNIX and SUPERPHÉNIX, ASTRID will meet a safety level at least equivalent to that of Gen III PWRs. Some design changes are necessary to fulfil this objective. The development and use of better CFD based safety assessment tools will contribute to the demonstration of this higher safety level and the conservativism applied in the reactor design's safety demonstration will be reduced through the more precise predictions of CFD based tools. Such tools will be applied to situations in which strong 3-D flows and mixing phenomena are expected in the reactor, either under nominal or accident conditions. The following reactor regions and physical phenomena [40] are assessed using the commercial CFD code STAR CCM+ and the in-house CFD code TrioCFD [34]:

- Subassembly thermal hydraulics.
- Core thermal hydraulics.
- Hot pool thermal hydraulics:
  - Core outlet region;
  - Entire upper plenum region;
  - Heat exchanger inlet regions;
- Decay heat removal.
- Gas entrainment.
- Thermal fatigue.

Multiscale problems are treated using the CATHARE/TrioMC/TrioCFD coupled code system [42].

Even though the CEA carried out many experiments in the 1990s in the context of the European Fast Reactor project, new tests, specific to the ASTRID design, are required for code validation. Experimentation with sodium is very difficult due to its opacity and its violent reactivity with water. As water and sodium are very close in terms of their mechanical properties, i.e. density and viscosity, most fluid flow experiments are performed using water. In this framework, the PLATEAU loop was built in 2012 [43]. The first mock-up, MICAS [44], commissioned in 2015, represents the upper plenum of the ASTRID reactor at a 1/6 scale, and is focused on studying the principal thermal hydraulic issues, such as gas entrainment at the free surface, flow around the intermediate heat exchangers, the behaviour of the jets rising from the core, and the flow penetrating the above core structure.

3.4.2. Canadian Nuclear Laboratories

The Canadian Nuclear Laboratories (CNL, formerly Atomic Energy of Canada Limited) has initiated a programme of work to develop CFD analysis capability for nuclear applications. The CFD analyses are focused on simulating nuclear fuel bundle geometry under subcritical and supercritical flow conditions due to its relative importance to the safe operation of the Canadian reactor designs.

Among its recent activities, CNL analysts have simulated a 28 element CANDU fuel bundle with spacers, as well as other configurations, including four rod and seven rod bundles [45, 46], and wire wrapped bundles [47, 48]. CNL has also participated in an international blind benchmarking exercise organized by the OECD/NEA [49]. A reference (or preferred) CFD code for the Canadian nuclear industry is yet to be identified for fuel bundle applications. In the interim, the commercial CFD code STAR-CCM+, marketed by CD–Adapco, is currently being used, principally because of its advanced mesh generation capabilities. Recently, a code to code comparison exercise between STAR-CCM+ and ANSYS-FLUENT was also performed to evaluate the suitability of commercial CFD codes generally for simulating fuel bundles [46].

Within the framework of the Generation IV International Forum, CNL is leading the effort in developing a Canadian supercritical water cooled reactor (SCWR) and has developed a fuel assembly concept for it [50]. In this project, CFD is used to examine the capability of existing turbulence models to predict the flow and heat transfer characteristics for the proposed fuel bundle design.

Due to a lack of experimental data in connection with Canadian SCWR fuel bundles, CFD assessments have been limited to partial bundle geometries (or subassemblies) of curtailed length, for which experimental data are available.

3.4.3. Korea Atomic Energy Research Institute

There are many applications of CFD codes in various research areas at the Korea Atomic Energy Research Institute (KAERI). The institute began an in-house project within the CFD working group that ran from June 2015 to May 2017. The primary objective of this project was to exchange experience of CFD simulation in different application areas, and to assemble an appropriate experimental database for verification and validation (V&V) of related CFD applications. A secondary objective was to establish a strategy for sharing the licenses of commercial CFD codes. In this context, the CFD working group at KAERI holds regular meetings and has hosted seminars from CFD experts on these issues.

KAERI has participated in international benchmark exercises in the framework of CFD V&V and has performed subchannel and CFD analyses of void distribution for the BWR fuel bundle test benchmark, organized by the OECD/NEA and the United States Nuclear Regulatory Commission [51]. KAERI has also participated in the OECD/NEA benchmark based on the Nuclear Power Engineering Corporation PWR subchannel and bundle tests. W.K. In et al. [52] have reported on the steady state void distribution benchmark based on the PWR subchannel and bundle tests. In addition, KAERI has provided test data from the MATiS-H experiments on turbulent mixing in a rod bundle with vane spacer grids for the OECD–KAERI CFD benchmark exercise [53]. More recently, KAERI has provided data from the OFEL experiments of flow mixing and heat transfer in 4 × 4 regular and tight lattice rod bundles for this CRP [1].

Further CFD applications at KAERI include the investigation of the flow distribution at the core inlet region of the system integrated modular advanced reactor (SMART) using the commercial code

ANSYS-FLUENT 12.0 [54], and analysis of the cooling performance of the annular linear induction pump for the Prototype Gen IV SFR currently under development at KAERI [55].

The group has also recently developed its own 3-D thermal analysis code (CUPID) but, in addition, over the years has accrued considerable expertise in the use of the commercial CFD code STAR-CCM+ 9.02. J. Yoon et al. [56] reported steady state CFD analyses of a large sodium pool system of the STELLA-2 test section under normal operating conditions: STELLAR-2 is a sodium integral effects test facility currently under design for Prototype Gen IV Sodium Cooled Fast Reactor development at KAERI. A coupled code system has been developed [57] (known as CORONA) to simulate the prismatic, gas cooled very high temperature reactor; and predictions of fuel temperature and heat transfer coefficient compared with those of detailed CFD calculations.

Numerical analysis using a commercial CFD code to predict the flow distribution and pressure drop in a plate type fuel assembly for the Jordan research reactor has also been performed [58], and the CFD predictions compared with the experimental measurements taken in the KAERI hydraulic test Omni Flow Experimental Loop. Currently, analyses are being carried out [59] using ANSYS CFX to assess the temperature distribution for normal operation of the Kijang Research Reactor, which is under construction in the Republic of Korea. Finally, researchers have developed a CFD methodology for predicting the overpressure caused by a hydrogen explosion [60]. This is aimed at improving the error range in such analyses, which is currently at approximately 30%.

3.4.4. Paul Scherrer Institute

CFD is currently being used at the Paul Scherrer Institute (PSI) in Switzerland for the safety assessment of current plants in support of the design of Gen IV reactors, but also in the general context of turbulence and numerical, multiphase model development.

One safety issue into which PSI has put a large amount of effort is PTS, which is being covered in the framework of two national projects sponsored by the Swiss Federal Nuclear Safety Inspectorate. These are STARS and PISA. The main focus of the STARS (Safety Research for Transient Analysis for the Reactors in Switzerland) project is an in-depth analysis of the dynamic behaviour of Switzerland's five operating reactors and entails both neutronics studies coupled to thermal hydraulic and fuel behaviour. CFD analysis is an integral part of this strategy. Pressure Vessel Integrity and Safety Analysis (PISA) is aimed at demonstrating that the integrity of the RPV continues to be guaranteed during normal operation, and also in the case of operating faults and (postulated) severe accidents. Specifically, PISA aims to assess the state of knowledge in the area of brittle fracture safety for RPVs. To this end, extended measurements and model calculations involving stress analysis, coupled with CFD, are currently being carried out [61].

PTS was also the focus of a recently concluded project launched by the Goesgen power plant, for which PSI performed the safety assessment of the RPV [62] for the case of a small break loss of coolant accident.

The first use of CFD for the design of a nuclear facility at PSI was associated with the MEgawatt PIlot Experiment (MEGAPIE) project [63]. The project was launched in 2000, by nine participating institutions, with the goal of demonstrating the safe operation of a liquid metal (lead–bismuth eutectic) spallation source target bombarded by a ~1 MW proton beam. The experiment was carried out at the spallation neutron source SINQ target facility at PSI. CFD simulations performed by the Laboratory of Thermal Hydraulics at PSI [64] were able to confirm the continued cooling of the spallation target and contributed significantly to the final design of the MEGAPIE vessel, and its internals, under a variety of operational and accident conditions.

Another example of the use of CFD for design purposes relates to the innovative reactor core assembly of gas cooled reactors in the framework of the MeAWaT project. The goal of this project is to design new fuel pins with internal cooling, thereby enabling an increase in the power density of the core. CFD proved to be important in assessing the pressure losses in and around fuel pins, and in determining optimal design parameters (pin spacing/pin diameter, inner/outer pin diameter ratio, wire pitch/pin diameter ratios) prior to experimental testing. This work has been duly reported [65].

Uncertainty quantification (UQ) of CFD simulations is a relatively new subject area. In one approach, model parameters, e.g. boundary conditions and physical properties, are considered as stochastic variables represented by probability density functions. PSI has ventured into this field using the polynomial chaos expansion approach (a spectral decomposition of the random variables) to obtain the response of the system in parameter space, and to calculate the most important statistical moments, such as the mean value and standard deviation of the physical variables. Use of this method enables the presentation of numerical results (e.g. temperature, velocity, pressure) with associated error bars based on standard deviations. PSI has successfully applied this method to simulate turbulent mixing in its own GEMIX test rig (mixing of two stratified streams), and to quantify the level of uncertainty introduced in the simulations by uncertainties in the boundary conditions [66, 67]. Measured data from this experiment have been used for the first OECD/NEA benchmark on UQ for CFD simulations [68].

3.4.5. Bhabha Atomic Research Centre

At the Bhabha Atomic Research Centre (BARC) in India, CFD is being used for analysing various current systems for advanced nuclear reactors. The approach is principally used for design optimization and safety assessment pertaining to these reactors. Some of the activities for which CFD is being used are described below.

3.4.5.1. Natural circulation in a water loop

In some advanced reactors, the core heat is removed under shutdown conditions through natural circulation of the coolant. A test facility has been set up to study such phenomena and supporting 3-D CFD simulations [69] have been performed, both under steady state and transient conditions. The CFD model includes pipe thicknesses and secondary side coolant passages, as well as the details of the primary side flow. Simulations have been performed for various configurations: vertical heater and vertical cooler; horizontal heater; horizontal cooler; etc. The effects of a sudden power increase and power step-back on the stability of the flow have also been investigated using CFD.

3.4.5.2. Hydrogen management

Hydrogen related issues pertaining to nuclear reactor safety have featured as an important research topic globally over the past decade. As a result, studies on hydrogen transport behaviour, and the development of hydrogen mitigation systems, are being actively pursued by BARC. CFD analyses [70] have been carried out to quantify hydrogen distribution under conditions of uniform injection of hydrogen over a specified period of time, as well as under time varying injection conditions. The results to date indicate that the process of hydrogen dispersion is primarily buoyancy dominated. Further, for the various injection rates encountered under severe accident conditions, the dispersion mechanism is quite poor, and most of the hydrogen actually accumulates in the fuelling machine vault area in the containment of a pressurized heavy water reactor. With regard to hydrogen mitigation, passive autocatalytic recombiners, consisting of catalyst coated surfaces, are also being investigated using CFD. Simulations have been performed for plate type passive autocatalytic recombiners to study their effectiveness [71]. A finite volume based, in-house 2-D CFD code has been developed to model and analyse the workings of such recombiners.

3.4.5.3. Moderator flow and temperature distribution studies

CFD simulations of moderator flow and temperature distribution in the calandria of a 700 MW(e) pressurized heavy water reactor have been carried out to investigate flow induced vibrations [72]. CFD studies have also been performed to determine the velocity distribution in the presence of various components in the calandria using the CFD-ACE+ code. Using the computed velocity distribution as input, flow induced vibration studies are subsequently performed.

3-D CFD analyses have also been performed to study the moderator flow and temperature fields in the calandria of an advanced heavy water reactor using the OpenFOAM CFD code [73]. The CFD model includes the calandria vessel, calandria tubes and inlet and outlet headers. Analyses were performed for cases of both uniform and non-uniform volumetric heat generation. The purpose of these studies was to confirm that the maximum temperature of the moderator in the calandria remained below the prescribed limiting value.

3.4.5.4. Liquid poison dispersion in moderator

In an advanced heavy water reactor, the Shut Down System-2 concept is based on liquid poison injection into the moderator. The liquid poison, at high pressure, is injected into the calandria through sparger tubes. The system is designed to shut down the reactor in a very short time, but its effectiveness depends on the dispersion of the poison in the moderator. Consequently, CFD analyses of poison injection and its dispersion have been carried out using OpenFOAM [74]. The CFD model was validated by comparing code predictions against experimental data. The investigations were performed specifically to quantify the performance of the poison injection system.

3.4.5.5. Liquid metal loop

In the case of the compact high temperature reactors currently being designed, core heat is removed by natural circulation of the lead–bismuth eutectic coolant. The test loop HANS (heavy metal alloy natural circulation study loop) has been built at BARC to study the thermal hydraulics of the heat removal process. Steady state and transient natural circulation characteristics have been investigated for different power levels. Natural circulation in the loop was simulated using the CFD code PHOENICS [75] and the predictions were found to be in good agreement with the experimental data.

3.4.5.6. Molten salt loop

Molten salts are increasingly receiving attention as possible reactor coolants, and as a storage medium in solar thermal power plants, due to the large difference between their melting and boiling points at atmospheric pressure. They are also used as fuel/blanket coolants in high temperature reactors. 3-D CFD simulations [69, 76] have been performed under steady state and transient conditions of operation of the molten salt natural circulation loop installed at BARC. The working fluid is a mixture of $NaNO_3$ and KNO_3. Various transients, including flow initiation, power step-up, power step-back, power trip and loss of heat sink, have been studied. From the CFD predictions, it was possible to understand the physics of the oscillatory flow patterns generated in the loop under various conditions, and thereby improve the design of such systems.

3.4.5.7. Flow accelerated corrosion

A CFD approach has been used to examine [77] the wall thinning degradation mechanism due to convective mass transfer in the feeder pipes of NPPs. Flow and mass transfer characteristics have been studied for a carbon steel elbow under high temperature and pressure conditions. The thickness degradation predicted as a result of mass transfer from the pipe wall in the numerical simulations was compared with those of measured data. In particular, the formation of eddies, and their interactions with the wall, were examined at the elbow. These results are useful for developing the targeted inspection plans in predicting possible vulnerable flow accelerated corrosion locations.

3.4.5.8. Future plans

The development of molten salt based high temperature reactors is in progress at BARC. These reactors aim to provide high temperature heat for thermo chemical splitting of water, and as a possible option for the third stage of the Indian nuclear power programme. The innovative high temperature reactor concept has been proposed for large scale hydrogen production. It will operate at high temperature, with molten fluoride salt as coolant. The fuel comprises Tri-structural Isotropic particle fuel coated particles machined into pebbles with graphite as moderator. The Indian Molten Salt Breeder Reactor is an attractive option for thorium utilization. It has a molten fuel salt mixture, which acts both as the fuel and the primary coolant in the reactor. The reactor system will also incorporate a blanket of molten salt for breeding purposes. CFD codes will be used extensively in support of the design and development of these reactor systems. The following paragraphs identify the areas where CFD codes are proposed to be used.

In pebble bed reactor designs, pebble geometry and coolant flow interact with each other through interaction forces, principally drag forces. The core geometry requires a tightly coupled simulation of the coolant flow over the pebbles in order to provide accurate predictions of the core dynamics. In realistic operations of pebble bed reactors, the above interaction is further complicated by the different modes of heat transfer (conduction, convection and radiation) and the resultant temperature distribution in the core. Advanced turbulence models are needed to study the complex flow dynamics in packed beds. Benchmark experiments also need to be carried out to qualify the advanced turbulence models adopted for these simulations.

In molten salt reactors, fissile atoms are dissolved in the molten salt coolant, and fission heat is generated inside the coolant itself instead of being transferred from fuel to coolant, as in the case of solid fuelled reactors. The phenomenon of non-uniform internal heating of coolant makes the thermal and dynamic behaviour of this system highly complex. Detailed analyses of the fluid flow and heat transfer processes can be carried out using CFD. It is proposed that neutron absorbing, gaseous fission products, such as xenon and krypton, may be stripped from the liquid coolant by bubbling through helium gas. This phenomenon can be simulated using two phase CFD models to optimize the various parameters for efficient stripping.

Concerning other advanced nuclear reactor systems, natural circulation is also an important phenomenon to study in the context of molten salt reactors. Heat removal from the reactor core by both natural circulation and forced circulation processes is possible and needs to be evaluated. Passive decay heat removal (i.e. by natural circulation of the molten salt) under postulated accident conditions is an essential requirement for the safe design of HTRs. Considering the challenges of possible flow instabilities associated with natural circulation of molten salts, studies need to be carried out for various core geometries. For this purpose, 3-D CFD modelling of the system is fundamental, with the involvement of suitable solvers and turbulence models, to ensure highly accurate predictions of the stability characteristics. The effect of the heat exchanger location, either outside or inside the reactor vessel, can also be studied using CFD. In liquid fuelled molten salt reactors, the stability of the natural circulation can be seriously influenced by the internal heat generated outside the core. CFD analysis may also help in this regard and contribute to the assessment of the overall stability of the system.

For high temperature applications in molten salt reactors, special types of heat exchangers need to be designed and developed. CFD is proposed as a tool to help in the design of such advanced heat exchangers. Established CFD models need to be enhanced for application to (high Prandtl number) molten salt, used as the primary fluid, and the (low Prandtl number) liquid metals used as secondary fluid. Similarly, CFD simulation of other fluids need to also be considered within the standard formulations.

For hydrogen generation, various thermo chemical processes are currently being evaluated. To carry out investigations on fluid flow, heat transfer and chemical reactions, CFD is a useful tool for optimizing various control parameters to ensure efficient reaction mechanisms take place. Hence, advanced CFD models can be utilized effectively for analysing the system during the design process.

4. STATUS OF VERIFICATION AND VALIDATION FOR THE USE OF COMPUTATIONAL FLUID DYNAMICS IN NUCLEAR POWER PLANT DESIGN

All CFD code developers and end-product users are acutely aware of the need for qualification of the numerical predictions of the code; i.e. the trustworthiness of these predictions. Originally, the qualification process was based on three clearly defined steps:

(1) Verification;
(2) Validation;
(3) Demonstration.

Verification is concerned with the reliable solution of the given equation set through a numerical algorithm. Note that there is no judgement here of how this equation set is representative of physical reality. This is covered by the validation step, which of necessity involves comparison of numerical predictions against experimental data. The demonstration step is to judge the capability of the code to provide numerical solutions for a given class of problems. This last step is obviously very problem specific and could involve 'user qualification' as well. In other words, how experienced is a CFD practitioner in applying the code in a reliable way? Best practice guidelines (BPGs) have emerged to provide some level of documented control over this final step.

More recently, one could add uncertainty quantification to the list, but this is largely undeveloped in CFD because of the excessive computation overhead involved. Throughout this publication, these concepts will arise multiple times. In this section, the individual involvement of two key NPP design organizations will be summarized, and some references given. A short mention of the technology gaps is also presented directly related to the specific design issues discussed. However, a more general, comprehensive, description of the technology gaps in the broader sense is given in Section 10.

4.1. DESIGN APPLICATIONS

4.1.1. Électricité de France

For each of its CFD codes (Code-Saturne, Neptune-CFD and Syrthes), EDF has assembled a catalogue of test cases. Code-Saturne solves single phase flows, whereas Neptune-CFD deals with two phase flows, both in the context of a Euler–Euler formulation. The Syrthes code is dedicated to solid conduction and face to face radiation and is often coupled with Code-Saturne or Neptune-CFD for conjugate heat transfer studies.

The V&V catalogues contain elementary cases, corresponding mainly to individual physical phenomena in simple geometries, as well as integral cases, coupling several physical phenomena on more representative domains. The elementary cases are typical configurations of forced, mixed and natural convection situations. For example, friction in a pipe, a sudden pipe expansion, pipe elbow flow, jets, a differentially heated cavity, stratified flow in pipes, and general flow mixing. The database can be analytical or experimental in origin and derive mainly from the literature or from in-house experiments. Integral test cases are generally linked to a specific reactor design and are performed in laboratories belonging to EDF itself or to its partners. The data from such integral tests are often not open, except for some joint actions (European programmes: e.g. FLOWMIX-R (boron dilution in the primary circuit [78]), PANDA (hydrogen behaviour in containment volumes [79]), and various OECD/NEA benchmark exercises).

However, for each new design study, a phenomena identification and ranking table analysis need to first be performed, highlighting the physical behaviour. The validity of the test cases also needs to be checked in terms of the characteristic dimensionless numbers (e.g. Reynolds, Rayleigh, Richardson). If the validation folder does not cover the new study, a new validation programme needs to be launched, according to the guidelines given in Ref. [80]. Such a programme can extend from simulating a simple test case from the literature to designing and operating a new mock-up experiment.

4.1.2. Westinghouse

V&V applied to CFD has found some limited application at Westinghouse. One recent example is a CFD benchmark and uncertainty programme carried out on the upper head of the reactor vessel internals of the AP1000® plant [81]. An uncertainty analysis, closely following the American Society of Mechanical Engineers (ASME) V&V 20 standard [82], was performed on the CFD results. This procedure included studies of mesh sensitivity, input sensitivity and turbulence model sensitivity.

Another vehicle for the development of V&V methods for CFD is participation by Westinghouse in the Validation and Modelling Applications focus area [83] of the CASL programme[2]. In particular, the use of the Dakota[3] computer programme for CFD V&V studies [84] is currently being explored. In addition, Westinghouse regularly participates in V&V conferences hosted by ASME to monitor developments in this area.

4.2. VALIDATION GAPS AND ISSUES INVOLVED

4.2.1. Électricité de France

The main technology gap is that validation cases are in the main related to scale models. Indeed, for obvious reasons, space, power, and flow rates are limited in testing laboratories. A generic length distortion generally used for the primary circuit is 1/5th scale [85, 86], e.g. ROCOM (Konvoi design) and JULIETTE (evolutionary power reactor). The characteristic number for mixed convection driving stratification and plume effects can be conserved using a heavy fluid representing the cold water of the reactor (e.g. by the addition of salt or sugar). However, the Reynolds number remains considerably distorted (by a factor of the order of 10 to 100) and this can be an issue for some low turbulent flows (parts of the reactor with low velocities or small characteristic lengths) so that unphysical re-laminarization could occur in the mock-up test, not present at full scale.

Another issue is that the use of CFD in support of reactor design is based on the assumptions that code validity can be scaled up from the mock-up to the full reactor size. In the absence of an integral test facility sufficiently representative of the full reactor scale, the hypothesis of code validity when several physical phenomena are coupled is, strictly speaking, an assumption.

For two phase flows, for which the characteristic dimensionless numbers are numerous, CFD can rely on simulant fluids for developing models, but the question of the transposition to water at PWR conditions still arises, since several dimensionless numbers will always remain distorted. For the more precise phenomenon of CHF, the use of a water/steam coupling is almost indispensable to maintain surface tension, contact angle and viscosity ratios. This leads to large, full scale experiments (e.g. the Kathy loop dedicated to CHF tests for BWR and PWR fuel assemblies [87]), and these are very expensive to build, operate and maintain. Such large mock-up tests are also not easily instrumented to provide the CFD grade data needed for CFD model developments, and only integral values can be compared (e.g. power leading to detection of CHF, and too thinly located temperature measurements).

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[2] See: http://www.casl.gov.

[3] See: http://dakota.sandia.gov.

For fluid structure interaction, elementary validation tests are not sufficient, and a coupled scale model test is mandatory for both representation of the structures and the fluid motion. Moreover, strict conservation of the Reynolds number is often necessary since, for example in the case of tube bundles, the Strouhal number, characterizing the oscillatory motion, itself depends on the Reynolds number. One also has to classify the nature of the interaction (i.e. as one or two way coupling, or in terms of small or large displacements).

4.2.2. Westinghouse

One advantage of CFD over alternative (and more traditional) numerical approaches, such as subchannel and system level codes, is that the technology provides much higher resolution of the geometry and physics. However, this advantage comes at the cost of much higher computational cost, and this overhead becomes a disadvantage with respect to performing V&V for CFD. Most V&V techniques require a large number of analyses to compute the needed sensitivity parameters, a procedure that is often impractical for industrial level CFD. Recent developments, such as the use of surrogate models [88] constitute a possible solution to this difficulty, but further research is required to make V&V techniques practical for industrial CFD applications.

Another difficulty with current V&V approaches (as defined in ASME V&V 20, for example) is that they are often based on the assumption of idealized numerical behaviour, something that does not always occur in practice. The most common example of this is the assumption of monotonic convergence of results with the degree of mesh refinement. This is especially important for turbulent flows in which some wall treatments, such as the use of wall functions, have changing sensitivity to mesh size. New approaches for computing mesh sensitivities in these situations are needed (see Ref. [89], for example).

5. FUTURE USE OF COMPUTATIONAL FLUID DYNAMICS FOR SELECTED REACTOR TYPES

5.1. SUPERCRITICAL WATER REACTOR

In the core of the SCWR, water under supercritical pressure is heated from below to above the pseudocritical temperature. Since no two phase flow appears in the SCWR core during normal operation, single phase CFD is adequate for the analysis of flow and heat transfer in the SCWR core, and for the design of the SCWR fuel assembly. Validation of CFD analysis of supercritical water heat transfer has been carried out on experiments performed principally in simple geometries, such as circular tubes and scaled rod bundles. The validation indicates that quantitative prediction is possible using the RANS turbulence models provided by the commercial CFD code vendors, including ANSYS-CFX, ANSYS-FLUENT and STAR-CCM+ [90–93]. Due to strong material property variations occurring near the pseudo-critical line, complicated flow and heat transfer phenomena occur when the bulk temperature approaches pseudo-critical levels. Heat transfer deterioration is well recognized as the main phenomenon limiting the heat removal capability, and CFD analysis can in principle represent this characteristic appropriately. However, to date the current range of validation is still not sufficient to enable the development of BPGs for CFD analysis of heat transfer in supercritical water.

At Shanghai Jiao Tong University, China, efforts to develop a reliable turbulence model for such applications are currently under way. Zhang et al. [94] have proposed to utilize the k–ε–kt–εt model (to avoid the restriction of setting a constant turbulent Prandtl number), with the buoyancy production of turbulence kinetic energy modelled based on the algebraic flux model. Zhang’s model has been widely utilized by the SCWR community. Xiong and Cheng [92] proposed using the algebraic flux model for both the turbulent heat flux and buoyancy production terms to reduce the complexity of the model. They showed that prediction of supercritical water heat transfer can be improved using this new model.

Since heat transfer experiments at supercritical pressure are extremely expensive, CFD has played an important role in the fuel assembly design for such reactors. Cheng et al. [90] have simulated heat transfer in triangular array and square array subchannels using ANSYS-CFX and pointed out that the circumferential non-uniformity of heat transfer needs to be considered more seriously in the fuel assembly design of the SCWR than hitherto supposed. Based on their CFD analyses using Star-CD, Yang et al. [95] tried to avoid any strong non-uniformity of temperature distribution by adjusting the pitch to diameter ratio, and by devising a special grid spacer. Complementing these studies, Zhu et al. [96] used STAR-CCM+ to evaluate the effect of a grid spacer on the maximum cladding surface temperature in a tight lattice bundle.

The Canadian Nuclear Laboratories, within the framework of the Generation IV International Forum, is leading efforts in developing the Canadian SCWR and has established a fuel assembly concept for the reactor [97]. In support of this effort, the CFD code STAR-CCM+ has been employed to simulate fluid flow and heat transfer characteristics in bare and wire wrapped fuel bundle configurations.

Currently, a fit for purpose turbulence model is not available for CFD simulations of supercritical flow and the associated heat transfer characteristics (i.e. heat transfer deterioration), thereby adding one more element of uncertainty in resolving turbulent flow and heat transfer in SCWR fuel bundle geometries. Consequently, one of the first steps undertaken by CNL was to perform sensitivity analyses of the commonly used two equation k–ω turbulence model and the Reynolds Stress Model (RSM) to assess their suitability for modelling bare and wire wrapped SCWR bundles [47].

The mesh requirements for supercritical flows differ significantly from those for subcritical flows. It has been found that a fine mesh, comprising wall adjacent cells of $y^+<1$, with a minimum of ten boundary layer cells, was required to capture the heat transfer deterioration phenomena encountered in supercritical flows. Based on the analyses conducted so far, the k–ω model has exhibited the potential to predict the correct trends of the heat transfer deterioration process, whereas the use of RSM resulted in a rather gradual rise of temperature, which appears to be unphysical.

Since the Canadian SCWR has remained at the conceptual design phase in recent times, it seemed premature to perform full scale experiments for the fuel assembly concept. Hence, the assessments of the CFD models have been made using data from recently available experiments for four rod and seven rod fuel bundle configurations only [46]. Overall, it was found that the simulations have underpredicted the experimentally measured wall temperatures, although the trends of the axial and circumferential temperature distributions were reasonably well captured by the k–ω model [46, 48]. As expected, the wire wraps resulted in stronger turbulent mixing across the bundle, leading to lower peak wall temperatures compared to those measured in the corresponding bare bundle tests [47].

5.2. WATER–WATER ENERGETIC REACTOR

A water cooled, water moderated nuclear power reactor, such as the water–water energetic reactor (WWER), is often referred to as the most prevailing type of LWR. In such reactors, water under high pressure is used both as coolant and moderator. The WWER has a number of distinct design features concerning both the component layout and the materials used. For example, horizontal steam generators and hexahedral fuel assemblies are employed. A schematic view of the primary circuit of the Gen III+ AES-2006/V-491 NPP is displayed schematically in Fig. 1.

Thermal hydraulics is an important field of knowledge for the future development of WWER type reactors. Advanced knowledge of coolant velocity, pressure and temperature distributions in the primary circuit is necessary for studying reactor plant conditions over the expected range of operating conditions. This knowledge helps to establish confidence that the NPP's design is both safe and efficient [99]. During the years of WWER development, various methods have been employed to study coolant behaviour: data from small scale and full scale experiments, data from an actual NPP in operation, and from the

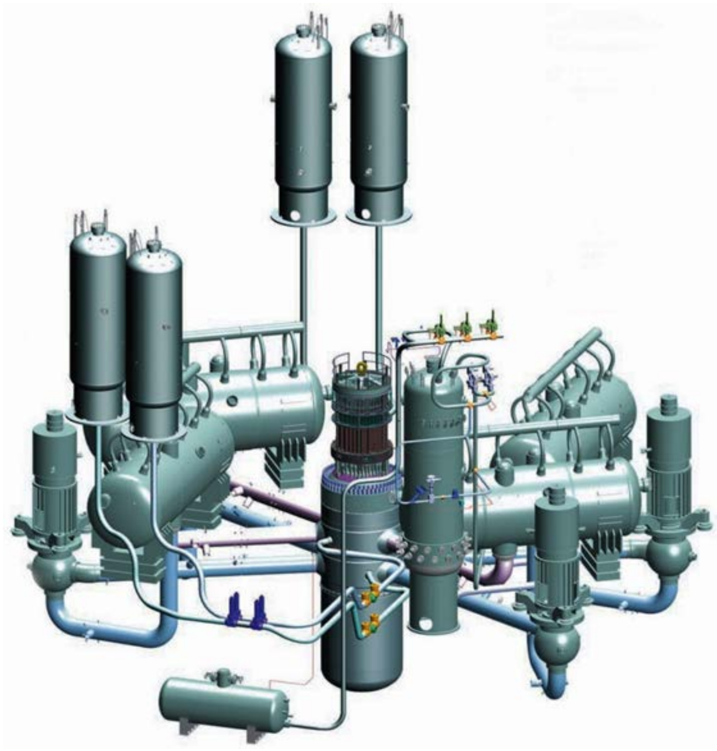

FIG. 1. WWER primary circuit component layout (courtesy of OKB Gidropress)[98].

results of system and subchannel code analyses. The growth of computing resources over the past 15 years has allowed CFD to also be used for this purpose. During this time, a set of computational models has been developed within various primary circuit research projects directed towards the advancement of numerical simulation of mass and heat transfer, e.g. in major reactor components, such as fuel assemblies and steam generators [98].

One dimensional engineering approaches are now widely recognized as not being able to predict coolant behaviour if important 3-D flow effects are present in the flow. Therefore, CFD has been used for the design optimization of various WWER components for which 3-D phenomena have a strong influence [99, 100]. CFD simulation allows one to obtain a number of thermal hydraulic parameters characterizing the reactor design, such as the mass flow distribution at the core inlet and outlet, the pressure loss coefficients through the fuel elements, the heat distribution within the different fuel assemblies in the core, etc. [100].

The use of CFD requires accurate and detailed V&V procedures of the numerical models. For the validation of CFD models at OKB Gidropress, the data obtained from experimental facilities specifically constructed for project justification have been employed. In turn, the validated CFD models allow more complete information to be obtained concerning the processes occurring in the experimental facility in the immediate vicinity of the sensor installation locations, as well as in the entire domain volume. Thus, validated CFD models can serve as a parallel, virtual analogue to the experimental test section [99, 101–103]. It is important to note that the use of CFD at the design stage of the experiment itself often improves the efficacy of the data measurement procedures and leads to better understanding of the underlying physical principles. For validation of the CFD models used, and enhancement of the qualification of OKB Gidropress generally, specialists participate regularly in international academic and industrial benchmark exercises [104, 105].

One of the chief benefits of using CFD in primary circuit design is the possibility of investigating the detailed processes of mass and heat transfer, and to optimize the design at state of the art scientific and technical levels on the basis of the limited experimental data available. However, inaccurate, or inappropriate, use of CFD may lead to erroneous conclusions. OKB Gidropress currently uses CFD to confirm applied technical solutions, and to optimize components. This approach significantly reduces the time involved in the design work, quickly identifies errors at early stages in the design process and fixes them.

5.2.1. Present limitations of computational fluid dynamics

As a priority for WWER support, a full scale coolant flow and mixing simulation in the downcomer, lower and upper plena of the reactor, as well as heat transfer in fuel assemblies, and in the core in general, has been set up. The experimental data obtained are being used specifically for the validation of the CFD models used in the simulation [98].

A large number of grids and, consequently significant computing resources, are required for any CFD simulation that takes into account all features of the design of the primary circuit. The complexity of anisotropic turbulence phenomena is also to be noted as an important aspect of CFD modelling and needs to be addressed appropriately. Many applications of multiphysics phenomena involving strong anisotropy can be modelled effectively using an RSM, LES and, in some cases, Hybrid RANS/LES turbulence models. Only a limited number of design issues can be studied with such complex models because of the high requirements of mesh resolution, small time steps, and user qualification.

For long, unsteady simulations, the required minimum number of control volumes causes runtime problems for the processor core, therefore often limiting the total practical simulation time. Further complications arise due to the presence of multiphysics phenomena taking place at different time scales; these often have significant influences on overall behaviour, and normally cannot be time averaged. Another important limitation restricting the application of CFD in the nuclear industry comes from the still immature state of multiphase CFD. While advanced and more general approaches are being developed and tested as part of large collaborative projects, and show promise in particular in the area of fuel design [106], well validated general closure models for both wall heat transfer and hydrodynamical behaviour are not yet readily available, and remain a central challenge in extending the application of CFD to highly turbulent flows.

5.2.2. Improvements needed

In some cases, consideration of the various physical phenomena in the primary circuit is required to produce more accurate modelling of the mass and heat transfer processes. The coupling of CFD with structural mechanics codes allows one to predict the deformation of certain design components in a specific fluid flow situation, and any mutual influence that may occur.

The coupling of CFD with neutron kinetics enables more accurate modelling of localized power surges in the core to be studied. One of the ways to achieve this is to couple CFD with 1-D thermal hydraulic codes, such as KORSAR/GP-LOGOS [106]. KORSAR/GP is used for the core simulation, and the CFD code LOGOS for hydraulic simulation of the downcomer and lower plenum regions. Special attention needs to be paid to the data transfer interfaces between the codes.

One of the main limitations of CFD is the absence of reliable two phase models for all boiling modes that may need to be represented over a wide range of simulations (e.g. critical heat flux prediction in the fuel assembly or core). Current efforts focus on trying to extend the generality of the physical representation of boiling phenomena and to abandon legacy approaches that have been incorporated in the first generation of multiphase CFD [107]. Work at EDF [108] and as part of the CASL project [109, 110], for example, show promising advancements in the predictions of critical heat flux using CFD.

5.3. SODIUM COOLED FAST REACTORS

The CEA has formed alliances with both French and international industrial companies in the technical development of the prototype reactor ASTRID (Advanced Sodium Technology Reactor for

Industrial Demonstration) concept: the reactor is already at the end of the conceptual design phase. Thermal hydraulics is recognized as one of the key scientific areas in the establishment of SFRs. Accurate knowledge of the velocity and temperature fields is needed for both nominal operation and during accident sequences to allow technical and economic progress to be made in terms of increased compactness and safety, in addition to reduced cost. Different methods are employed in the ongoing thermal hydraulic studies: scaled experiments, correlation approaches, and detailed CFD simulations. CFD is currently used in the conception and design of the reactor vessel and of the components for which 3-D flow effects are expected to occur. The use of a coupled calculation scheme built between the system code CATHARE and the CFD code TrioCFD is planned for some aspects of the licensing of the reactor.

Three dimensional effects may occur, for example, in the following regions in the reactor vessel (see Fig. 2):

— The hot pool above the core outlet, where multiple jets at different temperatures combine and impinge on the core structure.
— The entrance to the intermediate heat exchangers, where the cover gas (argon) can become entrained into the liquid sodium and be transported to the cold pool, with adverse consequences for reactivity control.
— The core inlet region under non-symmetrical flow conditions.
— The hot and cold pools under reduced flow conditions, for which large scale flow structures may influence the overall flow parameters.

Historically, in the context of SFRs, CFD has been used to better understand the physical processes and phenomena relating to the safety aspects of the reactor. Examples here, in the context of the PHÉNIX SFR, are CFD calculations to predict the onset of high cycle thermal fatigue in T-junctions [111], to estimate the negative reactivity effect during reactor shutdown, and to model the onset of natural convection in the primary circuit [112].

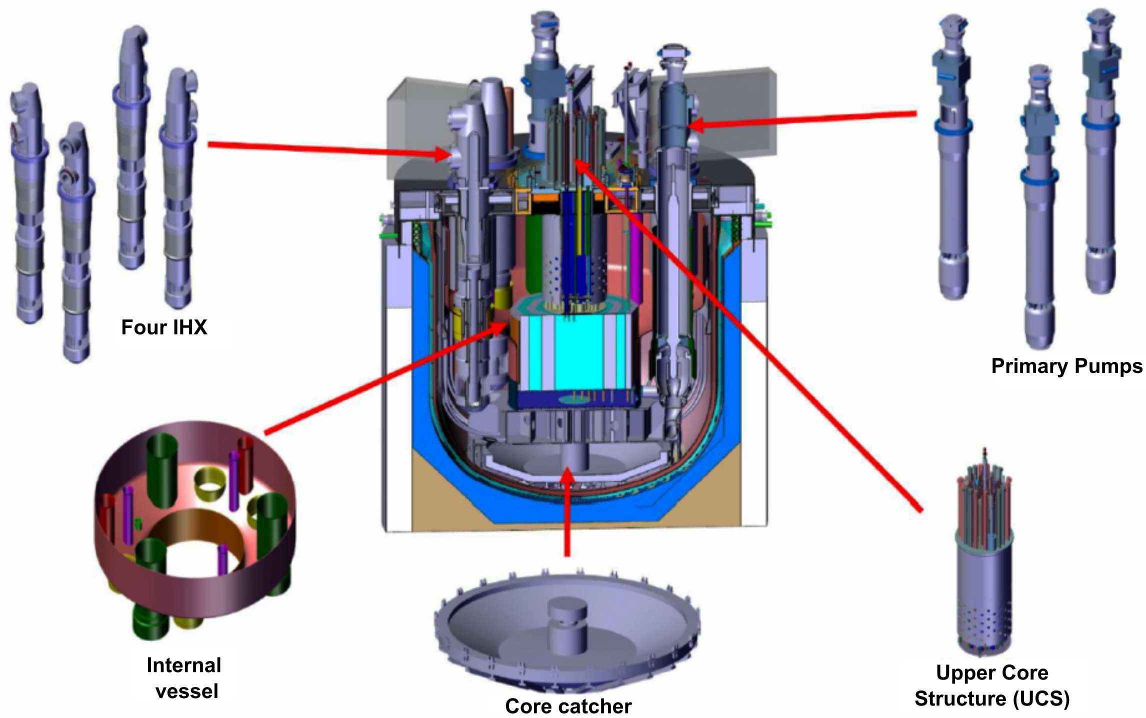

FIG. 2: Schematic of the ASTRID SFR concept.

5.3.1. Present limitations of computational fluid dynamics

An overview of the thermal hydraulic challenges in SFRs has been reported by Tenchine [34, 40]. A possible limitation in the use of CFD is the state of validation of the codes, due to the lack of appropriate validation experiments at high resolution, though a good database is available for reliable correlations to be utilized for system analysis purposes, and in the analysis of the global thermal hydraulic effects.

Within the European fast breeder reactor programme, experiments have been conducted at 1/20 scale in the RAMONA facility [113] to study decay heat removal. A larger water model at 1/5 scale, called NEPTUN, has also been constructed to address the scale effects, and to enable a better extrapolation to be made to the actual reactor scale [114]. A similar 1/6th scale water model is in operation in the context of the ASTRID project [43].

Similarity criteria are often used to extrapolate the results of water tests to sodium flow conditions. Such criteria for mixed convection have been evaluated at the CEA in two geometrically identical experimental facilities: SUPERCAVNA, for sodium flow, and JEAU for water flow. Thermal stratification and thermal fluctuations have been measured in both facilities and, in addition, velocity measurements have been taken in the water tests [115]. Selected steady state and transient experiments within the SUPERCAVNA programme have recently been analysed successfully using CFD [37].

Mixing of the submerged jets encountered at the core outlet has also been reported by Tenchine [40] for sodium. In addition, analytical experiments and detailed numerical simulations have been performed to study free-surface behaviour and air ingress of gas at the sodium/argon free surface in the presence of vortices [116].

A limitation for the use of CFD in such applications is the lack of knowledge of turbulence models that can simultaneously treat anisotropic effects, multiple interacting jets impinging on walls, the formation of thermal stratification, and its destruction by the impact of buoyant jets from below. Such multiphysics phenomena can be modelled using LES, but not by the classical turbulence models based on linear turbulence viscosity assumptions. However, non-linear eddy viscosity models are currently being developed for some specific applications: these show considerable promise. In particular, the model of Baglietto [117] appears to be successful when applied in specific situations (e.g. for tube bundles), but in general, at least at the current state of development, the models appear to not be capable of producing reliable predictions for other geometries.

5.3.2. Improvements needed

Several of the operational and accident transients that need to be analysed in the context of the ASTRID initiative involve strong 3-D fluid motions. In order to take these effects into account, code couplings have been developed between the thermal hydraulics system code CATHARE, the CFD code TrioCFD, and the core subchannel code TrioMC. These couplings allow one to account for the influence of local 3-D phenomena on global system behaviour without the need for fine-scale modelling of the complete primary circuit, which would entail excessive computational cost [118].

For the CFD component of the coupled code system, good candidates for improved turbulence modelling might be, for example, scale adaptive schemes (SASs) [119], improved RSMs, or partially integrated transport models [120]. Also, coupled RANS/LES approaches will become more feasible for modelling turbulence at industrial scales. Furthermore, in order to simulate long transients with persistent and/or slowly eroding thermal stratification, numerical schemes with very low numerical diffusion are needed, especially for flows in complex geometries, for which the gravity vector cannot always be guaranteed to be strictly normal to the mesh faces of the underlying computational grid.

5.4. PRESSURIZED WATER REACTORS

The Gen II PWR remains the most popular of the operating reactors in the world, though none were designed or optimized using CFD except for some post-manufacturing issues, such as cracking in T-junctions due to thermal stress. However, it is worth summarizing some common issues in the use of CFD in the design of future Gen III PWRs, and the challenges still facing its utilization and acceptance.

5.4.1. Present limitations of computational fluid dynamics

CFD predictions are not sufficiently reliable for a 'virtual reactor' to be constructed ahead of hardware manufacture, or more precisely if the configuration being simulated is not, or is only partially, covered by a validation catalogue. Moreover, only single-phase flow predictions (and not all of them), perhaps including conjugate heat transfer, are of sufficient maturity to be trusted for design purposes. However, some unstable flows (such as those occurring in the lower plenum of the reactor vessel, or in some T-junction configurations) cannot be represented in terms of simple, cost effective RANS techniques, which invariably lead to underestimation of the mixing phenomena. LES and similar models can help improve the reliability of the CFD predictions, but remain expensive in terms of computing time at industrial scales [121].

Another limitation is that generally large fluid domains are involved and the resultant size of the CFD simulation is again too expensive in terms of CPU time. This is particularly true of containment modelling using CFD, but also for some aspects of the primary circuit. Taking matters to the extreme, in the design of cooling towers, the fluid domain has to even include large parts of the atmosphere upstream and downstream of the power plant. The question also arises of the most suitable and reliable boundary conditions to be used.

Another technology gap is the need to minimize, as much as possible, user effects on CFD predictions. It is commonly recognized that this issue mostly manifests itself during the meshing procedure, even though general BPGs have been documented (e.g. for the modelling of boundary layers, managing local mesh refinement, and the use of non-conforming meshes). One of the important first steps in reducing the user effect is to utilize automatic meshing procedures, based as far as possible on numerical parameters, such as the gradients of the physical quantities. Automatic meshing also saves on model preparation time.

Finally, excessive CPU time still represents a gap in the technology that needs to be filled. In order to fully optimize any new NPP design concept, a number of CFD simulations (with geometrical variants) have to be performed (e.g. in the design of the reactor vessel internals, the cooling tower inlet, etc.).

5.4.2. Improvements needed

One of the major challenges to further advance the industrial application of CFD is its extension to the simulation of complex transients at affordable computational cost. A large number of component and system failures that have been observed are related to unplanned, unsteady flow and heat transfer events, which can lead to both mechanical and thermal fatigue [122]. The challenge here is to resolve complex coherent turbulent structures, which RANS based approaches cannot accurately reproduce. While turbulence resolving LES approaches have demonstrated good applicability to this class of problem [123], the associated computational cost does not yet make it amenable to large scale design applications. The industry has therefore been looking for a robust class of hybrid turbulence models to close this gap.

Detached eddy simulation (DES) and SAS turbulence models have had some success for specific flow configurations, but having been primarily developed to recognize massive flow separation phenomena (e.g. in aerospace and turbomachinery applications), they have been shown to have serious shortcomings when applied to typical nuclear related internal flow applications [123].

A class of model that promises more extensive applicability is Second Generation URANS (unsteady RANS) models [124], and some recent work has demonstrated its suitability to a number of nuclear related applications, which had, until recently, been limited to LES modelling only [125, 126].[4]

The need for more general multiphase physical closure models to allow robust application of multiphase CFD has already been discussed in Section 5.2.1 and remains of relevance for PWR applications.

The principal improvements needed in the use of CFD in NPP design are listed here.

- **Development of codes and models:**
  - *Unstable single phase flows.* The need here is not for new turbulence models, but for guidelines in setting up the most appropriate CFD approach when an unsteady calculation is required, i.e. which unsteady turbulence model to use — URANS, DES or LES — and the numerical empirical data to use.
  - *Two phase flows.* For 'simple' situations, i.e. those dealing with just one two-phase phenomenon (e.g. boiling, free surface modelling, bubbles of incondensable gas, adiabatic sprays, etc.), CFD codes have models that are included in their tool boxes. Parameters are set according to guidelines given in the literature (e.g. for drag and lift coefficients). However, CHF models remain to be improved and to be more reliable for designs which deviate from standard ones. For example, fuel mixing spacers featuring devices other than mixing vanes would need a dedicated validation programme.
  - *Flashing calculations, and two phase sonic flows originating from breaches of high pressure pipes.* Both of these require dedicated validation programmes. For more complex two phase flows incorporating several phenomena (e.g. PTS with a free surface, spill and vapour condensation, boiling in spent fuel pools (free surface, boiling by depressurization), sprays with interaction with steam (condensation on droplets and vaporization of them), or with wet air (cooling towers), model developments and associated validations are needed. In particular, the experiments have to deal with the different phenomena occurring simultaneously, and this remains a challenge. More generally, the developments required refer to the industrial domain size and not for the local bubble (or droplet) size.
  - *Fluid structure interaction.* Major developments needed here are in the coupling of the CFD and structural analysis codes, with particular attention to the numerical issues. Domain re-meshing (when two way coupling occurs) is also an item where progress is awaited. Fluid structure interaction has to also include in the future two phase flows (e.g. design as regards to vibration issues in the upper parts of steam generator tubes).
- **Coupling with system codes (and with neutronics codes).** The coupling with system codes is necessary to improve the specification of boundary conditions and to consider the feedback of the system. A typical situation is the modelling of the entire primary circuit using a detailed model for the core (considering the mixing of the flow from the different loops) and a 1-D system model for the rest of the circuit.
- **Models dealing with the different scales while maintaining reasonable computing times.** Typical configurations take into account the effects of fuel rod mixing grids in reactor vessel calculation and computing the local flows around the supporting plates in a steam generator. Classical porous media approaches cannot represent reliably all the important phenomena.
- **Faster codes** (i.e. more efficient algorithms for matrix inversion) and parallel machine architecture to deal with full scale simulations. To achieve this, massive parallelization has to be ensured.

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[4] The SAS model of turbulence is used in Framatome, and its appropriateness has been demonstrated over a wide range of flow situations, such as the flow distribution at core inlet and outlet, flow in the upper plenum, flow mixing in the vessel, boron dilution phenomena and PTS analyses. Results obtained with SAS are systematically as good as, or superior to, those obtained with the k–ε or k–ω RANS models.

— **Optimization algorithms.** These are embedded in CFD codes to limit the number of complete CFD runs needed for designing a specific component.
— **Performance of scale tests with CFD-grade data.** These are needed for reliable comparison with the numerical predictions.

6. BEST PRACTICE GUIDELINES IN THE USE OF COMPUTATIONAL FLUID DYNAMICS FOR NUCLEAR POWER PLANT DESIGN

6.1. BEST PRACTICE GUIDELINES FOR SAFETY ANALYSES

A report was prepared to support the CFD simulations undertaken within the European Union project entitled Evaluation of Computational Fluid Dynamics Methods for Reactor Safety Analysis (ECORA), under Contract No. FIKS-CT-2001-00154. The goal of the report was to provide BPGs for the simulation and documentation of the underlying verification, validation and demonstration test cases. One of the goals of the project was to provide a comprehensive evaluation of CFD codes for nuclear safety applications, though many of the conclusions are also relevant to NPP design using CFD. Any evaluation of CFD capability has to ensure that any source of error to which the simulation may be subject has been properly identified and, as far as possible, evaluated and controlled.

It is well known from exhaustive single phase studies of fluid flow that the identification, possible quantification, and certainly documentation, of possible modelling errors (e.g. the particular turbulence model to employ) is only achievable if the other major sources of error have previously been reduced to an 'acceptable' level; i.e. one within the stipulated tolerance levels of accuracy. In a perfect world, this would mean (among other requirements) that solutions have been provided for grids at the appropriate resolution to describe the physical phenomena being modelled and, for transient simulations, the time step(s) adopted have been chosen to capture the important transient phenomena taking place. Such idealized separation of the different sources of error, and the means to control them, is always difficult. Such challenges are greatly amplified by the inclusion of multiscale and multiphase physics. Nevertheless, any temptation to avoid the difficulties and to provide solutions on a single grid, with a single time step, and with accepted uncertainties in initial and boundary conditions not having been evaluated, will undoubtedly result in unreliable predictions: a strategy that would have been counter to the stated goals of the ECORA project.

An essential component of the quality assurance procedure underlying any CFD simulation is the definition of target variables. Ideally, these would have been identified in a preliminary phenomena identification and ranking table study of the task. These will mainly be defined in terms of scalar (integral) quantities (forces, heat transfer rates, peak temperatures, etc.), or 1-D distributions, such as the wall heat transfer rate along a specified line, for which measured data are available. Grid convergence studies are usually based on such target variables; obviously, suitable measured data are essential in this process. Target variables are particularly useful in assessing asymptotic convergence for unstructured meshes, for which the required degree of refinement may be difficult to define in advance, or mechanistic in origin due to automatic meshing procedures. Also important is the fact that target variables are of relevance to design engineers in evaluating model uncertainties from a physical standpoint. One danger of integral/global scalar quantities being used in the evaluation process is that compensation of errors may occur under successive grid refinement. Therefore, local measurements are very important for CFD validation procedures.

It is appropriate here to define the different sources of error that can impact a CFD simulation. Having done this, it is then necessary to identify the most obvious pitfalls to avoid in initially setting up the simulation, or at least to reduce the errors associated with them. Based on such approaches, procedures then have to be defined to be used for the test case simulations. Within the ECORA project, this was achieved by issuing templates to provide a uniform framework for the different partners to adopt within the project, given that it will certainly not be possible to rigorously perform the necessary error estimation and mesh reduction procedures demanded by strict adherence to BPGs. However, given the hardware resources available at the time, the best attempt possible needs to be made to avoid the acceptance of single grid strategies; i.e. those lacking grid sensitivity studies. It is even more crucial to follow a strict documentation procedure, to learn from past experiences, to identify deficiencies and uncertainties in the simulation procedures, and to provide guidance for future studies.

The strategies employed to identify, evaluate and reduce potential sources of numerical errors have been developed for single phase flows, and those associated with 1-D system code analyses for NPP safety considerations (see Section 9). Fundamentally, there is no procedural difference between those formulated for single phase and those needed for multiphase flow formulations. Both approaches are based on (ensemble) averaged governing equations and are mathematically similar, being parabolic, elliptic or hyperbolic in nature, depending on the particular application. From a practical standpoint, however, there are significant additional challenges in the case of multiphase flow, due to the interaction of the different phases, in addition to the obviously higher demands on computer time needed to represent them. An additional complication is the presence of interfaces between the phases, across which mass, momentum and energy exchanges will occur, and the degree of grid resolution required for capturing them, but still complying with computer hardware limitations.

In addition, multiphase flows have a higher affinity to physical instabilities, such as water hammer, enhanced Rayleigh–Taylor and Kelvin–Helmholtz instabilities, density wave and parallel channel instabilities, etc., all of which might be artificially suppressed if a coarse grid arrangement is employed, but which could appear under successive grid refinement. A parallel effect is often observed at the blunt trailing edge of an aerofoil in single phase flow, in which only successive grid refinement will capture the all important phenomenon of vortex shedding from the upper and lower wing surfaces. It is also to be kept in mind that brute force application of recognized numerical methods might lead to erroneous predictions. In such cases, the underlying philosophy, as documented in the BPGs, independently produced for different application areas, are to be followed as far as possible.

By definition, validation studies have to be based on experimental data. These data can themselves introduce significant errors into the comparison procedure. It is therefore necessary to select the project test cases with attention to potential error sources in standard measurement techniques, and experimental uncertainties. The main references used within the ROCOM document are Roache [127] on verification and validation, from which most of the definitions of the numerical errors have been taken, and the European Research Community on Flow, Turbulence and Combustion (ERCOFTAC) BPG [128]. The difference from the second document lies in the emphasis on validation in the OECD BPG report [129], since the ERCOFTAC initiative aims at the industrial end-user of CFD practitioners. The second difference is that some of the chapters in the OECD publication are dedicated specifically to reactor safety applications, some within the ECORA project.

The recognition of the importance of BPGs in CFD simulation enables its use for NPP design purposes to be placed on a firmer basis. The final aim of the BPGs for NPP design is the same as those formulated for safety considerations: the main difference and difficulty is to be confident enough in the numerical simulations without the need for accompanying experimental demonstration. The objective is to ultimately quantify the error involved, from the data obtained from the validation cases. At the design phase, this can be done by taking into consideration previous studies (supported by experiments) more than by the imposition of generic BPGs. For example, lessons can be learned from the CFD simulations performed of the different mock-up experiments of the cold plenum of a PWR [130, 131]. Former campaigns centred around numerical predictions of CHF, and pressure losses associated with fuel rod spacer designs, and their simulation, provide valuable information in the study of new design options.

CFD methodologies are being improved continuously by the application of BPGs. A trend towards unifying BPGs for several applications can be seen with the improvements in CFD code development, CPU cost reduction, and more refined experimental data [132].

6.2. SPECIFIC EXAMPLES

6.2.1. ROCOM test facility

For the analysis of boron dilution or main steam line break transients, coupled neutron kinetics/thermo-hydraulic system codes have generally been used. To consider coolant mixing phenomena in these codes in a realistic manner, analytical mixing models need to be included. In particular, the coolant mixing in the downcomer and lower plenum depends significantly on the construction details of the reactor vessel and internal components, as well as on the instantaneous flow conditions.

The models and assumptions for coolant mixing to be used in the coupled codes have to be validated against relevant experimental data, and detailed CFD calculations. Therefore, the Institute for Safety Research of the Forschungszentrum Rossendorf (now HZDR, Helmholtz-Zentrum Dresden Rossendorf) constructed a 1:5 mixing test facility ROCOM (Rossendorf Coolant Mixing Model) [85] representing the geometry of the German Konvoi type PWR (Table 1).

As mixing is less influenced by the absolute temperatures and static pressure than by density differences in the fluid and flow velocity, the vessel of the 1:5 scale test facility could be made from Plexiglas and operated at ambient pressure with cold water (Fig. 3). This choice allows flow visualization and laser Doppler anemometry (LDA) velocity measurements. The test facility is furnished with four separately controllable coolant pumps (Fig. 4) to simulate different flow conditions, from nominal coolant flow rate to natural convection and pump startup.

TABLE 1. COMPARISON ORIGINAL LWR — 1/5th SCALE MIXING MODEL, COOLANT MEDIUM WATER, 20°C

Dimension	Unit	Original	Model 1:5
Diameter of the pressure vessel	mm	5 000	1 000
Height of the pressure vessel	mm	~12 000	~2400
Inlet nozzle diameter	mm	750	150
Downcomer gap	mm	315	63
General mass flow of the coolant	m^3/h	92 000	1 400
Mass flow per loop	m^3/h	23 000	350
Speed at inlet nozzle	m/s	14.5	5.5
Speed at the downcomer	m/s	5.5	2.1
Re-inlet nozzle	—	8.4×10^7	8.3×10^5
Re-downcomer	—	2.7×10^7	2.5×10^5
Re-original/Re-model	—	1	~100

FIG. 3. RPV Plexiglas Model [2].

FIG. 4. Test facility ROCOM [2].

To study the mixing phenomena, plugs of salt water are injected into the RPV (initially filled with deionized water) through one of the four cold legs. The salt significantly changes the conductivity of the water, which can be measured using conductance methods. To this purpose, in the facility, a number of wire mesh sensors (WMSs) are installed. There is one sensor at the lower core support structure, two in the downcomer and another one in the cold leg where the injection takes place. The extensive instrumentation provided by these sensors permits high resolution images of the concentration field in the RPV to be made in space and time. The sensors are shown in detail in Figs 5–7. The downcomer sensors, and those in the cold leg, have 16 × 16 measurement points each. The sensor at the base of the core provides 193 measurement points. This means there is one concentration measurement at the bottom of each fuel element. All sensors provide 200 measurements per second and operate in the conductivity range of 10–500 µS/cm. In the experiments, a time resolution of 20 measurements per second is sufficient, i.e. 10 individual measurements are averaged to provide the recorded data.

FIG. 5. Sensor in the downcomer [2].

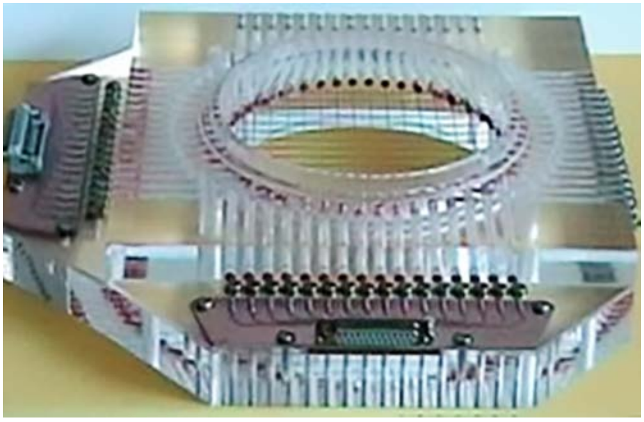

FIG. 6. Sensor at the inlet nozzle [2].

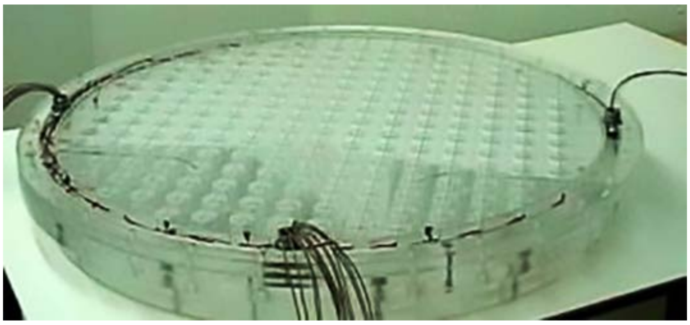

FIG. 7. Sensor at the core inlet [2].

The mixing measurements in the reactor model are obtained by the following steps. First, the test facility is filled with low conductivity (i.e. deionized) water. The required flow field is obtained by controlling the speeds of the main coolant pumps. After this, one pump injects a plug of salt water continuously, or discontinuously (i.e. to produce a slug), to the RPV through one of the cold leg loops. The concentration profile is measured by the WMS located in that cold leg. All processes, including the measurement of the mass flow rates, temperature and pressure, the tracer injection and the water cleaning with ion exchangers, are all computer controlled.

Two tests performed in the ROCOM series have been selected to provide the bases for CFD validation exercises within the framework of the current CRP, the results from which are reported in an associated IAEA publication [1].

6.2.2. HAWAC test facility

The horizontal air/water channel, or HAWAC [133], shown schematically in Fig. 8, is devoted to co-current flow experiments. A special inlet device, shown in Fig. 9, provides well-defined inlet boundary conditions by the separate injection of water and air into the test section. As the inlet geometry produces a number of perturbations in the flow (bends, transition from cylindrical pipes to rectangular cross-section, etc.), four wire mesh filters are mounted in each partition to provide homogeneous velocity profiles at the inlet to the test section.

Moreover, the filters produce a pressure drop that attenuates the effect of the pressure surge created by slug flow on the water and air supply systems. The 500 mm long blade separates the phases and can be moved up and down to control the free inlet cross-section for each phase. This allows the influence of the different cross-sectional areas on the evolution of the two phase flow regime to be investigated. Furthermore, the perturbation caused by first contact between gas and liquid can be either minimized or, if required, a perturbation can be introduced (e.g. a hydraulic jump). The cross-section of the entire channel is 100 × 30 mm² (height × width), and the test section itself is about 8 m long, leading to a length to height ratio of L/H = 80.

Both filters and inclinable blade provide well defined inlet boundary conditions for the subsequent CFD simulations and, therefore, offer very good validation possibilities. Optical measurements are provided by means of a high speed video camera.

In the context of this CRP, the HAWAC tests were not selected for detailed analysis. Higher priorities were set for the ROCOM and KAERI test data. Nonetheless, data from the tests were offered to participants on a bilateral basis once a common interest had been declared.

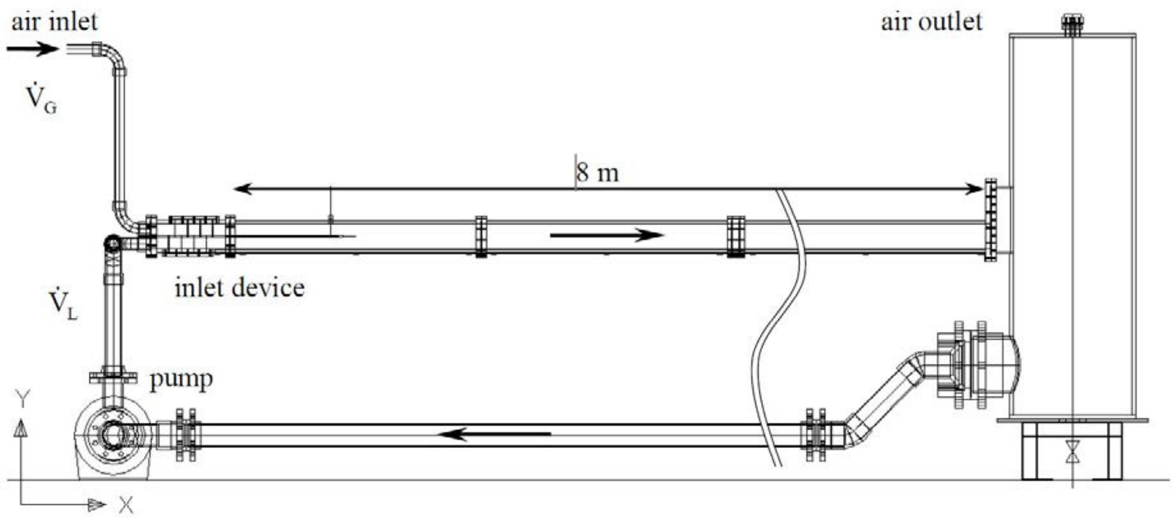

FIG. 8. Schematic view of HAWAC [133].

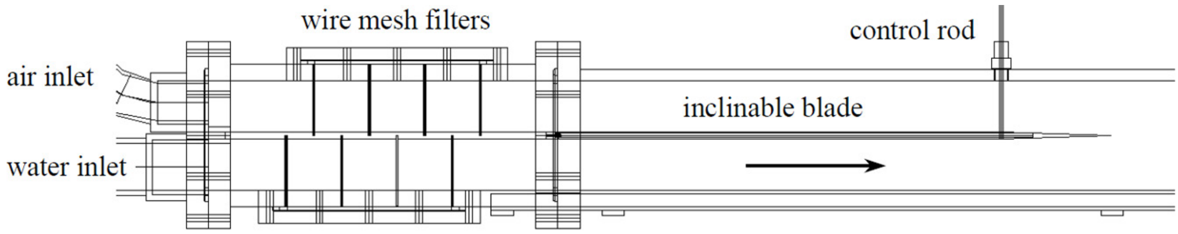

FIG. 9. The HAWAC inlet device (reproduced courtesy of HZDR [133]).

6.2.3. Vattenfall T-junction experiment

This experiment was the basis of an OECD benchmark exercise. The test section is constructed from plexiglass (Fig. 10) and the junction itself is one solid block into which the main and branch pipes fit (inset to Fig. 11). The dimensions are listed in Table 2. In the test, the temperatures of the water in the main and branch pipes were maintained at 15°C and 30°C, respectively, with minimal heat loss. Special care was taken to provide simple and well defined inlet boundary conditions to remove ambiguities in defining the CFD input data. Temperature fluctuations near pipe walls were measured using thermocouples. These were placed around the inner wall perimeter of the main pipe at seven stations downstream of the junction and at one station upstream (see Fig. 11). All thermocouples were positioned 1 mm from the wall.

Velocity profiles upstream and downstream of the junction were measured using a two component laser doppler velocimetry system. These were positioned at each inlet and at the outlet. Data are available in the form of mean values, root mean square (RMS) values and turbulence statistics.

The numerical prediction of thermal mixing and striping in terms of temperature amplitude and frequency using current CFD technology is computationally intensive, and thereby represents a challenging task. The flow is turbulent, and highly transient, and the thermal striping at pipe walls is affected by the formation and propagation of large scale turbulent structures in space and time. The aim is therefore to identify the most appropriate CFD turbulence model by means of detailed CFD/experiment comparisons. Turbulence model approaches studied in this context include URANS shear stress transport (SST) and scale resolving turbulence models (i.e. LES).

Vattenfall (in Sweden) provided time averaged temperatures and temperature fluctuations for all thermocouples. These were located at 0º, 90º, 180º, and 270º, two, four, six, eight and ten hydraulic diameters downstream of the T-junction, and at 0º and 180º, 15 and 20 hydraulic diameters downstream. In addition, time dependent temperature readings were provided two and four hydraulic diameters downstream at all four angular locations, at 0º, 180º, and 270º six diameters downstream, and at 0º, 90º, and 180º eight diameters downstream. These data were collected every 5 ms for 300 s.

Vattenfall also provided particle image velocimetry (PIV) data at 1.6, 2.6, 3.6, and 4.6 hydraulic diameters downstream of the T-junction (Fig. 11). In addition, time averaged and RMS fluctuations were recorded for the x and z velocity components (U and W) along a vertical line through the centre of the pipe at the four x locations. Time averaged and RMS fluctuations were also provided for the x and y velocity components (U and V) along a horizontal line through the centre of the pipe at the same four x locations. Time dependent PIV information was provided at the same four downstream locations, but only for a restricted number of points. All three velocity components were provided on the pipe centreline. The x and z components (U and W) were provided at $y = 0$ and $z = \pm 35$ mm, and the x and y components provided at $z = 0$ and $y = \pm 35$ mm. PIV data were sampled 60 times per second for 12 s, and two independent 12 s samples were provided for each velocity component at each location. The inlet velocity profiles are taken from an earlier test in which the volumetric flow ratio between the main and branch streams was 2. In the OECD test (flow ratio 1.5), the flow rate in the hot inlet was kept the same as before (6 L/s), whereas the one in the cold inlet was 9.0 L/s instead of the 12.0 L/s used previously. Since the velocity profile is fully developed in the cold inlet, the results could simply be scaled to fit the given flow rate. A non-dimensional temperature (mixing scalar) is defined at each thermocouple location and is the actual temperature minus the cold flow inlet temperature, divided by the difference between the inlet temperatures.

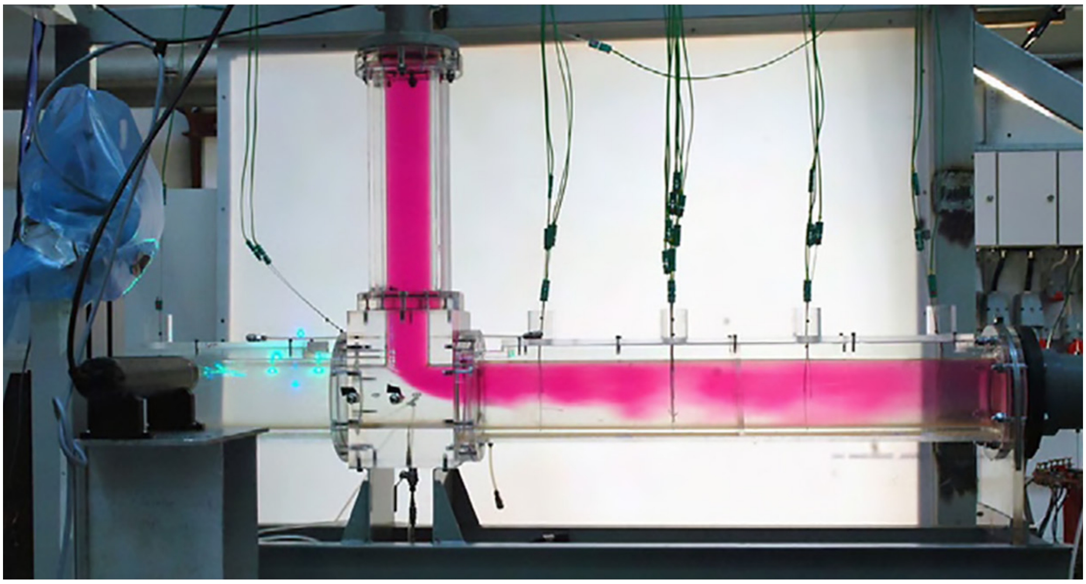

FIG. 10. Vattenfall T-junction experiment (reproduced courtesy of HZDR [123]).

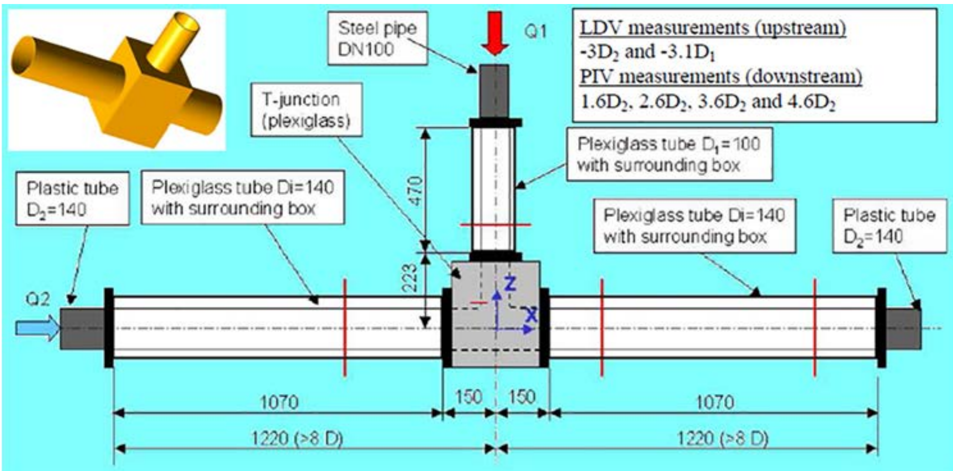

FIG. 11. Schematic of a T-junction with plexiglass sections (reproduced courtesy of HZDR [123]).

TABLE 2. DIMENSIONS OF THE T-JUNCTION TEST SECTION

Component	Material	Dimensions (mm)
Main inlet pipe	Plexiglass	Length: 1070; i.d.: 140; o.d.: 150
Branch inlet pipe	Plexiglass	Length: 470; i.d.: 100; o.d.: 110
Outlet pipe	Plexiglass	Length: 1070; i.d.: 140; o.d.: 150
T-block	Plexiglass	Length (x): 220; width (y): 285, height (z): 325 Main channel diameter: 140 Branch channel diameter: 100

(i.d.: inside diameter; o.d.: outside diameter)

Full details of the OECD T-junction benchmark exercise are described in the final CSNI publication [123]. Many of the members of the current CRP had previously participated in the benchmark activity, and benefited from the experience that would eventually feed into their respective CFD primary circuit design studies. It is noted that the thermal fatigue issues identified in the Civaux NPP in France resulted in expensive backfitting [134], which could in the future be avoided at the design stage by the appropriate use and interpretation of results obtained from the coupled fluid/structure codes.

6.2.4. Hybiscus-2 test

The Hybiscus-2 scale model experiment [135] (Fig. 12) is dedicated to integrity assessments of the French RPVs of their PWR fleet. Specifically, the experiment deals with PTS scenarios, following a small break loss of coolant accident, and the subsequent injection of cold water into the cold legs. During these transient scenarios, depending on the size of the primary leak and its location, a single phase or two–phase flow develops in the cold leg. The objective of the Hybiscus–2 programme was to simulate more completely the flow physics during a PTS event, with the following major objectives:

— Validation of the 3-D thermal hydraulic software platforms for both single phase and two phase situations;
— Construction of simplified correlations for the subsequent temperature transient, dedicated to the 1300 MW(e) RPV series.

The mock-up represents one-half of a French 1300 MW(e) (four loop) series vessel, half of the downcomer, two cold legs, two ‘pseudo-pumps’ and two cross-vessels, all at 1/2 scale. The transparent experimental loop is made from PMMA (polymethyl methacrylate acrylic glass) and operates at near atmospheric pressure, and between 10° and 45°C. Each cold leg is equipped with its own emergency core cooling system nozzle. In the downcomer, the obstructions of the two hot legs, one irradiation basket, and the two centring keys are represented. The volume of the lower plenum cavity is respected, but with a conical geometry. Two pipes connected to the lower plenum, designed to maintain the desired water level in the mock-up, allow water to be extracted by an overflow pipe for single phase tests, and a second pipe for two phase tests.

The mock-up is approximately 6 m high and contains 6 m^3 of water. Saturated brine (saltwater) is used to represent experimentally the density effect of safety injection in the cold leg. The initial hot fluid is represented by pure water. Moreover, the brine is heated so that the mixing can be measured by means of temperature (based on the hypothesis of identical turbulent diffusion between salt and temperature).

The scaling is based on the conservation of the ratio between gravitational and inertial forces, as represented by the densimetric Froude number; the scaling factors are listed in Table 3.

The instrumentation is made up of temperature sensors (120 thermocouples, each with a 12 ms response time), one platinum sensor, flow meters and density meters.

An uncertainty analysis of the measurements has provided the following information:

— Thermocouples <1 K;
— ECC temperature <0.2 K;
— Flowrates <0.3%;
— Density <0.5%.

6.2.5. Summary

It was not within the scope of the present CRP to formulate a set of BPGs specifically oriented towards NPP design studies. Indeed, design engineers will have access to highly proprietary ‘design codes’, built up over the years within their respective organizations, to accelerate the design process. These will differ for each reactor vendor and will not be readily available outside of the respective design office.

FIG. 12. View of the Hybiscus 2 mock-up (reproduced courtesy of EDF [135]).

TABLE 3. HYBISCUS 2 SCALING FACTORS

Length	Velocity	Flow rate	dρ/ρ
0.5	0.486	0.12	0.47

What has been described in this section is the common input gained from the application of BPGs to the design process, essentially based on reactor safety studies, knowledge from which is of benefit to all, and can be fed back into design thinking.

7. SUMMARY OF EXPERIMENTAL REQUIREMENTS FOR PRODUCING COMPUTATIONAL FLUID DYNAMICS GRADE DATA

7.1. GENERAL EXPERIMENTAL REQUIREMENTS

CFD grade experimental data are required for assessing the validity of any CFD calculation. As for the boundary conditions, the experimental apparatus needs to be well designed to establish an isothermal or thermal flow under either steady state or transient conditions. Ideally, the experiment will ideally provide measurements of the velocity and/or temperature profiles at the inlet boundaries. It is also often desirable to provide inlet boundary conditions for the turbulence parameters.

For the correct set-up of the outlet and wall boundary conditions in the associated CFD simulation, the test section needs to be carefully designed in shape and size and installed at an appropriate location in the test loop with well defined inlet conditions. For instance, the test section will ideally be long enough, with a constant cross-section, to guarantee fully developed flow at the outlet boundary. As for the initial conditions, the specifications have to describe in detail the experimental conditions (whether these be steady or transient), the test section, and the measuring equipment employed.

For a steady state experiment, the flow and/or temperature conditions have to be maintained at the constant target value. The test specifications have to also include as-built dimensions of the test section as well as the surface roughness and the material properties (including those of the heat transfer surfaces). It is likely that the as-built dimensions are somewhat different from those of the original design because of the manufacturing and machining processes. It is also necessary to have at hand specifications and calibration data of the test equipment for the final CFD assessment. The experimental data have to demonstrate repeatability, with small deviations in measurements from different trials of the same test. Error analysis are also to be performed to estimate the systematic (bias) errors and random errors of the localized data measurements. It is also important to ensure that the experimentation is reproducible, with different experimental apparatus and/or operating personnel.

7.2. VALIDATION OF TWO PHASE FLOW MODELLING FOR COMPUTATIONAL FLUID DYNAMICS

For the validation of modelling of momentum transfer, turbulence and mass transfer in single phase and two phase flows, a comprehensive experimental database is required.

7.2.1. General requirements

- Precise definition of the experiment geometry.
- Material properties for the ambient conditions relevant to the experiment.
- Boundary conditions at inlets and outlets: void fraction distribution (two phase flow only) and velocity profiles at inlet(s), and pressure at outlet(s).
- Mean values of all relevant data, including fluctuations at inlet(s), where appropriate.
- Error bounds on the measured data.
- Accurate measurements of the actual model dimensions (e.g. straightness, out of round characteristics, etc.).
- Surface roughness conditions, including imperfections or mismatches in components.
- Accurate location coordinates of all instrumentation (as opposed to requested location stated in the design drawings).
- Information relating to instrumentation mounting hardware.

7.2.2. Extra requirements for momentum transfer under two phase conditions

A suitable experiment for CFD validation will ideally allow the identification of the distinct physical mechanisms involved in the momentum transfer between the phases. For the validation of drag models, stratified, adiabatic, two phase flow with a smooth interface constitutes an ideal test case, since it allows for measurements to be made close to the interface, and for the fact that the momentum transfer is caused exclusively by interfacial shear.

Measurements of the following mean quantities will ideally be performed:

- Differential pressure between inlet(s) and outlet(s);
- 2-D velocity profiles for both gas and liquid phase (resolving boundary layers at solid walls and the free surface);
- Void fraction distribution and liquid height;
- Mean interfacial shear stress or drag coefficient derived from 3-D velocity measurements.

Experiments involving simple two phase flows provide a means for validating each momentum transfer model separately. In addition, more complex two phase flows, in which several momentum transfer mechanisms are superimposed, are essential for overall model assessment.

7.2.3. Requirements concerning the validation of turbulence models

Compared with the requirements for single phase flow (see above), additional mechanisms of turbulence generation and dissipation need to be taken into account in two phase flows, such as small wave turbulence and bubble induced turbulence. Each of these mechanisms is modelled separately in most codes and introduced into the turbulence model equations through additional source terms.

With regard to turbulence dampening at a free surface in stratified flow, a smooth interface is best suited in a first instance for model validation. Measurements of the following mean quantities will ideally be performed:

- 2-D velocity profiles in both the gas and liquid phases (and resolving boundary layers at solid walls at any free surface);
- Void fraction distribution and liquid height;
- Turbulence kinetic energy (for both phases);
- Reynolds stresses.

The complex interaction of turbulent eddies in the liquid phase and at a free surface is also of interest. Since all aspects of turbulence are invariably modelled using RANS based methods, the prediction of interface deformation requires intense modelling capability, including turbulence generation in wall boundary layers, transport across the liquid phase, and the turbulence dampening at the free surface.

8. USER QUALIFICATION

8.1. GENERAL REQUIREMENTS FOR PRACTITIONERS OF COMPUTATIONAL FLUID DYNAMICS

A highly evolved CFD code is the result of hundreds of person-hours of development and programming effort. Basic know-how on how to use such a sophisticated numerical tool will be just as demanding as learning to handle delicate measurement techniques, such as LDA, PIV, etc. CFD practitioners or users need the following general qualifications:

- Fundamental understanding of engineering design and current CFD techniques;
- Good understanding of commercial CFD solvers (ANSYS-CFX, ANSYS-FLUENT, or STAR CCM+);
- Good understanding of open source CFD solvers (e.g. OpenFOAM).

8.2. SPECIFIC KNOWLEDGE AREAS

In addition to the above general qualifications, CFD practitioners need specific knowledge and expertise in basic physics (fluid mechanics, thermodynamics), mathematics and computer science.

8.2.1. Basic physics

Adequate knowledge of the basic physics involved in the problem being simulated, including thermal hydraulics, fluid dynamics and heat transfer, is required. The code user needs to be capable of formulating an appropriate physical model, regardless of the solution methodology.

For excellence in physics, one needs not only to have a firm idea and appreciation of the physical processes involved, but also the ability to model these processes within the framework of a specific CFD calculation.

8.2.2. Mathematics

- *Linear algebra.* Any CFD simulation will require a significant amount of knowledge in this area on the part of the practitioner in order to choose the most optimum matrix inversion algorithm for the job in hand.
- *Differential equations.* Understanding of the characteristics of the governing equations (be they parabolic, elliptic or hyperbolic in nature) that will need to be solved; this will influence the choice of solver for the particular application.
- *Complex numbers.* For meshing purposes, transformation of coordinates, and the use of Fourier transforms, if needed.
- *Optional topics* (for additional mastery):
    - Probability theory;
    - Statistics.

8.2.3. Computer science and numerical analysis

- *Differential equations.* Selection of the appropriate solver.
- *Numerical methods.* The basis of CFD calculations.
- *Computational geometry.* For the generation and meshing of the body of fluid through which the flow is to be calculated.
- Additional topics:
    - Computer graphics;
    - Data science technology;
    - Compilers.

8.3. SUMMARY OF TRAINING COURSES IN COMPUTATIONAL FLUID DYNAMICS FOR REACTOR DESIGN

8.3.1. The HZDR multiphase flow workshop — short course and conference

Multiphase flows are of great interest for many industrial processes. Power generation, nuclear reactor technology, food production, chemical processing, aerospace and automotive industries are all driving forces in this complex field of study.

The goal of the annual HZDR workshops is to bring together experimental and numerical practitioners, and to foster discussion and exchange of knowledge between the various domains of expertise.

Experts from both areas are called upon to present their research and application results to a worldwide audience. Topics of interest include:

- Simulation technology for multiphase flows:
    - Phase interaction models;
    - Turbulence models;

  - Solution algorithms;
  - Multiscale modelling techniques;
- Application of specific simulation methods to multiphase flow problems.
- Experimental investigations of multiphase and magneto–hydrodynamic flows.
- Measurement methods for multiphase and magneto–hydrodynamic flows.

A typical workshop in the series is divided into two parts, starting with a 1.5 day short course, followed by a further 1.5 days for the conference itself, where individual presentations by participants can be made.

The short course is designed to provide knowledge on the use of numerical and experimental methods for multiphase flows. The experimental part provides guidance on the selection, implementation and use of modern gas–liquid measurement techniques and instruments, such as wire mesh sensors, needle probes, process microscopy and gamma ray computed tomography, along with the application of data analysis tools. The numerical part focuses on finite volume methods for Euler–Euler and Euler–Lagrange multiphase flow simulations, and on the associated mathematical models. The audience is typically composed of engineers, chemists, physicists and technicians active in NPP research and design who want to be informed on modern design methods and tools in active use for multiphase flow simulations. The first day focuses on general topics; while on the second day one group will specialize in experimental techniques, including standard laboratory practices, while the other group will delve into the intricacies of the multiscale modelling aspects.

The lecture topics include:

- Eulerian multiphase flow models;
- Lagrangian multiphase flow models;
- Interfacial heat and mass transfer models;
- Measurement techniques and experimental investigations for multiphase flows;
- Practical calculations of bubble column flow and jet spray propagation;
- Multiscale modelling techniques like the GENTOP, MUSIG and AIAD models.

8.3.2. IAEA training courses on computational fluid dynamics

IAEA training courses on CFD were held in Hungary (2008), Croatia (2009), and China (2010; 2011). Though these courses in their original format were oriented towards NPP safety issues rather than to design, much of the material remains of a generic nature, aimed at introducing young practitioners to the subject of CFD technology. The course was later modified and expanded to suit the needs of the reactor design community and relaunched within the context of this CRP. Therefore, the first of the new style CFD training courses was held at Shanghai Jiao Tong University in Shanghai, China, and the university delegate assigned to this CRP (J. Xiaong) obtained permission from the university to host the course, which subsequently took place from 29 August to 2 September 2016. A local organizing committee was set up at SJTU, the course material collected and evaluated, contacts made with possible sponsors and principal lecturers, and a prospectus produced for prospective students, including the legacy of system code approaches, turbulence modelling, the challenges of modelling two phase flow situations, and the compilation of assessment bases.

The purpose of the IAEA course was to present the fundamentals of the CFD approach to numerical prediction in the framework of NPP technology. The lectures included an introduction to the subject, the level of maturity of present day CFD codes, V&V of these codes, and the ongoing applications relevant to nuclear design and safety considerations. The course consisted of presentations and discussions on the central theme: the use of CFD in NPP design. The participants discussed and/or presented their personal experiences, and described the results they obtained. Time was also provided for the discussion of selected topics, and for discussions with the invited experts.

Attendance was expected from:

- — Engineering support organizations, including technical support companies, research institutes and vendor organizations involved in the use of CFD in NPP design, and those responsible for performing transient operational and accident analyses;
- — NPP staff responsible for modifying plant design as a result of pre-design postulated accident situations;
- — Regulatory body representatives responsible for reviewing/overseeing the use of the results of such analyses, and their influence on the design process.

The main areas covered in these courses were the following:

- — The continuing use of system codes in NPP design.
- — Best estimate approaches in system codes.
- — Introduction to CFD, and the history of its development, both inside and outside the nuclear industry.
- — The governing equations, physical modelling and numerical procedures.
- — Uncertainty quantification — the beginnings of the approach in single phase CFD simulations.
- — NPP issues for which CFD can bring real benefits for single phase simulations.
- — Error control, verification, validation and BPGs for single phase simulations.
- — Assessment databases for single phase CFD applications.
- — Identification of design and safety issues for which two phase CFD can bring benefits.
- — Introduction to two phase CFD modelling and the various modelling options available.
- — Application of two phase CFD to boiling phenomena, and the approach to CHF.
- — The role of CFD in two phase PTS scenarios, the state of the art and the gaps identified in the technology.
- — Hands-on experience of using CFD software: (i) mesh generation.
- — Hands-on experience of using CFD software: (ii) sample problem solving.

The last two items represent a new addition to the IAEA courses given previously. All have been well attended, and this trend continued during the present course: there were 60 registered participants in the course held at Shanghai Jiao Tong University.

8.3.3. Swiss Federal Institute of Technology short courses on multiphase flow

These courses have been offered annually since 1984 at the Swiss Federal Institute of Technology. They attracted a total of 1600 participants over the years. The courses have been continuously updated to reflect ongoing progress and developments, and the number of lecturers and content scope have gradually increased. They not only offer the opportunity to meet and interact with experts in the field of multiphase flow, but also with other co-workers sharing similar interests in different industries.

The lectures are organized in modular form, as intensive introductory courses for persons with a basic knowledge of fluid mechanics, heat transfer and numerical techniques. They also serve as advanced courses for specialists wishing to keep abreast of the latest advances in the subject. A tutorial text is sent to all registered participants before the course begins to introduce the basic concepts of the lecture material, and to fill any gaps in their background. This is intended to help them interact with the courses in the best possible way.

Part I of the training course is for all participants, covering the common background material and emphasizing the latest empirical and mechanistic models, as well as introducing the computational and instrumentation aspects relevant to multiphase flows. This series of lectures constitute the base level of the subject. There are 12 lectures in total, spread over three days, dealing with the following topics:

- — Introduction to multiphase flows;
- — Two phase flow instrumentation and visualization;

— Basic numerical models for two phase flows;
— Empirical and phenomenological models;
— Instability of the gas–liquid interface;
— Basics of phase transition and pool boiling;
— Flow boiling and condensation;
— Empirical and phenomenological models for multiphase flows with phase change;
— Thermal non-equilibrium flows and interfacial instabilities;
— Multifield models;
— Advanced two phase flow instrumentation;
— Numerical methods.

Participants are then offered a choice between two branches of the subject, depending on their personal interests: Part IIA or Part IIB.

Part IIA: New Reactor Systems and Methods. This is a course of eight lectures on the following subjects:

— Introduction and multiphase phenomena in design basis accidents;
— Advanced reactor concepts and phenomena;
— Closure laws in nuclear system codes;
— Advanced computational modelling of nuclear systems;
— Instabilities in two phase flow;
— Multiphase phenomena in severe accidents;
— Applications of interface tracking to nuclear safety problems;
— CFD modelling applied to reactor systems.

Part IIB: Computational Multi-Fluid Dynamics (CMFD). This is a course of eight lectures devoted to the following subjects:

— Introduction to CMFD;
— Introduction to interface tracking;
— Volume of fluid method;
— Direct simulations of multiphase systems;
— Applications of volume of fluid and lattice Boltzmann approaches;
— Embedded interface methods;
— Application of CFD codes to multiphase systems;
— Applications of CMFD to situations involving heat transfer.

Part III: CMFD within the context of commercial codes. This is a course of three lectures on the final afternoon and is attached to both Parts IIA and IIB. The participants can meet commercial code developers to discuss their interests for both nuclear and other applications. The titles of the formal lectures are as follows:

— Simulating industrial multiphase flows using the TransAT code;
— Validation of two phase flow models in ANSYS CFD;
— Modelling of industrial multiphase flows with STAR–CCM+.

The short courses are organized by the Institute of Energy Technology of ETH Zurich, and usually take place in January/February each year and last five full days; the course language is English. More information may be obtained on the following web site:
http://www.lke.mavt.ethz.ch/news–and–events.html

9. UNCERTAINTY QUANTIFICATION

9.1. OVERVIEW

Computational methods have supplemented scaled model experiments, and even prototypic tests, in studies of reactor systems for nearly 40 years. During this time, very trustworthy system codes, such as RELAP-5 [136], TRACE [137], CATHARE [138] and ATHLET [139], have been formulated for the analysis of primary circuit transients. Similar programmes (such as SCDAP [140], MELCOR [141], GOTHIC [142], TONUS [143], ASTEC [144], MAAP [145], ICARE [146], COCOSYS/CPA [147]) have also been written for containment and/or severe accident analyses. These traditional reactor system and containment codes are modelled on networks of 1-D or even 0-D elements. In particular, (primary) system codes have proven successful because of the very large databases of phasic exchange correlations that have been built into them. The correlations have been formulated from essentially 1-D separate effects tests (SETs), and their range of validity and confidence levels are now very well established.

Originally, the approach was to use such codes, which involved very simplified geometric modelling, and appeal to conservatism to cover the unknown factors, both from limitations in geometrical representation and from lack of accurate knowledge of the physical processes of relevance at the scales of interest. In this way, safety margins on the numerical predictions could be ensured. The advantage of this simplified modelling approach was that a large number of sensitivity studies could be carried out to determine how plant parameters need to be modified in order for the predictions to remain conservative. Sophisticated statistical methods, such as Latin hypercube sampling, have placed this practice on a firm mathematical basis. However, a key issue is then to determine the degree of conservatism needed to cover the lack of physics embodied in the simplified models. Information on the subject can be obtained from mock-up experiments of course, but considerable care is still needed in extrapolating results to full scale. Moreover, the experiments themselves, of necessity, contain simplifications, and judging the degree of conservatism involved in introducing such simplifications is in itself rather imprecise. In the dual contexts of NPP design and safety, such a conservative approach could easily lead to over-design and the installation of expensive safety features.

Consequently, over the years, there has been a trend to gradually replace conservatism by a best-estimate methodology, coupled with UQ. This transition took place in the context of system analysis codes already in the 1970s with the development of second generation system codes; for example, the transition from RELAP-4 [148] to RELAP-5 [136]. The emergence of commercial CFD codes in the early 1980s was not part of this transition since, from its very earliest conception, CFD is already a best estimate technology. Thus, of necessity, uncertainty quantification needs to be intimately involved in CFD predictions. However, progress has been slow, principally due to the high computational costs involved.

Within the confines of this CRP, an opportunity to make an original contribution to the subject initially presented itself in the context of two highly simplified experiments to be carried out at the University of Pisa: (i) flow through a sudden contraction of the pipe diameter, and (ii) re-laminarization in a diffuser. Both tests would involve pressure measurements at selected stations downstream, vital information for assessing CFD predictions. However, it was not possible carry out the tests within the time frame of the CRP. Consequently, no new inroads into the subject could be made. As a result, in this section the current state of the art on the subject is summarized, as derived from ongoing activities undertaken elsewhere, how they relate to the use of CFD in NPP design, and citations of the most important current work for future reference.

Of necessity, in the context of nuclear applications, the starting point historically is the use of UQ in system code applications, which has now reached a reasonable degree of maturity [149, 150]. However, it needs to be recognized that system codes are essentially 1-D in origin, whereas CFD is usually 3-D (2-D at a minimum). The associated computational overhead of undertaking UQ in the CFD domain has proven to be the ultimate limiting factor in developing the technology in the CFD context, until quite recently when advanced hardware platforms have become available to accelerate the computations necessary to complete the task. Despite these limitations, tentative first steps have been taken, albeit at a very modest scale, and the progress made is reported here.

The first reference is a recently concluded OECD study on the subject [151], which emphasized that the CFD community is inexperienced in UQ methodology, and conversely as the system code specialists are relatively unaware of the specific requirements of CFD modelling, some common ground needed first to be established. The two leading, traditional, UQ methodologies, inherited from system code experience, are: (i) propagation of input parameter uncertainty; and (ii) extrapolation of accuracy.

The first approach entails estimating the individual uncertainties of all the input parameters (or as many as can be handled) and how the uncertainties propagate within the CFD simulation. This process necessitates a multitude of ancillary simulations being performed. The second method attempts to assess the accuracies of code predictions based on the associated integral effects tests (IETs) underpinning the base study and extrapolating them to full scale reactor (design) applications.

For purposes of illustration, some possible sources of error and uncertainty in CFD predictions are listed here:

- Initial and boundary conditions.
- Material properties (e.g. heat conductivity in the case of liquid metals, which remains quite difficult to measure accurately).
- Physical models embodied in the code (e.g. knowledge deficiencies in material properties for high pressure systems); non-calculated physical processes (particularly with regard to turbulence modelling), etc.
- Numerical errors, such as discretization errors in space and time, approximate solving of algebraic systems of equations, iterative convergence errors, gradient reconstructions for unstructured grids, rounding errors, etc.
- Simplifications in geometry and/or limitations in details of the actual physical boundaries of the fluid domain.
- Possible chaotic behaviour resulting from unreliable determination in the short term for a particular simulation.

Despite this list, CFD remains the only method available to accurately simulate 3-D behaviour in fluids. However, the OECD concluded in 2016 [151] that the overall maturity of the UQ methods in CFD still remains low to very low due to the lack of appropriate benchmarking. Indeed, the experimental measurements needed to test the UQ principles in CFD simulations are themselves often deficient in UQ quantification: i.e. measurement errors and unqualified data confidence.

One advantage of CFD over traditional system code analyses is the ability to eliminate uncertainties originating from numerical errors, at least in principle. Best practice guidelines have been formulated on the subject [129], and good progress made in recognition of their need for implementation in CFD simulations. Nonetheless, other sources of uncertainty remain, principally in the choice of appropriate turbulence model, even for single phase calculations, and phasic exchange correlations in multiphase situations. Thus, while in theory UQ has to always be applied to best estimate numerical simulations, of which CFD is a prime example, practical limitations require compromises to be made to follow the theoretical principles.

The main problem in the CFD context is the computational overhead associated with 3-D or even 2-D UQ studies, which will always involve a multitude of simulations in order to obtain statistically meaningful results. The CPU restriction even applies to steady state calculations, while transient simulations will require considerable extra effort.

Some progress has been made in the broader sense of UQ, led by the positive conclusions derived from the BEMUSE project for system codes [150]. The first international CFD study in the nuclear domain centred on a very simple configuration: the mixing of two stratified layers of equal velocity in a horizontal channel. This exercise was based on the GEMIX experiment carried out at the Paul Scherrer Institute in Switzerland in 2015, and formed the basis of a blind benchmark activity, subsequently reported at the

CFD4NRS-6 conference at MIT in the USA in 2016 [152]. There were 21 participants in the exercise from 13 countries. Thirteen participants from nine countries submitted results, which formed the basis of the official report on the exercise [68]. The experiment was deliberately chosen for its simplicity so that the participants could attempt a UQ analysis within a reasonable time. Further details follow in Section 9.2.

9.2. ASPECTS OF UNCERTAINTY QUANTIFICATION

UQ studies can only begin once the various sources of uncertainty have first been identified; this could result from an initial phenomena identification and ranking table exercise. Information can also be derived from the SETs and IETs that have been carried out previously, most likely in the pursuit of V&V exercises associated with quantification and assessment of the particular CFD software packages being used. In many circumstances, measurement uncertainties may be lacking, so to do the job properly the experimental data need to be scrutinized thoroughly in advance. Subsequently, a number of sensitivity studies have to be carried out to produce data of statistical reliability. Note that 3-D CFD simulations already place heavy demands on computational resources, so, for the foreseeable future, even a commitment to undertake a genuine UQ exercise in association with a CFD design simulation of an NPP will represent a major difficulty.

9.2.1. Sources of uncertainty

9.2.1.1. Initial and boundary conditions

If flow enters the simulation domain from the notional outlet(s), the flow parameters are often uncertain. There can also be uncertainties associated with inlet flow; for example, the mass flow rate at a pump outlet, which is sometimes difficult to assess accurately because of uncertainties in pump characteristics, levels of turbulence, etc. Initial and boundary conditions may also have been prescribed from a previous system code calculation, which would only result in 1-D (i.e. area averaged) data, whereas CFD requires, at minimum, detailed 2-D inlet mean and RMS profiles. Upstream pipework, bends, branches and elbows will also have an effect on the inlet profiles in actual cases, but are usually unknown.

9.2.1.2. Uncertainties related to the physical models

Within the context of this CRP, Gen II reactors took preference and this resulted in little uncertainty in the specification of the physical parameters (density, viscosity, conductivity, heat capacity, etc.) of the base fluid — light water — at reactor operating conditions (at least for single phase flow). However, it was recognized that with advanced reactor types, this would not necessarily be the case, and that some uncertainty would prevail, even in the basic molecular properties of the materials: for example, the conductivity of liquid metals and densities near the critical point for supercritical reactors. In some cases, the basic physics would need to be revisited to provide some level of confidence in the parameters, or the uncertainties associated with them would have to be considered in any subsequent UQ study.

9.2.1.3. Uncertainties related to modelled physical processes

In all large scale, single phase simulations, a turbulence model will always be needed, and assumptions will be made on the details of the momentum and energy transfers taking place at bounding walls. It needs to be emphasized that accepted turbulence models (k–ε, k–ω, wall functions, etc.) have been derived almost exclusively in the context of (oversimplified) SETs, but how reliable are they in geometrically complex situations? The accepted approach is that the empirical constants built into the standard turbulence models are not to be modified to suit a particular CFD simulation. Cases in point are where there is boundary layer separation and/or significant recirculating flow. Rather, the model restrictions need to be followed (and some models perform better than others in particular situations), but then quantify the uncertainties in adopting a particular turbulence model formulated in an oversimplified geometric configuration to a complex geometry. Best practice guidelines have been developed over the years [129] which provide guidance on the particular turbulence model to be used in specified situations, but all are subject to inherent limitations. For example, the most popular eddy viscosity models, such as k–ε and k–ω, cannot predict non-isotropic turbulence, nor the inverse cascade of energy from small turbulence scales to large ones [153].

9.2.1.4. Choice among different physical model options

When the BPGs cannot provide strong arguments to propose the best model option to employ in a given circumstance, it is also possible to consider the model choice itself as a basic source of uncertainty. This uncertainty can be considered a 'categorical variable' and be treated as such in the uncertainty assessment.

9.2.1.5. Numerical uncertainties

Numerical uncertainties are related to the discretization of the exact differential equations governing the momentum and heat transfer processes for solution on a finite grid, and for finite time step advancement for transient simulations. Sources of uncertainty include the time and spatial discretization themselves, and how representative they are in capturing the relevant physical process taking place, but also the fact that inversion of the solution matrix will inevitably involve iteration procedures — direct solvers are of no use in CFD. There may also be uncertainties due to round-off errors, though with current advances in machine architecture these are now usually considered minor. BPGs give guidelines on how to control such errors [129]. However, in purely practical terms, a certain level of residual error may have to be tolerated, which introduces a further level of uncertainty in the numerical predictions.

9.2.1.6. Choice among different numerical options

In the cases in which strict BPGs cannot provide convincing arguments to support the choice of the best numerical options, one may consider all the possible options (partially compatible with BPGs) and then regard the choice as a further source of uncertainty, also classed as a 'categorical variable'.

9.2.1.7. Simplifications in the geometry

The intricacy of reactor geometries, or even of a SET or IET, may have an impact on the resulting flow predictions. In most code applications, some simplifications of the geometry may have to be accepted, and, in all cases, details of processes occurring at smaller scales than the mesh size cannot be represented explicitly; they have to be modelled in some way. These circumstances create uncontrolled errors that themselves have to be considered part of the UQ process.

9.2.1.8. Uncertainties resulting from scaling distortions

Situations may exist in which one can determine the uncertainties associated with the input parameters within a given range of flow conditions, as determined by the geometrical layout of the flow configuration, and the values of the non-dimensional numbers characterizing the flow. In most full scale reactor applications, the values of most of them will be well beyond the tested range. In such cases, one needs to assign some uncertainty resulting from the extrapolation process.

9.2.1.9. Uncertainties resulting from previously measured data

Information derived from previous experiments (principally SETs) is often used in subsequent simulations: for example, the physical properties of fluid and solids. At best, such information will have defined error bounds, which will ideally be included in the global evaluation of uncertainty in the code predictions.

9.2.1.10. Uncertainties arising from physical instabilities and/or chaotic behaviour

Under certain circumstances, non-linear dynamic systems, as embodied in the Navier–Stokes equations, can exhibit chaotic behaviour. Manneville [154] reminds us that chaos results in unpredictability in the long term, even though determinism guarantees predictability in the short term. Chaotic behaviour can be computed directly, provided there is adequate time and space resolution, by introducing small changes in the input data, and computing the consequences. However, the results need to be treated within a probabilistic framework, and though UQ provides a means of dealing with this, physical practicalities, such as lack of sufficient computing power, may force unwelcome compromises.

9.2.2. Uncertainty propagation methods

The American Society of Mechanical Engineers [82] and Électricité de France [150] have separately attempted to evaluate, and categorize the multitudinous sources of uncertainty in CFD simulations. Figure 13 illustrates the various sources of uncertainty that may arise within a given CFD simulation (details are taken from Ref. [150]). Note that not all the sources listed above have been represented. The colour scheme of the boxes has been chosen as follows:

— Blue fields represent the parameters fixed by the associated V&V procedures: i.e. the optimum turbulence model to be used, wall boundary laws, etc.
— Green fields denote inlet and boundary conditions.
— Orange fields show the relationship between the mesh and the numerical options available in the CFD code.

Note that CFD model uncertainty evaluation cannot be avoided through any route depicted in this figure.

In the context of CFD, UQ is always going to be challenging because of the computational power needed to perform multiple parallel simulations. Nonetheless, the foundations have been laid, based on previous experience (derived principally from system codes in the NPP simulation context), in the expectation that the necessary computing power will eventually become available. Notwithstanding the obvious disadvantages associated with UQ procedures in CFD, there are clear advantages in comparison to multiphase, system code applications. The most important are the following:

— Single phase CFD simulations incorporate relatively few physical models (i.e. turbulent viscosity and turbulent Prandtl number, wall functions, etc.), whereas multiphase, system code simulations include a large number of empirical closure laws for wall heat transfer, interfacial momentum and heat transfer for a multitude of flow regimes. Many of these depend on details of the flow geometry, which are not represented accurately in system codes.
— Single phase CFD simulations have multiple options for the non-resolved physical models, particularly turbulence models (e.g. k–ε, k–ω, RSM, SST, RNG k–ε, LES, DES), with guidance from BPGs on which model to use in particular circumstances. On the other hand, system codes generally propose just one set of standard closure laws.
— Single phase CFD tools incorporate multiple options to ensure numerical convergence, whereas system codes generally promote just one option (CATHARE, ATHLET, TRACE) or at most two

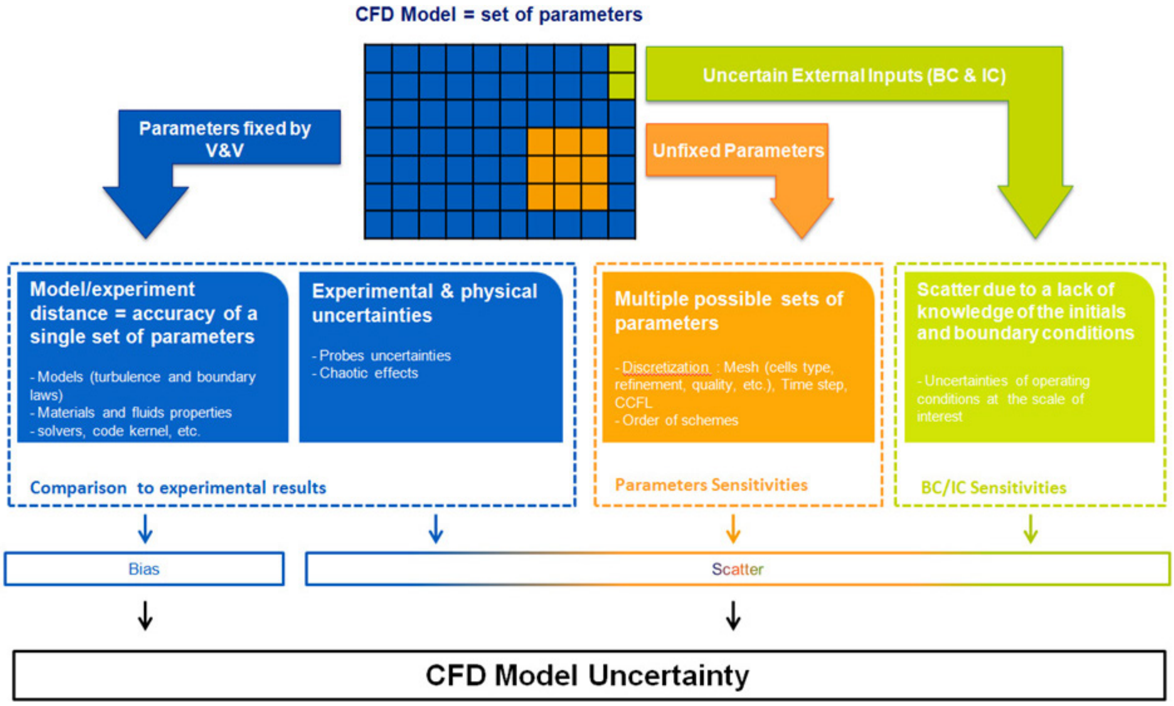

FIG. 13. Identification of sources of uncertainty [151].

(RELAP-5 and TRAC). The degree of convergence is also controlled better for CFD, since a backward-time 'differencing' is invariably applied, with internal iterations to ensure that truncation errors are minimized (this may not be true for direct numerical simulation (DNS) approaches). There is also the option currently of automatic mesh refinement to limit spatial differencing errors, which are monitored and subsequently controllable. Finally, the application of BPGs is now well established in CFD, which, if strictly observed, will ensure that the desired level of numerical convergence has been achieved.

— Single phase CFD codes do not involve a comprehensive validation matrix for each set of physical options, whereas for system codes a very large validation matrix is needed to gain confidence in the large number of closure laws needed for a typical two phase simulation.

The major drawback with the application of UQ to CFD is the associated computational overhead, which is the reason for its limited use (to date). The methodologies established within the essentially 1-D realm of system code analyses are often just too expensive to be applied to 3-D CFD applications. Typically, 100+ parallel simulations are needed in addition to each base CFD simulation to quantify the influence of the various uncertain parameters. This remains something for the future, except in grossly oversimplified situations. Nevertheless, the appropriate methodologies have emerged from 1-D system code simulations, since it is foreseen that these will form the bedrock of the UQ approaches within the CFD domain once the current computational restrictions have been lifted, or at least partially lifted.

9.2.3. Methods based on propagation of uncertainties

The methods using propagation of code input uncertainties follow the pioneering idea of scaling, applicability and uncertainty set out in Ref. [155]; the ideas were later extended by Global Research for Safety, in Germany [156]. This represents the approach to UQ used most often in the nuclear context. First, those input parameters judged to be of significant influence for the results of the simulation are listed: these include initial and boundary conditions, material properties, and (particularly) closure laws. Probability density functions (PDFs) are determined for each input parameter. Then the parameters are progressively sampled according to their PDFs, and simulations performed for each set. Global Research for Safety has proposed an extension in which a Monte Carlo sampling would be performed, with all input parameters varied simultaneously according to their respective PDFs.

Since the number of ancillary simulations would quickly get out of control, the Wilks Theorem is generally employed — a standard approach in statistics for assessing the log-likelihood ratio of two different events of statistical importance in order to bypass the least likely event [157]. Nonetheless, at least 100 code runs would need to be performed to reach an acceptable degree of confidence in the numerical predictions; in many cases, 150–200 code runs would be required.

With regard to uncertainty propagation methodologies, three principal themes have emerged:

(1) The Monte Carlo approach requires a large number of simulations to be carried out in which all uncertain input parameters are sampled according to their individual PDFs. The resulting PDF of the base code prediction is thereby obtained; the accuracy of the assessment does not depend on the number of uncertain input parameters.
(2) A second approach is the use of so-called meta models. This is an attempt to reduce the total number of code simulations by considering only the most 'influential' uncertain input parameters [151]. These methods demand fewer calculations for building the meta-model that is subsequently used as part of a Monte Carlo analysis to determine uncertainties. A typical example of this approach is the use of polynomial chaos expansion techniques. However, predicted results will ideally be viewed with some caution, since the underlying assumptions of regularity and continuity of model responses is not always justified [151].
(3) The third approach is to use deterministic sampling. Here, no attempt is made to propagate the exact PDFs, but rather to use statistical moments. For example, if only the first two moments are known (i.e. mean values and standard deviations), the uncertainty is deemed to be represented by these two moments alone. Then, given that four moments are required to produce a bona fide Gaussian distribution, higher order moments are added by considering so-called marginal simulations. This method avoids performing too many additional simulations, but one always has to justify the authenticity of the sampling, which often needs to be weighted according to a non-rigorous evaluation procedure.

Uncertainty propagation methods require considerable preliminary work, particularly using results from SETs and IETs. But, as has already been emphasized, such a database of experiments is in itself somewhat lacking in the context of even single-phase CFD, since the closure models are not as expansive or adequately documented as for two phase system codes. In summary, though the strategies for the application of UQ in CFD nuclear design applications derive from the advancements made in system code analyses, one cannot be overly confident in the methodology.

To make economies on the required computational effort, some short-cuts are currently being investigated. For example, though the base run has to be undertaken with strict adherence to BPGs, subsequent runs within a Monte Carlo methodology could be performed using coarser meshes, relaxed numerical convergence criteria, larger time steps, etc. Obviously, this approach is for the pragmatist, and not the purist, which is why some care is needed in its application, together with a measure of user experience.

9.2.4. Accuracy extrapolation methods

These methods, which were also developed in the context of 1-D system codes, are based on the concept of propagation of code output errors based on extrapolation of accuracy. The most popular approaches are uncertainty methodology based on accuracy extrapolation [158] and CIAU [159]. Both rely on extensive SETs and IETs, which have previously served to judge the accuracy of code predictions in a wide variety of situations.

In both approaches, a metric for accuracy quantification is defined using Fourier transforms. The experimental database includes results derived at different scales, and once the accuracy of the code predictions is assumed not to depend strongly on scale, accuracy is extrapolated to reactor scale.

For CFD, the ASME V&V20 guidelines state that “the concern of V&V is to assess the accuracy of a computational simulation” [82]. This view is clearly compatible with extrapolation from validation experiments. In current industrial (non-DNS) CFD applications, results derive from solving a subset of the Navier–Stokes equations, supplemented by modelling those parts of the calculation that cannot be simulated directly due to problems of scale representation, in particular, fully developed turbulence. Verification of the equations — called solution verification by Oberkampf and Roy (2010) [160] — can still be considered ‘tractable’, even for some complex flow configurations. Beyond that, however, physical model uncertainty becomes of genuine concern.

Overall, UQ approaches based on extrapolation of validation data represent a rather poor mathematical description of the concept, but the comparison with reality offered, even in scaled experiments, may still give an idea of the impact model inadequacy will ultimately have on code predictions, even those at full scale. Nonetheless, extrapolation of UQ data obtained from scaled experiments to full scale will remain open to challenge.

9.2.5. Comparison of methods

One difference between the methods based on propagation of uncertainties and extrapolation from scaled information is the possibility of performing sensitivity analyses. Propagation methods allow such analyses to be carried out using data from previously performed uncertainty calculations, but this luxury is not afforded to methods based on extrapolation, for which individual contributions to the overall uncertainty cannot be identified.

The UMS [161] and BEMUSE [150] projects, initiated by the OECD, have resulted in an acceptable degree of maturity of UQ methodology for system codes, even though the quantification of uncertainties of the closure laws still remains challenging for propagation of uncertainty methods. However, it is to be remembered that the move to derive a best estimate of uncertainty quantification for 1-D system codes is nearly 50 years old, a period that has witnessed unparalleled advancements in computer hardware technology. Though the development of general purpose CFD codes stems from this same period, the computational overhead associated with even a single CFD run is far greater than for the system codes (more so for transient simulations), and all the UQ approaches, which inevitably involve multiple code runs around a specified base case, thereby remain in their infancy. It is not the UQ methodology that is missing. it is simply a question of lack of computing power. Nonetheless, a test case for CFD in the form of a benchmark exercise has been attempted, sponsored by the OECD (see Section 9.3).

Overall, though the methodology has firm foundations, due to CPU limitations the level of maturity of UQ in CFD is still extremely low. Initially, progress has to be made in the context of very simple single phase test cases to gain experience. Such an exercise is described here.

9.3. THE GEMIX BENCHMARK

As part of the UQ initiative promoted by the OECD and linked with the international series of CFD conferences under the acronym CFD4NRS, a very simplified mixing experiment, GEMIX (Generic Mixing eXperiment) was carried out at the Paul Scherrer Institute in Switzerland in 2015–2016. This involved the turbulent mixing of two horizontally stratified layers in a square channel geometry (50 × 50 mm) under isokinetic conditions. The experiment was well instrumented in the mixing region (see Fig. 14), but for the original tests the specification of the inlet conditions (i.e. mean velocity profiles and turbulence levels) had not been measured; only the overall mass flow rates to the upper and lower channels were available. This deficiency was partially corrected for the subsequent exercise that would form the basis of an international uncertainty analysis benchmarking activity.

Blind benchmark conditions were imposed for the base test by making the upstream test specifications available to participants in advance, together with precise geometric details of the flow configuration. However, the downstream measurements were kept secret until the CFD simulation results had been received by the benchmark organizers and assessed. Nonetheless, in support of the extrapolation methodology of UQ, both upstream and downstream data were supplied to participants, derived from similar tests in the same facility [68].

The GEMIX test was conducted under very simplified conditions of isokinetic flow in each inlet channel under conditions of stable density stratification. Nonetheless, the exercise was still challenging. A more detailed view of the test configuration is presented in Fig. 15.

As shown schematically in Fig. 15, the two liquid streams are initially separated by a splitter plate in the inflow section. Both streams pass through identical honeycombs and grid structures to minimize the rotational components of the velocity field and to promote the generation of narrow boundary layers. The only difference between the streams is the 1% density increase of the lower stream, to provide stably stratified conditions for the test. The density gradient in the mixing streams has practical significance in many NPP design issues. As the two streams pass over the tip of the splitter plate, they merge with one another and form the mixing layer, which widens downstream. The main objective of the benchmark was that participants were expected to provide mean velocity, turbulent kinetic energy and concentration profiles at selected downstream locations, given only the upstream conditions. Since some UQ methodologies require information concerning measured data from similar tests, information from three similar open tests were provided to participants in advance.

It has to be emphasized from the outset that though the methodology of UQ in the CFD context derives from the experience gained using system codes, each CFD predictive simulation might require orders of magnitude additional computational effort to produce results of similar reliability.

Several flow tailoring devices were installed in the two inlet channels: a honeycomb, two identical coarse grids and a single fine grid, to ensure that the two streams meeting at the splitter plate tip are free of rotational components. Each inlet channel was supplied with the same volumetric flow rate,

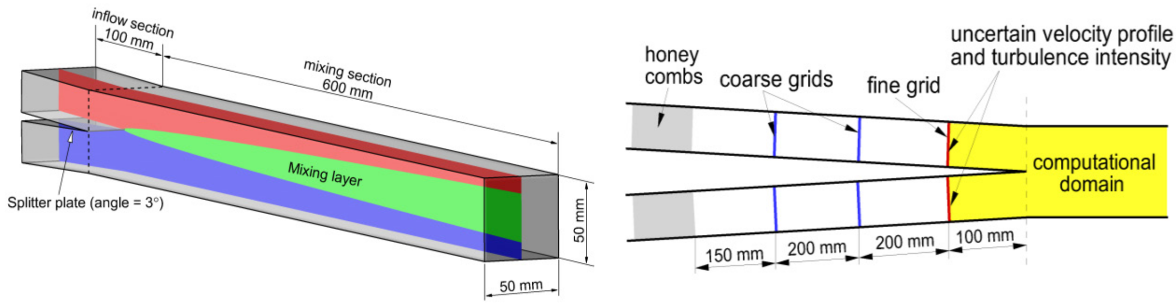

FIG. 14. Schematic of the GEMIX test section [68].

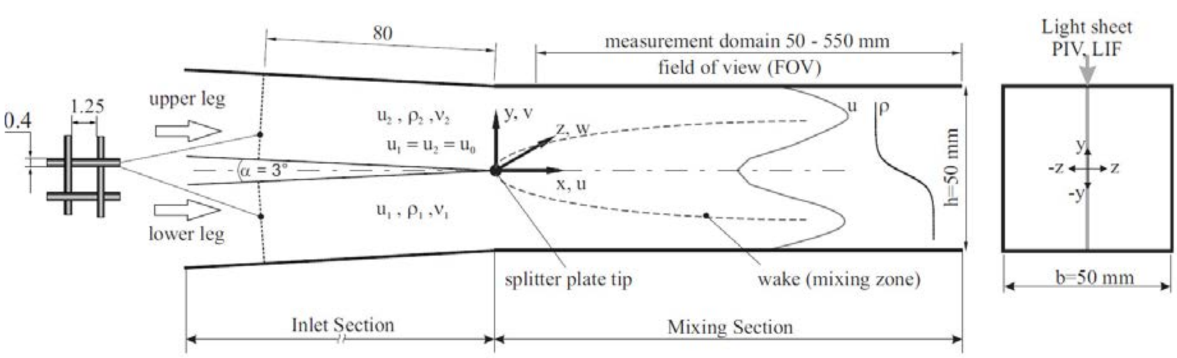

FIG. 15. Details of the GEMIX test section [68].

though at different densities. Advanced instrumentation techniques were used to measure the inlet flow conditions precisely: PIV; LDA; and laser induced fluorescence (LIF). In addition, WMSs were installed in the mixing region to measure concentration levels. Note that since WMSs are intrusive, only one was installed at each downstream measuring location (50 mm, 150 mm, 250 mm, 350 mm, 450 mm), which meant that multiple, notionally identical, tests had to be carried out for each WMS station.

In such an exercise, it is imperative to quantify the measurement uncertainties, which was done. For example, the volumetric flow rates to the separate channels were judged to be accurate to within ±0.15%, a credit to the experimental team. The error in the density measurements was estimated at ±0.01%. The relative error corresponding to the isokinetic assumption was ±1.0%. The CFD predictions need to lie between these experimental uncertainty bands to be considered accurate. The major discrepancy lies with the predicted and measured levels of the turbulent kinetic energy (TKE), which was consistently underpredicted: no satisfactory explanation has been forthcoming. For the measured data, more effort is required in estimating the uncertainties associated with changes in refractive index for streams of different densities. Consequently, TKE predicted levels were excluded from the ranking process of the blind simulations.

As mentioned above, in the original GEMIX tests, only mean flow rate data were available for the upper and lower inlet channels. More precise data were made available for the benchmark exercise. As a consequence of limited optical access, mean velocity and RMS profiles were measured in just one quadrant of the upper inlet channel (see Fig. 16).

Symmetry arguments were used to provide information in the other quadrants, both for the upper and lower channels. Since the volumetric flow rates were identical, as well as the flow geometries, this was considered a reasonable assumption. Note that, as a consequence of the set-up, all three components of the velocity fluctuations cannot be measured simultaneously within one test run.

There were 21 registered participants in the benchmark exercise: all received the specifications and measured data files relevant to the tests. Of these, 13 participants from 9 countries were able to submit results within the time frame of the exercise. Of these, four were from France, two from the USA, and one each from the Republic of Korea, Netherlands, Poland, Russian Federation, Spain, Sweden and the United Kingdom. From these submissions, conclusions were drawn by the organizers concerning applications of this type.

Surprisingly, since this was the very first, and international, UQ benchmark activity of its kind undertaken in the CFD domain relating to NPPs, there was a scattering of results that was very large, which is quite encouraging. All the submissions were ranked according to the maxims of the benchmark

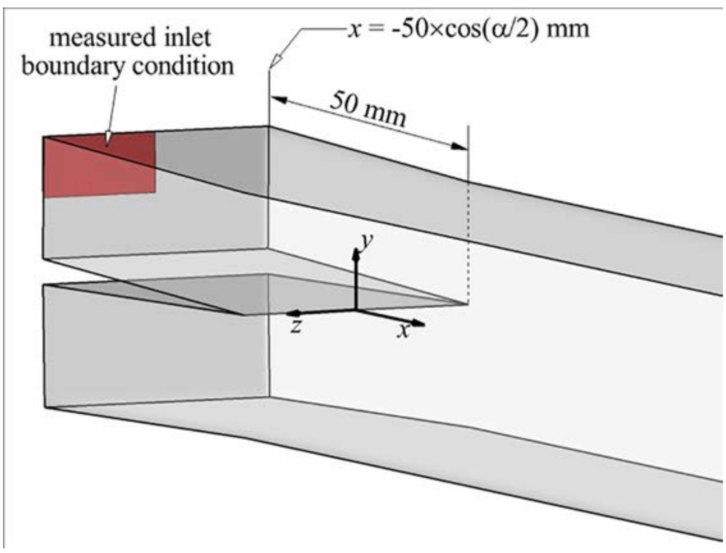

FIG. 16. Location of LDA measurement plane in a quadrant of the upper inlet channel [68].

organizers. The details of the ranking procedure are not included here, but the interested reader is referred to the definitive report on the activity [68]. Of the most highly ranked submissions, the number of ancillary simulations employed to complete the UQ analysis was astonishingly wide, ranging from 4 to 836. This difference requires further investigation, since it is likely significant savings could be made on code runs in the future. Most participants employed RANS turbulence models: the most popular were variants of the k–ε model (5), k–ω (4), RMS model (1), though LES was also featured (2), and surprisingly required only 22 parallel simulations to produce meaningful UQ results.

Of the 13 participants included in the synthesis, ten relied on a single propagation step, while the other three used extrapolation plus propagation. Of those using the propagation approach, four used polynomial chaos expansions, two used a Monte Carlo approach, and two used deterministic sampling.

The principal source of discrepancy between experiment and calculation concerns the TKE levels, for which the measured values were significantly larger. Similar trends have also been noted in the two active benchmark exercises associated with the present CRP [1, 2]. Nevertheless, results from the GEMIX benchmark are encouraging, and seem to indicate that the methodology taken over from the system code applications is respectable and trustworthy within the CFD context. One advantage with CFD is the use of BPGs [129], which, if properly applied, will mitigate, to a certain extent, the uncertainties associated with numerical errors in the solution procedure. This is generally not true for system codes.

As with the earlier PANDA benchmark [162], LES did not provide any advantage over the RANS model approach, though its application was vital in producing good results for the earlier T-junction benchmark [123], also sponsored by the OECD. Two users provided data from 2-D rather than 3-D simulations, but these proved not to be very successful.

It is to be noted that the uncertainty bands obtained from the GEMIX benchmark (±2 standard deviations) do not conform to the rigours of NPP safety philosophy, for which uncertainty bands are constructed from confidence intervals of (5%, 95%). This issue will need to be addressed in investigating UQ methods in CFD for NPP design purposes (as well as for safety considerations), and for each of the advanced reactor types, for which it is anticipated that UQ methods in CFD simulations will be more strictly applied than for the Gen II situations reported here.

In summary, this first of a kind blind international CFD UQ exercise produced better results than expected. Though the flow configuration was deliberately oversimplified, several important physical processes were still represented: stratified flow and turbulent mixing of parallel streams, which is of interest in many NPP applications, e.g. above core mixing. Exceptionally well qualified experimental data were provided, derived from advanced measuring techniques — LDA, LIF, PIV, WMS — which formed the basis of the subsequent numerical comparisons.

The benchmark synthesis team even proposed a new measure, fidelity, which may help with the assessment of results of future CFD UQ exercises: namely, the convolution of the probability distributions of a predicted value and the corresponding experimental value, both assumed to be Gaussian. They also identified four essential components of a successful CFD UQ analysis: uncertainty identification, calibration, extrapolation and propagation.

9.4. CONCLUSIONS

By definition, CFD is a best estimate methodology, so numerical results derived from its usage has to be accompanied by UQ to be regarded as meaningful in NPP design and safety issues. However, the advancement of UQ for CFD simulations has been severely hampered by the computational overheads associated with a typical CFD computation. UQ methodologies have been developed over many years in the context of the recognized system codes, but these are essentially 1-D in origin, and the CPU demands of even a single 3-D CFD run are orders of magnitude greater. As illustration, a typical system code ‘nodalization’ of an entire NPP primary circuit might consist of several hundred hydraulic volumes and junctions, while a CFD simulation of just one component of such a circuit would involve tens of millions of control volumes. The major computational effort in a CFD simulation is associated with the inversion of the solution matrix which, though sparse, is very large, and certainly not tridiagonal, given the typical differencing schemes employed in representing the basic equation set. In addition, system codes generally require just one step for time advancement (forward time differencing), whereas CFD invariably involves backward time differencing, which entails a number of internal iterations before the time step can be updated. Not surprisingly, progress has been slow in the application of UQ to CFD predictions.

The three principal methodologies, derived from system code UQ studies, have been outlined in this section. All involve multiple numerical simulations of the base case in order for code predictions to be considered reliable, given the individual uncertainties associated with the models and numerical procedures employed in the calculation; typically, 100 or more parallel runs. This computational overhead is totally unfeasible in the CFD context, except for highly simplified flow situations. Nonetheless, a start has been made with the blind GEMIX benchmark, which involves the isokinetic mixing of two parallel, 'stably stratified' streams in a square channel. Highlights have been included in Section 9.3. Overall, results are quite encouraging, given that this represented a first of a kind international UQ exercise relevant to NPP design and safety issues.

No doubt, further progress in the subject will be made in the near future, in parallel with advances in CPUs and machine architecture and, probably to a lesser extent, more efficient software algorithms. However, it seems the methodology for the application of UQ to CFD predictions is well in place, and further benchmark activities of the type represented by the GEMIX exercise will increase confidence in the application of the technology.

10. GAPS IN COMPUTATIONAL FLUID DYNAMICS TECHNOLOGY APPLIED TO NUCLEAR POWER PLANT DESIGN ISSUES

10.1. VERIFICATION AND VALIDATION

Any CFD assessment matrix for a given application requires three groups of items:

— Verification problems, in which code predictions are compared against analytical solutions (there are not many in fluid dynamics) or against 'highly accurate' solutions derived by independent means;
— Highly instrumented validation experiments (SETs) and associated CFD simulations;
— Demonstration simulations, possibly with some suitable supporting experiments (IETs).

Identification of gaps in the assessment matrices for a given application is possible only after thorough examination of the corresponding exact solutions and experiments and their CFD counterparts has been undertaken. The verification exercise, i.e. to check whether the relevant coding is free of 'bugs', is primarily the responsibility of the code developers, though independent checks can be carried out; for example, using the ERCOFTAC database [163]. Code verification activities can be further subdivided into numerical algorithm verification, and software quality assurance practices. There is a hierarchy of confidence in the 'highly accurate solutions' that have been assembled over the years [5], ranging from exact analytical solutions and/or the application of the method of manufactured solutions [164], in which artificially produced benchmark solutions are created by adding algebraic source terms to the governing equations to satisfy an artificial situation for which the analytical solution is already known. One simply feeds the solution into the differential terms to determine the source terms that have to be included on the right hand side of the equations for them to represent the given solution; attention has to also be paid to the boundary conditions. Since no differential terms are added, potentially changing the characteristics of the governing equations, the approach is attractive, and often rewarding, since it adds a new component to the verification process. Specified source terms (and perhaps artificial boundary conditions) are programmed into the code during this exercise.

Not all CFD computer codes (principally the commercial ones) provide access to the source modules to those users developing their own physical models, but adding algebraic source terms is usually not a problem, and the commercial CFD codes (e.g. ANSYS-CFX, ANSYS-FLUENT, STAR-CCM+) provide the necessary means to do this. For open source programmes, such as OpenFOAM, such access is in any case totally transparent.

Analytical solutions (closed solutions in the form of an infinite series, complex integrals and asymptotic expansions of the governing partial differential equations represented in the conceptual model) are the basic tools of the verification procedure. Typically, for CFD, the database consists of inviscid or laminar viscous flows in simple geometries, so only limited features of the CFD computer codes (or, more precisely, of the conceptual models) can be verified in this way. The verification process has to be considered 'open', in that new trustworthy data have to be made available for comparison as new numerical models are introduced into the CFD codes, for example in the context of application to possible Gen IV reactor design concepts, such as supercritical reactors (not considered within the present project), for which the underlying physics is still not fully understood, or reliably modelled.

The application of numerical benchmarks to underpin the assessment procedure requires thorough and well-documented verification of code performance in simple cases, comprehensive numerical error estimation, and accurate calculations of the same base cases, via independent experts, preferably using different numerical approaches and computer codes. There is, however, a tendency to use some SETs not only for the development and validation of the physical models, but also for conceptual model verification. Here, similar requirements to those related to numerical benchmarks have to be met, not only by the computational solutions but also by the quality of the experiments themselves, which need to involve highly resolved data measurements necessary for CFD validation: for example, inlet conditions and data relating to resolved wall boundary layers. Only well designed, well executed and fully documented experiments will ideally be used to advance understanding and model development. Such a scheme represents in fact an interface between the verification and validation procedures.

The primary responsibility for a numerical algorithm verification procedure will ideally be placed upon the code developers, though code users also have to have access to the relevant (and adequately documented) information. In most cases, this is a status now clearly recognized by the code development teams, whom, it is to be remembered, are in direct competition with each other in the commercial CFD world. With this more open approach to V&V, this particular technology (or information) gap is closing rapidly.

Basic verification problems in CFD are limited to very simple geometries and involve a restricted number (preferably one) of the important physical processes involved in the flow characterization; supporting experiments are frequently aimed primarily at the development of the physical models embodied in the code. Validation of a conceptual, physical model within a particular CFD code would need to start at this level. Repeated experimental runs are required, to ensure that systematic errors in measurement data can be identified and eliminated. All the important code input data, especially initial and boundary conditions, can, in principle, be accurately measured in advance of the actual test, though often this has not been undertaken. In some cases, multiple CFD computations are needed to enable confidence in the output quantities to be established as a consequence of a lack of precise input specifications. Possible technology gaps arise as a consequence of: missing significant flow information (e.g. the location of boundary layer separation); precise measurement of such parameters has been performed but at unsuitable locations; measurement error analysis is missing or has been ignored; and, in the CFD simulations, important data items are missing (e.g. turbulent kinetic energy levels at input) because it was not possible to measure them directly at the levels required during the experiment, often due to optical access limitations.

Turning to validation benchmark cases, these typically involve only two or three types of flow interaction mechanisms, but in more complex geometries than for idealized verification tests and involving more complex physics. Possible technology gaps in this context are similar to, though requiring more computational capability than, those encountered in the verification exercises: e.g. demonstration of grid independence of the CFD solution.

For practical NPP design simulations involving CFD, grid independence cannot be guaranteed in the majority of cases as a consequence of the computational overhead involved. However, this situation will ideally improve with advancements in computer hardware technology and more efficient software algorithms. As a result, this particular technology gap is expected to close rapidly. Furthermore, it is often impossible to trace the origin(s) of differences between measured and computed data in validation tests (SETs or IETs) simply because it has not been possible, through earlier V&V exercises, to estimate how closely the conceptual model simulates reality in the given context.

Generally, with the current status of computer hardware, it is computationally not possible to model the entire primary NPP system using CFD alone. Hence, there is a need to couple the well-established and well-validated system codes, which have been specifically constructed to model the entire NPP circuit, with detailed CFD simulations of specific components for which 3-D modelling is necessary, such as in the case of pumps, heat exchangers, core subchannels, etc. Verification and validation of such coupled code approaches is more complicated than that for the CFD or system codes individually. The coupling methodology itself can often be a source of additional error. The validation of the coupled code system will ideally be able to detect any such errors, if they are indeed present. The unsteady nature of many of the NPP design issues requiring numerical analysis ahead of experimentation, makes such identification considerably more difficult than for steady state situations. This field warrants more extensive research before application of such coupled code approaches becomes a matter of routine.

10.2. RANGE OF APPLICATION OF TURBULENCE MODELS

CFD simulations of NPP design issues will inevitably involve strongly turbulent flow conditions, and the need to apply the most reliable turbulence model for the specific application will always be required. The turbulence research community has assembled and classified a large selection of generic flow situations over the years (jets, plumes, flows through T-junctions, swirling flows, separated flows, etc.), and BPGs have been assembled to provide guidance on which turbulence model(s) is/are most appropriate to a particular simulation case. As emphasized several times, currently CFD is not capable of modelling entire reactor systems, which means that sections of the system have to be isolated for detailed CFD analysis, where this becomes necessary. The range of scales can be large (e.g. in containments), and/or the flow phenomena can be rather special (e.g. ECC injection relating to PTS and boron dilution issues), or simply be used as an aid to spacer grid design in core bundles. It is necessary to extend the database of recognized flow configurations to include those particular to NPP applications of CFD and build a suitable validation base to fine-tune the modelling approach.

In most industrial applications of CFD, two equation RANS models of turbulence (e.g. k–ε and k–ω) are still employed some 50 years after their initial development [165]. The reason is simple: the models are robust and computationally efficient (in the CFD context), and, when used in accordance with BPGs [129], can be trusted to give reliable predictions. However, due to the averaging procedures involved, valuable local flow information will often become lost. A case in point relates to thermal fatigue in T-junctions. A comprehensive study carried out by the OECD in collaboration with Vattenfall [123] showed that only LES models of turbulent behaviour were capable of capturing the relevant flow phenomena and, hence, the thermal fatigue characteristics. However, application of LES is an order of magnitude more computationally demanding than using RANS models, so any decision to employ this particular turbulence model needs to be justified. What is needed is a screening of NPP design applications and BPGs on which particular turbulence model to apply in a given situation, both in terms of efficiency and accuracy. This is an ongoing process.

Advances are also being made with respect to the formulation of non-isotropic turbulence models. The most complex are second moment closure (SMC) models [166]. Here, instead of two equations for the two principal turbulent scales, the solution of seven transport equations for the independent Reynolds stresses that make up the definitive stress matrix, together with one length (or length related) scale, is required. The challenge for the user of CFD codes is to select the optimal model for the application at hand, and the least computationally demanding, from the different models available. It is not a trivial task to provide general rules and guidance for the selection and use of specific turbulence models for complex applications. Two-equation models often offer a good compromise between complexity, accuracy and robustness, but definitive guidance in the form of BPGs will always be required, backed up of course by data from appropriate experiments. There has also been some progress in the development of non-linear k–ε models [167] to relax the assumption of isotropy of the turbulent motions. This approach needs to be further explored.

In particular, a significant weakness of the present two equation RANS turbulence models is that they are insensitive to streamline curvature, boundary layer separation, and induced rotation [168]. Particularly for swirling flows, this deficiency can lead to over-prediction of turbulent mixing and to a strong decay of the core vortex in swirling flow simulations. Curvature correction models are now becoming available [169], but lack comprehensive validation data for complex flow situations. In contrast, SMC models, which need to be more reliable in such circumstances, are much less robust numerically. A standard modus operandi for their use is to first perform simulation based on the robust k–ε model and use this as a starting point for the detailed SMC solution. However, such an approach is hardly feasible for transient simulations, which are often required for NPP design applications.

The first alternative to RANS is URANS and to LES it is VLES (very large eddy simulation). The former is more descriptive of the actual technique of application, i.e. to carry out an unsteady RANS analysis even if the boundary conditions are steady. Thus, if a steady state RANS calculation does not converge, it may be that some intrinsically unsteady behaviour is present in the flow, such as periodic behaviour, plume or jet meandering, vortex shedding, etc. A URANS calculation can often identify the unsteady component, but it has to be remembered that averaging over all turbulence scales remains implicit in the method and may not be appropriate to reliably capture all the important non-steady phenomena. A situation in point is when a straightforward RANS approach leads to a falsely averaged solution, and a URANS, LES or DES model would be more appropriate. This situation often manifests itself in the form of non-convergence of the residual errors. This can occur as a consequence of poor mesh construction or of non-steady physical phenomena relating to turbulent behaviour not being captured by the model applied. Prime examples here are flows in T-junctions, and in lower plenum flows.

The amount of information provided by the turbulence model can be reduced if the large time and length scales of the turbulent motion are resolved explicitly. In LES, the equations are filtered, rather than simply averaged, usually with respect to the grid size of the chosen computational cells. All scales smaller than that provided by the resolution of the mesh are modelled using a suitable subgrid scale (SGS) model, and all scales larger than the cells are computed explicitly. Away from boundaries, LES appears attractive, even with very simplistic SGS models, such as that of Smagorinsky [170]. The base maxim with LES is that the major turbulence energy cascade process is being computed directly, including all the complexities of non-steady, non-isotropic flow characteristics, while only the much smaller scale dissipation processes need to be modelled. It is argued that these small scale processes are geometry independent, and can be represented by an oversimplified, isotropic turbulence model, with more justification than in the case of RANS models, for which averaging over all scales is implicit in the method. Several SGS models have been proposed which are much cruder than those associated with RANS approaches, but are still adequate [170]. But problems remain in the modelling of wall regions: pure LES becomes very inefficient due to the need to scale the lateral dimensions in the same way as in the normal direction just to capture the smaller scale eddies. This is not necessary in RANS because the flow parallel to the wall changes much less abruptly than in the normal direction, and an appropriate model has been formulated accordingly, i.e. with the use of wall functions [171]. Also, lack of sophistication of the SGS models may be tolerated in the bulk flow, but near walls the SGS stresses become much more important and need to be accounted for with increasing accuracy.

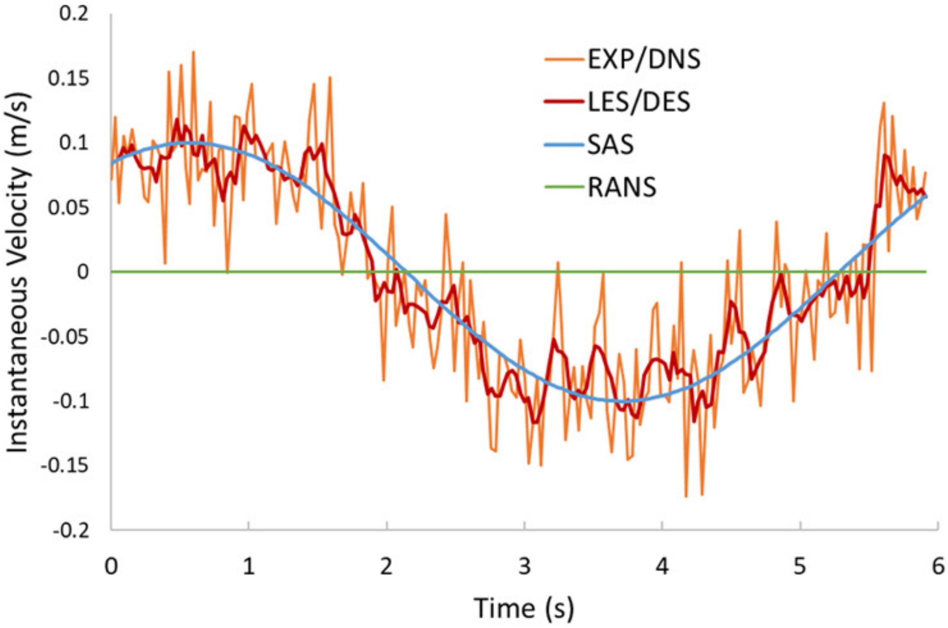

FIG. 17. Representation of instantaneous velocity by turbulence models.

An alternative is to entrust the entire boundary layer treatment to a RANS model for the 'attached' eddies, and only use LES away from the walls, where the eddies are 'detached'. This approach has become known as detached eddy simulation and is employed principally in the aerofoil industry [172]. DES provides considerable savings in CPU time over traditional LES approaches. The case for continued use of LES in near-wall regions, probably in combination with a more complex SGS model, has to be judged in terms of the possible loss of information from using DES against the extra computational effort involved in attempting something more exact, such as DNS. Again, this remains an active research area, of some relevance to NPP design, but probably emphasized somewhat less compared with other industries, in which precise boundary layer modelling is a paramount consideration.

The SAS model is a hybrid approach similar to DES but it functions without an explicit grid dependency. The controlling parameter is the ratio of the turbulent length scale L, for example, derived from the two-equation *k–kL* RANS model of Rotta [173], and the von Karman length scale (LvK), which is determined in the usual way from the first and second velocity gradients. In regions where the flow tends to be unstable, LvK is reduced, increasing the length/scale ratio L/LvK. This leads to a reduction in the magnitude of the eddy viscosity. The flow will become more unstable, and hence transient in these regions, with vortices down to the scale of the local grid size being resolved explicitly, resulting in LES like capture. In stable flow regions, LvK remains large, which leads to high values for the eddy viscosity. In these areas, the model acts like a RANS model. Due to the model's ability to resolve the turbulent spectrum, it is termed a 'scale adaptive simulation' model, hence the name. It has similarities to the DES model, but has the advantage that it is not based on the local grid size and therefore avoids grid sensitivity issues. However, the SAS turbulence model has proved to be inadequate for the OECD T-junction benchmark [123] and needs to therefore be used with caution.

Figure 17 illustrates how each of the different approaches to turbulence modelling is expected to capture an instantaneous velocity signal, either measured experimentally, or calculated via a detailed DNS.

As a general observation, LESs do not easily lend themselves to the application of grid refinement studies. The main reason for this is that the turbulence model adjusts itself to the resolution of the grid. Two simulations on different grids may not be compared using asymptotic expansion techniques as they are based on different levels of eddy viscosity and, therefore, on a different resolution of the turbulent scales. From a theoretical standpoint, the problem can be avoided if the LES model is not based on the actual grid spacing but on a pre-specified filter width. This would allow grid independent LES solutions to be obtained. This can be done in phase space, though to date only in simple geometries, but the concept is important enough to be further explored.

10.3. STRATIFICATION AND BUOYANCY EFFECTS

Buoyancy forces develop for heterogeneous density distributions in the flow field, caused by differences in temperature or concentration levels. Many important events related to NPP design involve thermally stratified flows, which result from differential heating (e.g. in heat exchangers), or from incomplete mixing of flows at different temperatures (e.g. thermal stratification). For single phase flows, there are important stratified flow conditions developing in the case of PTS, for hot leg heterogeneities, and for conditions for promoting important natural convection phenomena. The issue with hot leg stratification is particularly relevant for reactor design, since the core outlet temperature is invariably used as an input variable for monitoring core performance. Specifically, if the flow is stratified, and the measurement is made in the 'wrong' part of the flow field, misleading information could be fed back to the plant operators, and erroneous decisions could be made for core control.

In many cases, the issue is to derive a modelling strategy which is able to handle all the situations of relevance to NPP design, and suitable operational parameters to be defined appropriately. These complex phenomena are difficult to take into account (and justify) using a 1-D system code approach alone, and CFD is often needed, in particular, to estimate the mixing rate between flows at different temperatures, often controlled by 3-D fluid phenomena. Further, situations may exist in which thermal stratification may limit, or even suppress, the role of turbulent exchange processes affecting heat and momentum transfers, while buoyancy may, in some cases, actually promote turbulent mixing; e.g. in thermally unstable configurations.

For example, the standard $k–\varepsilon$ model is known to poorly accommodate mixing in strongly buoyant situations, and more complex closures (e.g. RSM) may then be proposed for obtaining satisfactory results [172]. Unfortunately, RSM is much less robust that the pure RANS $k–\varepsilon$ or $k–\omega$ models, and it may be difficult, or even impossible, to obtain converged solutions in situations involving complex geometries. One further troublesome issue is the application of standard wall functions [171] in cases where there are strong buoyancy effects. This also remains an active research area. In some cases, in addition to the mean flow conditions, details of the thermal fluctuations are also needed, including their spectral distribution (which is a central characteristic for thermal fatigue issues). This remains a challenge, especially in cases where instability is due to buoyancy (e.g. heating from below in narrow channels).

10.4. COUPLING SYSTEM/COMPUTATIONAL FLUID DYNAMICS CODES

This remains an active research area, since NPP simulations using CFD alone are, in the majority of cases, beyond the capabilities of present computer hardware. Use of a less detailed, though less computationally demanding, system analysis code to produce initial and boundary conditions for a localized application of a CFD code appears to be the only practical alternative. Such multiscale coupling is indispensable in the case of demonstration simulations, examples of which are provided in Table 4, as it is, of course, in the application of a CFD code to many other industrial scale problems. It is frequently necessary to simulate not only the thermal hydraulics, but also phenomena belonging to different fields of physics, such as water chemistry.

If the system code is used to supply 'inexorable' boundary conditions to the CFD code, meaning that the boundary conditions do not change as a consequence of any feedback from the detailed CFD simulation predictions, the approach is quite straightforward, and indeed good progress has already been made using this approach [174]. However, the issue of V&V for the coupled code system — even if there have previously been extensive V&V exercises performed for the two codes separately — still needs to be addressed. In particular, the associated V&V tests will have been carried out at very different time scales, and to match these at an interactive level may require some new experiments. A start has been made, but to date at a rather academic level [175]. More effort is needed, including suitable data from IET and SET experiments, to put the technology on a firm basis. Particular issues will often be very design specific, so a general approach, involving non-proprietary test data, might be difficult to obtain, and document.

An example of the extensive research already being carried out in the field of code coupling is the development of a methodology for coupling of the RELAP5 and RELAP5-3D codes to different CFD codes, as described in Refs [176, 177]. The standard approach is to couple the separate codes through an executive program, based on a generic coupling methodology, but this has now been replaced by a semi-implicit coupling, as described in Ref. [175]. RELAP5-3D can act as either master or slave during the coupled code computation, as dictated by the particular application. In the case of the coupling between RELAP5-3D and the CFD code ANSYS-FLUENT, the executive programme monitors the progress of each code during the simulation, determines when both codes have converged according to their separate convergence criteria, controls the information interchanges between them, and issues instructions to allow each code to move to the next time step. The first round of a successful validation matrix for the RELAP5-3D/FLUENT coupled code was reported in Ref. [178].

One of the problems of multiscale coupling, i.e. the transition between 1-D and 3-D descriptions of the flow dynamics, and the matching of the interface(s) between them, has been reported in Ref. [179]. Enforcement of uniform profiles for transmitted quantities at the interfaces (the only option available for input from system codes) is common practice. The referenced emphasizes the vagaries associated with such an approach, which can lead to erroneous estimates of important parameters, such as estimation of pressure drops and temperature distributions.

Clearly, a start has been made in the validation of CFD codes, coupled to system and neutronics codes for NPP design issues. Despite the advances in computer hardware, it is anticipated that coupled system/CFD codes will be used ever more frequently for NPP design issues, at least during the early stages of the design process, because of the need to produce reliable results quickly in order to distinguish between several design options simultaneously. Nevertheless, validation of the coupled technology will remain a key issue, and some serious experimentation specifically addressed at interactive coupling will be needed to place the approach on a firm foundation. Finally, it is generally not sufficient to perform

TABLE 4. EXAMPLES OF COUPLED SYSTEM/CFD CODES

System code	CFD code	Scenario or experiment
RELAP5	COBRA/TF	LOFT L2–3 LOCA experiment
ATHLET	FLUBOX	UPTF experiment
ATHLET	ANSYS–CFX	MSLB analysis
RELAP5	CFDS-FLOW3D	Subcooled boiling experiments
Authors' 1-D code	NPHASE	Pipe flow experiments
RELAP5	ANSYS-FLUENT	Pipe blowdown experiment
RELAP5	GOTHIC	IRIS reactor 4 in. pipe break
CATHARE	TrioCFD	SFR applications
KORSAR/GP	LOGOS	WWER localized power surges

Note: 1 in. = 25.4 mm.; LOCA: loss of coolant accident.

V&V exercises for the component (CFD) parts of a coupled code system, unless explicit coupling is acceptable for the application (i.e. feedback effects are negligible or at least insignificant). Rather, a V&V for the coupled code system itself has to be carried out, and this currently represents a technology gap.

10.4.1. Multiscale and multiphysics considerations

Often, at both the system and component levels, multiscale and multiphysics coupling need to be represented, especially in the case of new NPP designs within the Gen III and Gen IV reactor concepts. In many cases, a demonstration simulation is a necessary step in application of a CFD code to a specific NPP design issue; indeed, such a simulation can provide insights into problems that will likely be encountered in the future. These problems can then be taken into account, at least partially, during planning of a code/model validation strategy. However, such an approach remains to be documented in detail, and may remain proprietary in origin.

It is of particular benefit if demonstration simulations for the same problem are performed using two or more CFD codes and involving different CFD specialists; only then can some idea of the effectiveness of the different algorithms and the 'user–effect' issue be evaluated. Since the requirements put on the demonstration simulations are often very 'relaxed' in comparison with the strictures of the model validation exercises, it is not always straightforward to discuss code 'deficiencies' in the context of a specific application. All too often, 'expert judgement' is applied to situations in which there is a lack of a strict validation philosophy. This gap needs to be closed to maintain proper adherence to established V&V principles.

10.4.2. Isolating the computational fluid dynamics problem

Traditional 1-D system codes often need to be 'manipulated' to account for genuine 3-D effects, when it is recognized that multidimensional aspects need to be taken into account to justify code predictions. A potential technology gap arises in being able to isolate the 3-D analysis from possible feedbacks to the 1-D system code prescription of the reactor circuit, which could alter the boundary conditions used for the standalone CFD simulation. If strong feedback from the system parameters is anticipated, a consistent coupling algorithm is required between the CFD and system code requirements. Such a coupling could be computationally expensive. The problem is well recognized, and progress is being made with implicit, fully consistent coupling algorithms of the system and CFD codes during a transient simulation. For example, flows in the upper and lower plenums and downcomer regions of the RPV, and to some extent the core region, are all essentially 3-D in character, particularly if driven by non-symmetric loop operation. Natural circulation and mixing in containment volumes are also essentially 3-D phenomena. The number of meshes required to model these phenomena precisely using CFD is well beyond the capabilities of present computer platforms. Closure relations for 3-D multiphase situations are often non-existent, and criteria for defining flow regimes at the fine mesh, CFD level remain largely underdeveloped. Moreover, no readily available CFD code has yet an acceptable neutronics modelling capability. With CFD not yet mature enough to model the entire system, an alternative strategy is needed. The most attractive option is still to couple the existing 1-D system codes with the 3-D CFD codes.

The most cost effective way to do this is to use the system code to provide input data to the CFD simulation in terms of (perhaps transient) inlet boundary conditions, and then run the CFD code in isolation. However, a problem remains in specifying the initial conditions (i.e. profiles of velocities and field variables, for which only area averaged quantities would be available) for the CFD run in the 3-D context. To complete the link, the procedure has to be extended by feeding averaged exit boundary conditions from the CFD computation back to the system code and continuing with the transient system analysis. This is an iterative process and itself is computationally demanding, but, again, progress is being made with the logistics of the coupling, though proper validation is still lacking.

10.4.3. Direct coupling of system codes with computational fluid dynamics codes

Multiple attempts have been made to directly couple CFD and system codes, rather than providing a simple interface construction between them, an exercise that is necessary because:

- The recognized system codes have proven reliability in the field, at least for Gen II and Gen III PWRs;
- Such codes are computationally efficient;
- CFD simulations will, of necessity, be restricted to local or component applications, at least in the foreseeable future, due to computational overheads and lack of validation matrices.

Current practice is to use less detailed, though computationally less demanding, system code analyses to produce initial and boundary conditions for the subsequent detailed CFD analysis. Such multiscale coupling is indispensable in the case of demonstration simulations and, of course, application of a CFD code to real NPP design issues. However, problems still exist in respect to the very different spatial and temporal scales involved, and some code development is needed to couple the two simulation techniques in a consistent manner, especially if there are important feedback effects.

Progress is being made, and Table 4 [180] summarizes some of the current efforts for specific cases. Problems remain in that system codes generally employ explicit time differencing, which of necessity are CFL limited, while CFD codes almost exclusively involve backward time differencing, which is stable (at least in principle, regardless of the size of the time step), but necessitates the use of internal iterations for consistency, adding significantly to the computational overhead. However, in many practical cases, the time step for the accuracy of CFD predictions matches that of stability of the overlying system code, so, from a pragmatic viewpoint, common ground can often be found. Explicit coupling between the system and CFD codes is the easiest to programme compared with implicit coupling, but it is more prone to numerical instabilities, especially if the time scales of the different physical processes to be represented are disparate.

To take this point further, independent of the details of the particular coupling strategy, validation and assessment of the coupled code are also required. The individual codes are usually employed to solve problems with different spatial and time scales but, particularly if two way coupling is involved, it is not enough to validate or assess the codes individually. Effort is still required in conducting experiments representing cases of strong coupling between the two multiscale situations. In this regard, experimental data remains lacking.

One of the problems of multiscale coupling, i.e. the transition between a 1-D and a 3-D description of the flow at the interface between the separate numerical representations, at system and local levels, was originally studied by Gibeling and Mahaffy [179]. Application of uniform profiles for transmitted quantities at the interface between the separate computational domains remains common practice. Reference [179] recorded for the first time that such an approach often leads to erroneous pressure and temperature field predictions. More effort has been devoted to this issue in recent years [181].

Clearly, a start has been made in the comprehensive validation of CFD codes coupled with system codes relevant to NPP design issues. It is anticipated that coupled codes will be used much more frequently in the future, but validation remains a key issue, representing a technology gap in the approach. It is necessary to perform V&V exercises for the individual component parts of a coupled code, but this is not sufficient to claim that V&V standards have been achieved for the coupled code itself; additional effort is required for this.

10.5. COUPLING WITH OTHER PHYSICS CODES

10.5.1. Coupling of computational fluid dynamics code with neutronics codes

Precise prediction of the thermal loads to fuel rods and of overall core behaviour result from a balance between the thermal hydraulics and the neutronics. Basic understanding of the interactive nature of the processes consists of recognizing that the thermal hydraulics is coupled with the neutronics through the heat release due to neutron activity (nuclear power distribution and evolution), and that the neutronics is coupled with the thermal hydraulics through temperature (i.e. of the fuel and moderator), density (of the moderator material), and the possible concentration level of neutron absorber material (e.g. boron).

The difficulty is to perform a coupled simulation, involving a particular (often commercial) CFD code, not principally developed in-house, and with a specific NPP application in mind, with a chosen neutronics code, most likely developed in-house, without considering CFD issues concerning fluid flow conditions. Despite the divergent origins of the numerical models, some progress can be reported in this field. The current state of the art on the subject is a coupling between a subchannel description of the thermal hydraulics of the core region and neutron diffusion at the assembly level. As an example, direct coupling between an in-house CFD code (Trio_U) and an established Monte Carlo neutronics code has been tested, and results obtained so far compare well with the available experimental data [182].

CFD/neutronics coupling has been proposed in the case of STAR-CD (later STAR-CCM+) and the neutronics code VSOP [183] in the case of lead–bismuth modular reactors. Another example is the coupling between core thermal hydraulics and neutronics within the SAPHYR system [184], based on the FLICA4 3-D two phase flow model and the CRONOS2 3-D diffusion and transport models.

Several benchmarks on the coupling issue have been initiated: PWR Main Steam Line Break [185], BWR Turbine Trip [186] and, more recently, for the WWER-1000 Coolant Transient [187]. CRONOS2 and FLICA4 have also been successfully applied to the TMI Reactivity Insertion Accident benchmark [188, 189], with pin by pin modelling, and within the EU Framework Programme NACUSP [190].

Though limited at present, substantial efforts are being made in this area, the results and confidence levels from which will directly feed into the use of CFD in NPP design in the future. In this regard, taking into account the interaction between the neutronics of core performance and local thermal hydraulics would result in more cost effective designs, more efficient core management procedures, and improved safety margins.

Possible lines of further research include:

- Coupling of CFD codes with more advanced codes (i.e. deterministic or stochastic transport) neutronics.
- Development of a multiscale approach to optimize the level of description under the prevailing conditions since, in many 3-D cases, the power output is often peaked (during rod ejection, boron dilution, steamline break, etc.), but in practical terms fine scale modelling could only currently be applied in limited regions.
- Development of efficient time step management procedures (e.g. subcycling) for complex transients for which the thermal hydraulics and neutronics timescales may be very different.

10.5.2. Coupling of computational fluid dynamics code with structural analysis codes

Flows in the primary circuit components of Gen II and Gen III reactors are often strong enough to induce vibrations in, or damage to, confining or nearby structures, which may have consequences, both regarding plant safety and economical operation. In cases in which the thermal and mechanical loads to the structures result in no significant changes in flow geometry — i.e. explicit coupling — the technology is now quite well established. The CFD team determines the (mechanical and thermal) structural loads, transfers the information to the structural dynamics team, which subsequently performs the stress analysis. A case in point here is thermal loading in T-junctions in Gen II PWRs [123]. Since there is no significant feedback of the structural deformation of the confining walls on the fluid dynamics and wall to fluid heat transfer, the CFD and SM simulations can be performed independently, and only a suitable data interface needs to be constructed between them. Good progress has been made in this area [191].

However, there are several instances in which the structural deformation of the confining walls could significantly modify the geometry of the fluid domain. If the timescales of the structural and fluid dynamical responses are similar, an explicit coupling procedure between determining the loads and the structural responses may no longer be appropriate, and an implicit coupling between the two will be needed. A tightly coupled CFD/SM simulation is considerably more challenging, not least due to the fact that the corresponding development teams will have become accustomed to working independently but will consequently have to learn to work together. Thus, the human factor again becomes important.

An added complication is that changes in the wall boundary conditions applied to the 3-D CFD simulation, linked either to structural response, or perhaps crud buildup, especially in the region of spacer grids, could result in serious changes to the flow dynamics, and could feed back to the umbrella system code simulation used initially to provide the boundary conditions needed by the CFD code, or even to the neutronics calculation undertaken in support of the system code parameters in defining, for example, fuel rod heat fluxes and surface rod temperatures. If there is a positive feedback due to changes in flow geometry to heat input from nuclear reactions, obviously these processes need to be computed simultaneously, and this remains a challenging task, and as such remains an ongoing research activity.

Interactive coupling between CFD and SM codes has accelerated in the commercial world as a consequence of the corporate alliances between the respective technologies. For example, the finite element SM suite ANSYS now includes both the finite volume CFD codes ANSYS-CFX and ANSYS-FLUENT. Similarly, STAR-CCM+ has been coupled directly to the SM code ABAQUS. As a result, this particular technology gap is closing rapidly, and it is anticipated that coupled CFD/SM simulations, even with positive feedback effects, will soon become quite routine, for example in the context of flow induced vibrations or water hammer.

However, note that it is still possible to couple simplified SM models into a CFD code, and this is possible even in the case of commercial codes. For example, a 1-D cantilever beam can be introduced without recourse to a general purpose 3-D coupling algorithm. The mesh generation and run times are consequently strongly reduced, which is always advantageous.

10.6. COMPUTING POWER LIMITATIONS

Parkinson’s Law [192]: “Work expands to fill the time available for its completion”, was first articulated by C. Northcote Parkinson in his book of the same name, and is based on an extensive study of the British civil service. One of the observations in the book noted that as Britain’s overseas empire declined in importance, the number of employees at the Colonial Office actually increased. From this have arisen a number of variants. Two pertinent ones from the sphere of information technology are: Parkinson’s Law of Data — ‘Data expands to fill the space available for storage’; and Parkinson’s Law of Bandwidth Absorption — ‘Network traffic expands to fill the available bandwidth’. The application of CFD methodology also deserves a mention. Perhaps Parkinson’s Law of Computational Fluid Dynamics could read: ‘The number of meshes expands to fill the available machine capacity’. A corollary is that the extension of the computational domain, the discretization, and the total simulation time, of a particular CFD calculation is often influenced by the planning. Hence the need for an initial phenomena identification and ranking table exercise and, as far as possible, possible limitations in the application of strict BPGs applied to CFD calculations at an early stage in the planning.

Best estimate system code analyses began in the early 1970s, which, by modern standards, was a period of very limited computing power. Typically, good turnaround times (i.e. overnight runs) could only be achieved using the supercomputers of the day. Now, such system code calculations are made on workstations or even PCs and tablets. However, even with the advances made in computer hardware, it is difficult to see how CFD codes could become capable of simulating the entire primary or secondary loops of an NPP at the design stage of the reactor: well validated system and component codes will remain the main design tools for some time. However, for those occasions for which CFD is needed — for example, for thermal fatigue in core subassemblies or T-junctions — the necessary computations will stretch computing resources to the limit, and ever more demands will be made, as predicted by Parkinson's Law.

The CFD codes focus on specific zones of a reactor coolant circuit, or may alternatively be used as a tool to derive new closure relations for more macroscopic approaches, reducing the necessity for expensive associated experimental programmes. Coupling between CFD and system codes may also be an efficient means to improve the description of small scale phenomena while living within the current computer limitations. When the necessary computer speed becomes available, DNS can be used to establish better understanding of small scale physical processes, and to formulate new computational models at mesoscale and eventually on a large scale.

Currently, CFD simulations using 100 million nodes are common in many industrial applications, e.g. in aerofoil design. Such calculations are most often steady state and single phase. In NPP design applications, issues such as containment mixing and stratification are of relevance, e.g. in the efficient placement of hydrogen combiners. CFD codes are computationally demanding, both in terms of memory usage and the total CPU time required. Since the accuracy of a solution can be improved by refining the mesh, and by reducing the time step, there is a tendency to use whatever computational resources are available (at the limit of their capacities), and there is a never ending demand for faster machines, improved parallelization, and more memory: Parkinson's Law again.

By way of illustration of the demands of strict adherence to BPGs, in such circumstances for a 3-D CFD simulation, with N meshes in each coordinate direction, the total number of grid points is N^3. The time step, though usually not CFL limited, remains, for purely practical reasons, roughly proportional to 1/N, so the number of time steps is also proportional to N. Current commercial CFD codes are generally based on a pressure velocity coupling algorithm, which entails the iterative solution of a large linear system of equations. Much of the CPU overhead (sometimes more than 90%) derives from this process. Typically, the number of iterations M to convergence within a time step is not strictly proportional to N, since the solution matrices are meagre, but the actual algorithm employed could result in a significant algebraic multiplying factor having to be applied to the overall CPU estimate. Certainly, the run-time for the CFD code needs to scale according to:

$$t \propto N^4$$

Despite the continual improvement in processor power, the commodity computer market still falls very short of the demands of CFD. Traditionally, CFD codes were written to run on a single processor in a serial manner, with one operation occurring after the next. One way to speed up the process is to divide the programme so that it runs on a large number of processors, running in parallel, these days typically on a cluster of machines. However, studies have indicated [193] that the scaling up of performance with the number of processors is strongly dependent on the size of the system arrays (i.e. number of meshes in the case of CFD), as well as on the details of the computer architecture and memory. Good performance is guaranteed in the case of small array sizes that fit into the processor's cache. However, when this is not the case, performance drops dramatically due to internal machine communication difficulties.

Even accepting the 'perfect' optimum of linear speed-up with the number of processors available, the N^4 (perhaps with a large preceding coefficient) dependence of run-time on number of meshes in one coordinate direction, doubling the number of processors, and keeping total run-time the same, the number of meshes in each direction can be increased by only 19%, say from 100 to 119. This is hardly adequate for a mesh size independence study within the dictates of the established BPG strategy. Conversely, doubling the mesh density, say from 100 to 200 meshes in each coordinate direction, again keeping total run-time constant, means that the number of processors has to be increased by a factor 16.

Given these statistics, it is evident that the pursuit of quality and trust in the application of CFD to transient NPP design issues, adhering strictly to the dictates of a BPG philosophy of multimesh simulations, will stretch available computing power to the limit for many years to come. In the medium term, compromises will have to be made: for example, examining mesh sensitivity for a restricted part of the computational domain, or to a specific period within a given transient. Certainly, expanding efforts will ensure that Parkinson's Law will prevail for CFD for some time yet.

This applies in particular to the current major missing component of the CFD best estimate philosophy: uncertainty quantification. This issue is so important, an entire chapter of this publication has been dedicated to it (Section 9).

11. CONCLUSIONS

This CRP, which was set up to document the role of CFD codes in future NPP designs, officially was developed at a kick-off meeting at IAEA Headquarters in Vienna in December 2010. The primary objective was to showcase and report on current efforts in the field. The status of CFD as a technology was at that time already a widely accepted design tool in many diverse industries, including those related to turbomachinery, automobile and aerospace design. It seemed therefore inconceivable that such an important, advanced technological tool is not also of value in the design of new, even innovative, nuclear reactor concepts, particularly those designated as Gen III and Gen IV reactors. At the meeting, participants came to the consensus opinion that the topic was worthy of further pursuit in the context of a formal CRP.

While the CRP was being organized, the accident at the Fukushima Daiichi nuclear power plant took place, in March 2011. It was recognized that the role of CFD in NPP design would be primarily directed towards Gen III+ and Gen IV design concepts, but in a rather academic context, and would not play a part in the development of advanced PWR and BWR designs. Rather, it would be restricted to highly localized design issues, such as fuel spacer technology. However, as countries reassessed the role of nuclear power generation in future electricity production, it was recognized that there were still issues in current NPP technology development where CFD could still play a part, though continuing to focus on classical Gen II PWR technology. This was the framework upon which the CRP was reoriented, while reporting on contributions that could be made to future design issues within the present Gen II and Gen III PWR reactor concepts.

This publication is not intended to be a state of the art publication on the subject. That was considered to be too bold a venture within the newly emerging climate of NPP design considerations following the Fukushima Daiichi accident. Rather, it represents a first look at the role of CFD in possible future NPP design issues, while the focus remains on current water cooled reactor technology. Discussions of future design options, i.e. those not involving current water cooled reactor based technologies, are left to future initiatives.

This publication serves to underpin the origins, scope and objectives of the regenerated CRP, as well as the limitations to which it is subject, and represent the ultimate achievements of the endeavour. It was first necessary to identify those issues for which CFD could be regarded as a legitimate design tool: primarily, as in other industries, as a cost effective method to eliminate overspeculative design options, and later to identify those options worthy of subsequent, though necessarily expensive, experimental investigation.

It was considered necessary in this publication to include the first hand opinions and suggestions of those directly involved in reactor design issues of the potential role of CFD in NPP design. Consequently, EDF (France), KAERI (Republic of Korea), OKB Gidropress (Russian Federation) and Westinghouse (USA) were welcome participants in the group's activities. Many national research organizations were also instrumental in achieving the project's objectives and contributed positively to these objectives. These include CNL (Canada), Shanghai Jiao Tong University (China), HZDR (Germany), BARC (India), KAERI (Republic of Korea), PSI (Switzerland) and MIT (USA). Their individual contributions to the overall knowledge base are acknowledged here and the individual contributions summarized.

This publication is divided into different sections, as originally identified by early roundtable discussions. They include current activities in which CFD is being used to support NPP design. The principal contributions are from EDF (France) and Westinghouse (USA), with additional material supplied by CNL (Canada), BARC (India), KAERI (Republic of Korea) and PSI (Switzerland). Also documented is the current status of the V&V procedures serving to underscore the use of CFD in NPP design, followed by a synopsis of the projected uses of CFD for particular reactor types, among them supercritical reactors, sodium cooled fast reactors and advanced LWR designs.

Best practice guidelines in the use of CFD as a design tool for nuclear reactors are yet to be formalized but have been established in other industrial application areas: the first of these (ERCOFTAC) were focused on turbomachinery design. However, the scope has broadened considerably over the years and those relating to NPP safety (though not specifically aimed at design issues) are also now well established, through the efforts of the OECD. The transfer of the know-how to design related topics is discussed in this publication.

Of course, the application of CFD to NPP design also has to be underpinned by appropriate experimental validation data, and this important topic is addressed in detail in the present publication. Principal contributions here relate to the experiments carried out at HZDR (Germany) and KAERI (Republic of Korea) and the data released by these institutions, which have formed the bases of two major code comparison exercises organized, undertaken and reported in the context of this CRP. Both have been issued as IAEA technical documents (TECDOCs) associated with this CRP. In addition, the lessons learned from the Vattenfall T-junction test, which is important in connection with the issue of thermal fatigue, is also reported here but for guidance purposes only, though some members had actively participated in the OECD benchmark study.

Another important issue relates to the specific requirements of test data derived for CFD validation purposes from experimental tests. The availability of suitably qualified data is not a trivial issue, nor is it usually within the perspectives of the experimenters. A section in this publication is devoted to this important topic with the intention of setting the ground rules for what the CFD community would regard as trustworthy test data from the viewpoint of CFD validation.

It was generally recognized by the group that ‘user qualification’ is not as important an issue for CFD practitioners as it is for those using system codes, provided that BPG shortcuts are strictly observed. In practical terms, however, certain ‘work-arounds’ tactics may need to be employed when performing a CFD simulation in order to provide meaningful results within a reasonable time. Such tactics also need to be properly scrutinized so that the CFD results can be considered totally substantiated. This issue is also discussed in the publication.

The principal technology gaps, still regarded by the international community as being open with regard to the application of CFD to NPP design, have been identified in the course of this CRP and are summarized here. Also, lists are available of the ongoing research activities aimed at closing these gaps. At least for single phase applications, the main problems appear to be the identification of the most appropriate turbulence model to adopt in a given situation, and how to represent the near wall effects, especially when convection currents are important, though BPGs do provide some guidance on the issues. A section here is dedicated to this subject.

However, the one most important consideration associated with any so-called ‘best estimate’ numerical approach, of which CFD is one, is the question of the uncertainty quantification of the predictions. This remains uncharted territory in the application of 3-D CFD codes due simply to the current lack of computing power to perform the necessary support calculations to quantify the uncertainties, and the application of CFD to NPP design is no exception. However, at least in the nuclear area, firm foundations have been formalized in the context of the recognized, and well validated, system codes developed in the context of NNP safety, though these are essentially 1-D in origin despite claims to the contrary by the code developers. The specifics of the challenges remaining are detailed within this publication, which at least at this time will serve as a reminder of the issues to be faced in the future of CFD predictions providing trustworthy data upon which NPP design decisions can be based. This may prove instrumental in pursuing future NPP design options.

To reiterate, this publication is not intended to be a state of the art publication on the role of CFD in NPP design; a task considered to be beyond the brief of this CRP. Rather, it is, as the title suggests, a summary itemizing the various activities still requiring attention, and in some cases being actively pursued, within the framework of the CRP, as discussed and supported by its sitting members. Certainly, CFD is destined to become a frontline technology in many future NPP designs. The challenges involved in this method achieving a reliable status are outlined in this publication.

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ABBREVIATIONS

ASME	American Society of Mechanical Engineers
ASTRID	advanced sodium technological reactor for industrial demonstration
BARC	Bhabha Atomic Research Centre
BPG	best practice guidelines
BWR	boiling water reactor
CEA	French Alternative Energies and Atomic Energy Commission
CFD	computational fluid dynamics
CHF	critical heat flux
CRP	coordinated research project
DES	detached eddy simulation
DNS	direct numerical simulation
EDF	Électricité de France
ERCOFTAC	European Research Community on Flow, Turbulence and Combustion
HWR	heavy water reactor
IET	integral effects test
KAERI	Korea Atomic Energy Research Institute
LDA	laser Doppler anemometry
LES	large eddy simulation
LWR	light water reactor
NPP	nuclear power plant
NRS	nuclear reactor safety
OECD/NEA	Nuclear Energy Agency of the Organisation for Economic Co-operation and Development
OFEL	omniflow experimental loop
PDF	probability density function
PIV	particle image velocimetry
PTS	pressurized thermal shock
PWR	pressurized water reactor
RANS	Reynolds averaged Navier–Stokes
ROCOM	Rossendorf coolant mixing
RPV	reactor pressure vessel
RSM	Reynolds Stress Model
SAS	scale adaptive scheme
SCWR	supercritical water cooled reactor
SET	separate effects test
SFR	sodium cooled fast reactor
SGS	suitable subgrid scale
SST	shear stress transport
UQ	uncertainty quantification
URANS	unsteady Reynolds averaged Navier-Stokes
V&V	verification and validation
WMS	wire mesh sensor

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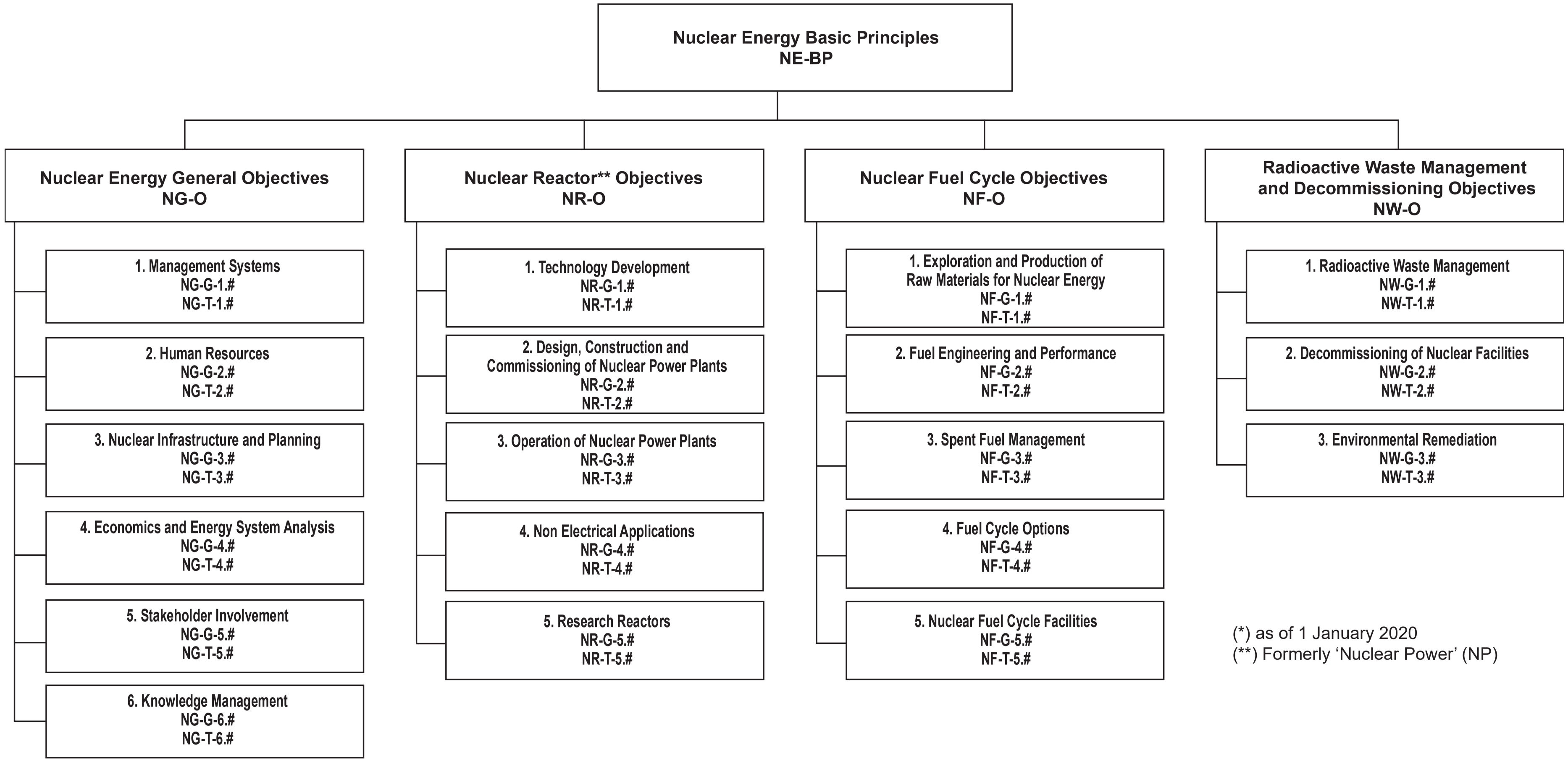

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