Nuclear Safety
NEA/CSNI/R(2020)3
February 2022
www.oecd-nea.org

# Requirements for CFD-Grade Experiments for Nuclear Reactor Thermal Hydraulics

OECD
BETTER POLICIES FOR BETTER LIVES

NEA
NUCLEAR ENERGY AGENCY

Nuclear Energy Agency

**NEA/CSNI/R(2020)3**

**Unclassified** **English text only**

**16 février 2022**

**NUCLEAR ENERGY AGENCY**
**COMMITTEE ON THE SAFETY OF NUCLEAR INSTALLATIONS**

# Requirements for CFD-Grade Experiments for Nuclear Reactor Thermal Hydraulics

This document is available in PDF format only.

**JT03489666**

### ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT

The OECD is a unique forum where the governments of 38 democracies work together to address the economic, social and environmental challenges of globalisation. The OECD is also at the forefront of efforts to understand and to help governments respond to new developments and concerns, such as corporate governance, the information economy and the challenges of an ageing population. The Organisation provides a setting where governments can compare policy experiences, seek answers to common problems, identify good practice and work to co-ordinate domestic and international policies.

The OECD member countries are: Australia, Austria, Belgium, Canada, Chile, Colombia, Costa Rica, the Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Israel, Italy, Japan, Korea, Latvia, Lithuania, Luxembourg, Mexico, the Netherlands, New Zealand, Norway, Poland, Portugal, the Slovak Republic, Slovenia, Spain, Sweden, Switzerland, Turkey, the United Kingdom and the United States. The European Commission takes part in the work of the OECD.

OECD Publishing disseminates widely the results of the Organisation's statistics gathering and research on economic, social and environmental issues, as well as the conventions, guidelines and standards agreed by its members.

### NUCLEAR ENERGY AGENCY

The OECD Nuclear Energy Agency (NEA) was established on 1 February 1958. Current NEA membership consists of 34 countries: Argentina, Australia, Austria, Belgium, Bulgaria, Canada, the Czech Republic, Denmark, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Japan, Korea, Luxembourg, Mexico, the Netherlands, Norway, Poland, Portugal, Romania, Russia, the Slovak Republic, Slovenia, Spain, Sweden, Switzerland, Turkey, the United Kingdom and the United States. The European Commission and the International Atomic Energy Agency also take part in the work of the Agency.

The mission of the NEA is:

– to assist its member countries in maintaining and further developing, through international co-operation, the scientific, technological and legal bases required for a safe, environmentally sound and economical use of nuclear energy for peaceful purposes;

– to provide authoritative assessments and to forge common understandings on key issues as input to government decisions on nuclear energy policy and to broader OECD analyses in areas such as energy and the sustainable development of low-carbon economies.

Specific areas of competence of the NEA include the safety and regulation of nuclear activities, radioactive waste management and decommissioning, radiological protection, nuclear science, economic and technical analyses of the nuclear fuel cycle, nuclear law and liability, and public information. The NEA Data Bank provides nuclear data and computer program services for participating countries.

## COMMITTEE ON THE SAFETY OF NUCLEAR INSTALLATIONS

The Committee on the Safety of Nuclear Installations (CSNI) is responsible for the Nuclear Energy Agency (NEA) programmes and activities that support maintaining and advancing the scientific and technical knowledge base of the safety of nuclear installations.

The Committee constitutes a forum for the exchange of technical information and for collaboration between organisations, which can contribute, from their respective backgrounds in research, development and engineering, to its activities. It has regard to the exchange of information between member countries and safety R&D programmes of various sizes in order to keep all member countries involved in and abreast of developments in technical safety matters.

The Committee reviews the state of knowledge on important topics of nuclear safety science and techniques and of safety assessments, and ensures that operating experience is appropriately accounted for in its activities. It initiates and conducts programmes identified by these reviews and assessments in order to confirm safety, overcome discrepancies, develop improvements and reach consensus on technical issues of common interest. It promotes the co-ordination of work in different member countries that serve to maintain and enhance competence in nuclear safety matters, including the establishment of joint undertakings (e.g. joint research and data projects), and assists in the feedback of the results to participating organisations. The Committee ensures that valuable end-products of the technical reviews and analyses are provided to members in a timely manner, and made publicly available when appropriate, to support broader nuclear safety.

The Committee focuses primarily on the safety aspects of existing power reactors, other nuclear installations and new power reactors; it also considers the safety implications of scientific and technical developments of future reactor technologies and designs. Further, the scope for the Committee includes human and organisational research activities and technical developments that affect nuclear safety.

# *Acknowledgements*

The authors of this document are the principal contributors. They are listed below. Many other members of the Nuclear Energy Agency (NEA) Committee on the Safety of Nuclear Installations (CSNI) Working Group on the Analysis and Management of Accidents' Task Group for Computational Fluid Dynamics (CFD) application to safety and of the SILENCE network contributed to discussions and their assistance is gratefully acknowledged.

Main author:

D. Bestion (French Alternative Energies and Atomic Energy Commission [CEA])

Principal contributors:

R. Camy (Électricité de France [EDF])

S. Gupta (Becker Technologies GmbH)

C Heib (Institute for Radiological Protection and Nuclear Safety [IRSN])

O. Marfaing (French Alternative Energies and Atomic Energy Commission [CEA])

F. Moretti (NINE Nuclear and Industrial Engineering)

T. Skorek (Gesellschaft für Anlagen- und Reaktorsicherheit [GRS])

# *Table of contents*

## Figures

# *Executive summary*

The Nuclear Energy Agency (NEA) Committee on the Safety of Nuclear Installations (CSNI) launched an Action Plan on the "Application of Computational Fluid Dynamics (CFD) Codes to Nuclear Reactor Safety (NRS) Problems" in 2003 with mandates to perform the following tasks:

- provide a set of guidelines for the application of CFD to NRS problems;
- evaluate the existing CFD assessment bases and identify gaps that need to be filled in order to adequately validate CFD codes for application to NRS problems;
- summarise the extensions needed to CFD codes for application to two-phase NRS problems.

It was necessary to carry out a review of uncertainty methods for CFD application to nuclear reactor safety. The report was issued in 2016 (NEA 2016a).

In parallel, as a spin-off activity, an international workshop was organised every two years to provide a forum for numerical analysts and experimentalists to exchange information in the field of NRS-related activities related to CFD validation. The CFD4NRS workshops started in 2006 and significant progress was reported every two years in modelling, validation and verification. In addition, blind benchmark exercises were also proposed based on some experimental tests related to safety issues such as thermal fatigue, turbulence in rod bundle flow, hydrogen behaviour in a containment, mixing with buoyancy effects, and mixing in pressurised water reactor cold leg and downcomer in relation to pressurised thermal shock. This benchmarking activity highlighted the need to have very well-designed and instrumented CFD-grade experiments for model validation. Thus, the working group on CFD application to nuclear safety of the CSNI Working Group on Analysis and Management of Accidents (WGAMA) decided to establish some requirements for CFD-grade experiments able to properly validate the single-phase CFD tools. The SILENCE network also supported this initiative and contributed to this work. This document reports the results of this activity.

When looking for a validation experiment for CFD application to reactor simulation for either design or safety studies, it appears that available data often suffer from a lack of local measurements, an insufficient number of measured flow variables, a lack of well-defined initial and boundary conditions, and a lack of information on results uncertainty.

This report first analyses the gap between available data and what can be called CFD-grade experimental data. The objectives of the validation are recalled and put in the context of a best estimate plus uncertainty methodology. It then defines the objectives of a CFD-grade experiment. The scope of this analysis is given with an emphasis on single-phase CFD.

The report then discusses the requirements and gives recommendations for both separate effect tests and combined effect tests concerning boundary and initial conditions, flow parameter measurements, measurement uncertainty of quantities of interest, and boundary and initial conditions in view of minimising the validation uncertainty. The report

concludes with guidelines and recommendations and proposes a roadmap for the design of a CFD-grade experiment.

The main outcome of this work is the following:

Clear objectives should be first defined with reference to a reactor application, an analysis of the process to be investigated and a selection of the type of turbulence model that may be used for the simulation. Then a discussion between experimentalists and the CFD code practitioners is necessary to define the test section geometry, the initial and boundary conditions, and the quantities of interest with their locations, so as to define the requirements on the measurement uncertainty. The choice of measurement technique stems from these specifications.

The acceptance criteria should be defined in accordance with the required accuracy and the sensitivity of the measurements to the uncertainty in the experimental conditions.

Preliminary CFD simulations are necessary to confirm the most appropriate measurement locations, experimental conditions and overall the interest of the experiment for the physics to validate. Iterations may be necessary to reach an optimised design of the experiment.

CFD-grade experiments should be able to validate CFD and one important concern is to minimise the validation uncertainty on some selected figures of merit.

It is expected that this document will contribute to building more helpful future experimental programmes, although the presented guidelines and recommendations still need to be complemented and improved.

An important effort should be made in the future to establish practical guidelines for estimating the experimental uncertainty, which seems to be the weak point in the current roadmap. This could justify a future activity to write a guide for experimentalists that gathers all the available knowledge on sources of uncertainty for every type of sensor used in CFD-grade experiments.

# *Acronyms and abbreviations*

| | |
|---|---|
| ASME | American Society of Mechanical Engineers |
| ASN | Autorité de Sûreté Nucléaire (Nuclear Safety Authority, France) |
| BIC | Boundary and initial condition |
| BWR | Boiling water reactor |
| CEA | Commissariat à l'énergie atomique et aux énergies alternatives (French Alternative Energies and Atomic Energy Commission, France) |
| CET | Combined effect test |
| CFD | Computational fluid dynamics |
| CFD4NRS | Computational fluid dynamics for nuclear reactor safety |
| CSNI | Committee on the Safety of Nuclear Installations (NEA) |
| EDF | Électricité de France |
| FoM | Figure of merit |
| GRS | Gesellschaft für Anlagen- und Reaktorsicherheit (Association for Plant and Reactor Safety, Germany) |
| IAEA | International Atomic Energy Agency |
| IC | Initial condition |
| IET | Integral effect test |
| IRSN | Institut de Radioprotection et de Sûreté Nucléaire (Institute for Radiological Protection and Nuclear Safety, France) |
| ISP | International standard problems |
| KAERI | Korea Atomic Energy Research Institute |
| LES | Large eddy simulation |
| NEA | Nuclear Energy Agency |
| NRS | Nuclear reactor safety |
| OECD | Organisation for Economic Co-operation and Development |
| PCE | Polynomial chaos expansions |
| PIRT | Phenomena and Identification Ranking Table |

| | |
|---|---|
| PSI | Paul Scherrer Institute |
| PWR | Pressurised water reactor |
| RANS | Reynolds-Averaged Navier-Stokes |
| rms | Root mean square |
| SET | Separate effect test |
| SILENCE | Significant Light and Heavy Water Reactor Thermal-hydraulic Experiments Network for the Consistent Exploitation of the Data |
| UMAE | Uncertainty Method based on Accuracy Extrapolation |
| UQ | Uncertainty quantification |
| URANS | Unsteady Reynolds-Averaged Navier-Stokes |
| V&V | Verification and validation |
| VLES | Very large eddy simulation |
| WG | Writing group |
| WGAMA | Working Group on the Analysis and Management of Accidents (NEA) |

# 1. Introduction

Following the conclusions of the Exploratory Meeting of Experts on the Application of Computational Fluid Dynamics to Nuclear Reactor Safety (NRS) Problems that took place in Aix-en-Provence in 2002, the Nuclear Energy Agency (NEA) Working Group on the Analysis and Management of Accidents (WGAMA) initiated activities the following year in order to promote the use of computational fluid dynamics (CFD) for nuclear safety. Three separate writing groups (WG) were created. WG1 established the "Best Practice Guidelines for the Use of CFD in Nuclear Reactor Safety Applications" (NEA, 2007a; 2015) with a set of guidelines for a range of single-phase applications of CFD. WG2 produced a document on the "Assessment of CFD Codes for Nuclear Reactor Safety Problems" (NEA, 2008a; NEA, 2014a) with a compendium of current application areas and a catalogue of experimental validation data relevant to these applications. A list of the NRS problems for which CFD analysis is expected to bring real benefits was compiled, and reviewed critically. Validation data from all available sources have been assembled and documented. Assessment databases relating to specific NRS issues has been catalogued separately, and more comprehensively discussed. Gaps in the existing assessment databases were identified. WG3 treated the "Extension of CFD Codes to Two-Phase Flow Safety Problems" (NEA., 2006; Bestion, 2010; NEA, 2010; NEA, 2014b). Then a review of uncertainty methods for CFD application to nuclear reactor thermal hydraulics was written (NEA, 2016a).

International benchmarks were also organised to test CFD capabilities to address reactor issues. A first benchmark was based on a mixing Tee experiment from Vattenfall (NEA, 2011a) for investigating thermal fatigue. The second benchmark addressed flow in a rod bundle with specific influence of spacer grids and was based on a MATIS-H test of the Korea Atomic Energy Research Institute (KAERI) (NEA, 2013). The third addressed physical processes (particularly stratification erosion) occurring in a containment following a postulated severe accident in which there is a significant build-up of hydrogen in the containment atmosphere. It is based on a PANDA test of the Paul Scherrer Institute (PSI) (NEA, 2016b). The fourth benchmark was the first uncertainty quantification exercise on a rather simple mixing problem in the presence of buoyancy effects. It was based on the GEMIX mixing layer experiment of the PSI in the presence of density differences. The ongoing fifth benchmark is the second benchmark with uncertainty evaluation and is devoted to cold leg mixing processes associated to emergency core cooling system injection with high density differences. It uses an experiment of Texas A&M University.

The writing groups proposed to extend the work by organising a new series of international workshops to provide a forum for experimenters and numerical analysts to exchange information. The first of the workshops, which all specifically focused on the application of CFD to NRS issues, took place in Garching, Germany in September 2006 under the acronym CFD4NRS (NEA, 2007b), sponsored jointly by the NEA and the International Atomic Energy Agency (IAEA). Papers describing CFD simulations were accepted only if there was a strong validation component. Most related to the NRS issues highlighted in this paper, such as pressurised thermal shock, boron dilution, hydrogen distribution, induced breaks and thermal striping. Selected papers of each workshop appeared in a special issue of *Nuclear Engineering and Design*.

The second workshop in the series, XCFD4NRS (NEA, 2008b), took place in Grenoble, France in 2008. Here, the emphasis was more on new experimental techniques and two-phase CFD. CFD4NRS-3 took place in Washington, DC in 2010 (NEA, 2011b), followed by the CFD4NRS-4 workshop in Daejeon, Korea in 2012 (NEA, 2014c). The fifth workshop took place in Zurich, in 2014 (NEA, 2016c). Another workshop took place in Cambridge, Massachusetts, in 2016 and the CFD4NRS-7 workshop took place in Shanghai, People's Republic of China, in September 2018. The CFD4NRS workshops are a very useful addition to the more general conferences aimed at the nuclear technology community in that they are highly focused on CFD applications to nuclear safety issues and the separate effect and integral experiments that validate them. The papers reporting experimental findings must contain data from local measurements of parameters of interest, suitable for CFD validation, and the use of error bounds on the data are very desirable.

In parallel to the WGAMA activities, the SILENCE (Significant Light and Heavy Water Reactor Thermal-hydraulic Experiments Network for the Consistent Exploitation of the Data) network was created for co-operation among teams of experimentalists managing significant experimental projects in nuclear reactor thermal hydraulics. Its objectives are:

- Optimising the funding available worldwide for experiments, recognising their vital role for the design and the safety of existing and coming nuclear power plants.
- Co-ordinating the efforts of teams of experimentalists in order to provide support for international institutions, like the NEA and the IAEA, namely for launching and possibly organising International Standard Problems (ISPs).
- Addressing the scaling issue and providing an agreed view from the side of experimentalists. This also implies the design and execution of counterpart tests.
- Setting-up a centre of expertise for supporting experimental programmes in "embarking countries" with an interest in the area of large thermal-hydraulic experiments.
- Maintaining, expanding and using the database of experiments already available from various parts of the world possibly in co-operation with the international institutions (notably the NEA where the NEA Data Bank is available).
- Improving the existing measurement techniques.

One of the activities of the SILENCE network towards fulfilling the above-mentioned objectives was to organise the "Specialists Workshop on Advanced Instrumentation and Measurement Techniques for Nuclear Reactor Thermal-Hydraulics (SWINTH)", which was held in Italy in 2016. The workshop covered the technology of experimentation in nuclear thermal hydraulics, including both separate effect and integral test facilities, with coarse as well as CFD-grade measurements, and not limited to light water-cooled reactor technology (www.nineeng.org/swinth).

Both the WGAMA CFD Task Group and the SILENCE network identified the need to establish more detailed guidelines and requirements for future "CFD-grade experiments" and this paper is an effort in that direction.

In the present report, the role of validation in resolving a thermal-hydraulic issue with CFD is recalled and the objectives of a CFD-grade experiment are defined. The scope of this analysis is given with an emphasis on single-phase CFD.

The report then proposes a list of requirements for both separate effect tests (SET) and combined effect tests (CET) about boundary and initial conditions (BIC), flow parameter measurements, measurement uncertainty of quantities of interest and BIC, with a view of minimising the validation uncertainty. Finally, the report provides guidelines and recommendations and proposes a roadmap for the design of a CFD-grade experiment.

## 2. Objectives of computational fluid dynamics code validation

Safety demonstration of the nuclear reactors requires the analysis of complex problems related to accident scenarios. Often, the experiments cannot reproduce at a reasonable cost the physical situation without any simplification or distortion and the numerical tools cannot simulate the problem by solving the exact equations. Only reduced scale experiments are feasible to investigate the phenomena and only an approximate system of equations may be solved to predict time and/or space averaged parameters with errors due to imperfections of the closure laws and to numerical errors. Complex methodologies are therefore necessary to solve a problem, including:

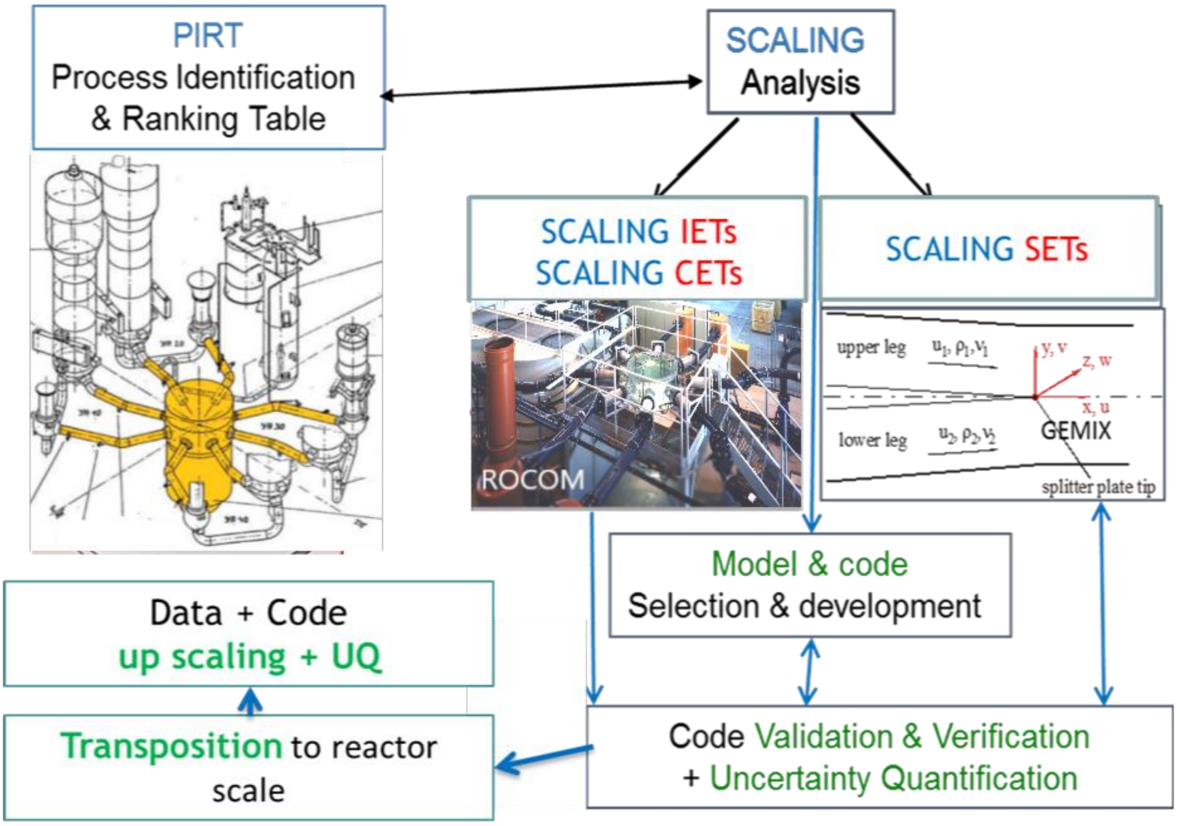
- a Phenomena and Identification Ranking Table (PIRT) analysis;
- a scaling analysis and the selection of scaled integral effect tests (IETs), combined effect tests (CETs) and separate effect tests (SETs);
- the selection of a numerical simulation tool;
- the verification and validation (V&V) of the tool;
- an analysis of transposition for use of the tool in the intended reactor case (ASN and IRSN, 2017) (including identification of the geometrical [scale effect] and physical differences between the validation cases and the scope of utilisation);
- an assessment of the ability of the models to remain predictive (or penalising) taking account of the differences identified between the validation range of the tool and the utilisation range, including notably the justification of the transposition of the adjustments and the uncertainties and assuring the consistency of modelling choices in the safety studies with the choices adopted for the validation cases;
- the code application to the safety issue of interest and the use of an uncertainty method to determine the uncertainty of numerical prediction.

This global approach is illustrated in Figure 1.

Verification answers the question ‘Do we solve the equations correctly?’

Verification of a code allows assessing the correct implementation of all numerical and physical models in a CFD method. Verification assessment is generally performed in two steps: 1) to confirm that the software is working as intended; and 2) to verify the calculation performed by numerical calculations and quantification of numerical errors, if any. For the second step, usually simple test cases with analytical solutions or with manufactured solutions are simulated. It may also include the calculations of experiments to test all the relevant implementation aspects of a CFD code and the models implemented. This step is conducted by the code developers.

**Figure 1. Methodology for solving a complex reactor thermal-hydraulic issue**




Note: UQ: uncertainty quantification; IET: integral effect test; CET: combined effect test; SET: separate effect test.

Source: Adapted from Höhne, T. and S. Kliem, (2020), "Detailed Simulation of the Nominal Flow and Temperature Conditions in a Pre-Konvoi PWR Using Coupled CFD and Neutron Kinetics", *Fluids* 2020, 5, 161, https://doi.org/10.3390/fluids5030161 and courtesy of S. Kliem (HZDR).

Validation answers the question: Do we solve the right equations?

Validation of a code is a process to assess the accuracy of the tested physical models of the code based on comparisons between computed results and experimental data. The validation is performed to provide confidence in the ability of a code to predict the values of the safety parameters or parameters of interest. It may also be used to estimate a bias on the specific configuration under concern. The results of a validation may be used to determine the uncertainty of some constitutive laws of the code. The validation can be conducted by the code developers and/or by the code users. When it is performed by the code developers it is called developmental assessment and when it is performed by the code users it is called independent assessment. A validation matrix is a set of selected experimental data for the purpose of extensive and systematic validation of a code within the limits of a given application scope. The validation matrix usually includes:

- basic tests;
- SETs;
- IETs;
- nuclear power plant data;

SETs are experimental tests that intend to investigate a single physical process, either in the absence of other processes or in conditions that allow measurements of the effects of the process of interest. An SET may be used to validate a physical model independently from the others.

IETs are experimental tests that intend to simulate the behaviour of a complex system with all interactions between different dynamic phenomena occurring in various system components. An IET relative to reactor accidental thermal hydraulics can simulate the whole primary cooling circuit and simulate the accidental scenario through initial and boundary conditions.

SETs may include single effect tests where only one process is investigated and may also include CETs where a few processes are investigated, implying several physical models having a significant influence. Although CET is not a standard nomenclature in the Committee for the Safety of Nuclear Installations' documents, we use it here to distinguish them from SETs and IETs. CETs also simulate interactions between various flow and heat transfer processes occurring in various system components without simulating the whole system or reactor circuit of interest. It may simulate the flow in several components of a reactor, including various geometries and various phenomena. Examples are the ROCOM or HIBISCUS test facilities used to investigate phenomena in pressurised water reactor cold legs and pressure vessels in boron dilution or pressurised thermal shock scenarios.

In the validation, the comparison of simulation results with measurements from experiments is a key point starting with the metric definition. Depending on the metric, agreement can appear poor or good. The choice of the metric should be goal oriented. Quantification of a bias on IET can contribute to uncertainty quantifications. Quantification of biases on different SETs can be used for calibration if performed.

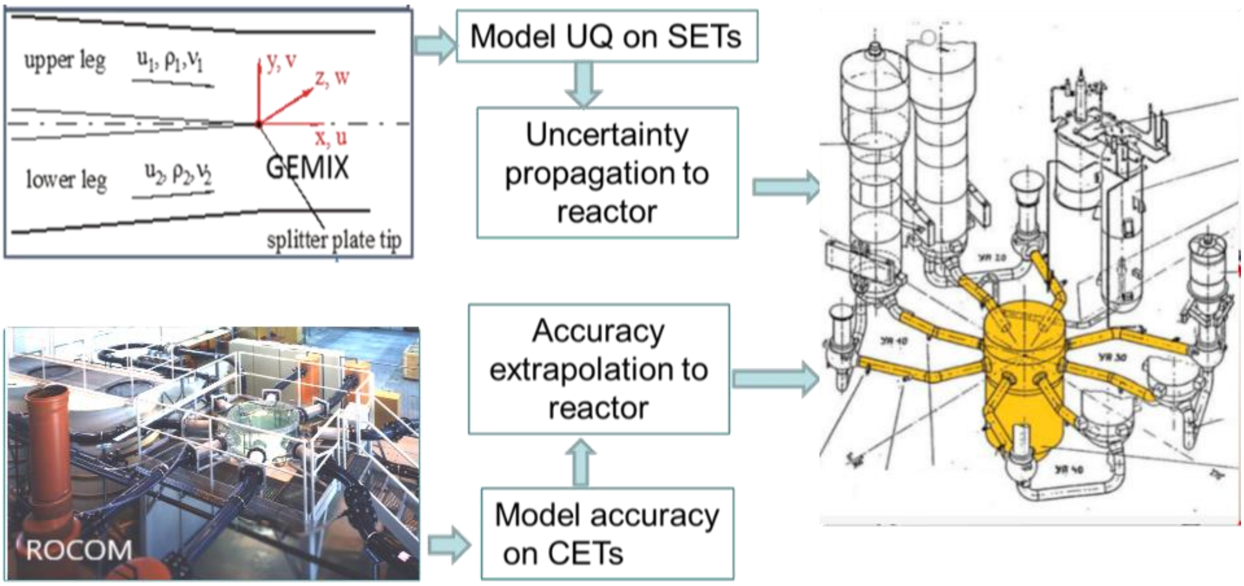
One may list the following sources of uncertainty of single-phase CFD application (NEA, 2016a):

- Initial and boundary conditions.
- Uncertainties related to the physical models:
  - Uncertainties related to the parameters of physical models: wall functions − if used − to express momentum and energy wall transfers and parameters of turbulence models (e.g. C1, C2, Cm, Prk and Prε of the k-ε model) are sources of uncertainties.
  - Uncertainties related to non-modelled physical processes and uncertainties related to the form of the models: models may have inherent limitations. For example, any eddy viscosity model like k-ε or k-ω cannot predict a non-isotropic turbulence nor an inverse-cascade of energy from small turbulence scales to large ones.
- Uncertainties related to the numerical solution: they are related to spatial discretisation errors, time discretisation errors, iteration errors and round-off errors.
- Simplification of the geometry: non-modelled geometrical details may have some impact on the resulting flow.
- Uncertainties due to scaling distortions: when the uncertainty or the accuracy is determined in a given range of flow conditions characterised by a geometry and extrapolated to a reactor with a different geometry and different values of some non-dimensional numbers.
- Uncertainty due to physical properties of fluid and solids.

- Uncertainty arising from physical instabilities/chaotic behaviour: non-linear dynamic systems (like Navier-Stokes equations) can, under certain circumstances, have a chaotic behaviour.

Code validation requires comparison with experiments of various types: SETs, IETs, possibly including CETs. The determination of code uncertainty also uses comparison to data of the various types to get the basic information for an inverse model uncertainty quantification. Two types of methods are considered for model uncertainty quantification in the review of uncertainty methods for CFD application to nuclear reactor thermal hydraulics (NEA, 2016a): an accuracy extrapolation and an input uncertainty propagation, as illustrated in Figure 2. Table 1 summarises the characteristics of the methods and shows what type of experiments (SETs, CETs and IETs) are necessary. One may observe that input uncertainty propagation methods require SETs to get information on the uncertainty of the parameters of the models, while extrapolation methods require more prototypical experimental data to measure the accuracy of the model in conditions close to the reactor application. For example, one can validate and determine the uncertainty of the parameters of a turbulence model by calculating a set of experiments with basic flow configurations, such as a boundary layer, a free jet, an impinging jet, a wake, a mixing layer, a grid turbulence decay and so on. This may be useful in a best estimate plus uncertainty approach using a propagation of input uncertainties approach. One can also determine the code model accuracy on a specific target value by calculating CET tests that simulate the reactor situation of interest with a scaled geometry and then propagating by some method the uncertainties determined on the target value to the reactor application. Since these two types of tests are rather different, they are not treated in the same way for the initial and boundary conditions, the number and quality of measurements, and the measurement uncertainty. This has to be taken into account in the requirements for CFD-grade experiments.

**Figure 2. Illustration of the two methods for taking model uncertainty into account in a computational fluid dynamics simulation of a reactor issue**




Note: UQ: uncertainty quantification; SET: separate effect test; CET: combined effect test.

Source: Adapted from Höhne, T. and S. Kliem, (2020), "Detailed Simulation of the Nominal Flow and Temperature Conditions in a Pre-Konvoi PWR Using Coupled CFD and Neutron Kinetics", *Fluids* 2020, 5, 161, https://doi.org/10.3390/fluids5030161 and courtesy of S. Kliem (HZDR).

**Table 1. Synthesis of the various methods on uncertainty of computational fluid dynamics**

| Basic methodology | Used methods | Address the sources of uncertainty | | | | | | Use of separate effect tests | Use of integral effect tests or combined effect tests |
|---|---|---|---|---|---|---|---|---|---|
| | | Initial condition and boundary conditions, | Physical models | Non-modelled processes | Numerical errors | Geometrical simplifications | Scaling distortions | | |
| Propagation method | Monte-Carlo random sampling | OK | OK | No | OK | OK | OK | Can use many | Possible |
| | Use of metamodels (e.g. PCE) | Only a few of them | | | | | | Can use many | No |
| | Deterministic sampling | Only a few of them | | | | | | Can use many | No |
| Extrapolation method | Extended UMAE | Not fully | All of them are collectively accounted for, though not explicitly and individually addressed | | | | | Must use | Must use |
| | Based on ASME | In principle may address all<br>May depend on how ASME method is extended | | | | | | No | Must use |
| Combined propagation and extrapolation method | Use of metamodels or not | A few by propagation<br>Others by extrapolation | | | | | | Can use | Must use |

Note: PCE: Polynomial chaos expansions; UMAE: uncertainty methodology based on accuracy extrapolation; ASME: American Society of Mechanical Engineers.

Source: Based on NEA, 2016a.

# 3. Objectives of a computational fluid dynamics-grade experiment

The American Society of Mechanical Engineers (ASME) has worked on a standard for verification and validation (V&V) and uncertainty quantification (UQ) for computational fluid dynamics (CFD) and heat transfer application (ASME, 2009).

The ASME VV 20 Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer states that: "The concern of V&V is to assess the accuracy of a computational simulation." In current industrial CFD modelling (non-direct numerical simulation), results come from a solved part of Navier-Stokes equations and from a modelled part of these equations. Verification of correct solving of equations (called solution verification) can be considered "tractable" even for complex flows and once it is done, uncertainty arising from physical model uncertainty is a legitimate concern.

Practically, the standard VV 20-2009 affirms that "The ultimate goal of V&V is to determine the degree to which a model is an accurate representation of the real world". This standard is strongly based on the use of experimental data for V&V and consequently for UQ. With this approach, the ASME places a strong link between V&V and UQ.

Therefore, one may define some requirements for a CFD-grade experiment by considering the requirements of the ASME standard.

The comparison error $E$ in any validation process is defined as the difference between the simulation result denoted by $S$, and the experimental value $D$:

$$E = S - D$$

If we denote $T$ as the true value, then the comparison error can be split into:

$$E = S - T - (D - T)$$

Then, one defines the experimental data error $\delta_D$ and the simulation error $\delta_s$ as follows:

$$\delta_D = D - T; \; \delta_S = S - T$$

The simulation error $\delta_s$ has three components: the error due to the physical modelling $\delta_{model}$; the numerical solution error $\delta_{num}$ produced by the numerical algorithm; and the discrete mesh used to solve the modelling equations and the input data errors (initial conditions, boundary conditions, properties, etc.) $\delta_{input}$. $E$ can be expressed as the overall result of all the errors coming from the experimental data and the simulation:

$$E = \delta_{model} + (\delta_{input} + \delta_{num} - \delta_D)$$

It is assumed that $D$ is based on an average of individual measurements, and that the error $\delta_D$ is computed using the ordinary methods of the experimental fluid dynamics, and the same assumption is valid for the experimental uncertainty $u_D$. Therefore, the uncertainty of the comparison error is given by the expression:

$$u_E = \sqrt{u_{model}^2 + u_{input}^2 + u_{num}^2 + u_D^2}$$

The components of the simulation uncertainty that can be estimated are the numerical simulation uncertainty $u_{num}$, the input data uncertainty $u_{input}$ and the experimental uncertainty $u_D$. However, there is no established method to estimate the physical modelling uncertainty $u_{model}$.

To solve this problem, the unknown error $\delta_{model}$ produced by the modelling is isolated:

$$\delta_{model} = E - (\delta_{input} + \delta_{num} - \delta_D)$$

*E*, its sign and its magnitude are known. Next, the validation uncertainty $u_{val}$ is defined as an estimation of the standard deviation of the combination of errors $\delta_{input} + \delta_{num} - \delta_D$, if these errors are really independent, the combined validation uncertainty is given by the expression:

$$u_{val} = \sqrt{u_{input}^2 + u_{num}^2 + u_D^2}$$

$u_{model}^2$ may be given by:

$$u_E^2 = u_{model}^2 + u_{val}^2$$

The ASME standard gives solutions to evaluate every term of the comparison error (E) and the validation uncertainty ($u_{val}$).

Propagation methods are mainly used to evaluate code result uncertainties coming from input parameters. Uncertainties of numerical solutions are given by the solution verification step. The standard indicates how to use the E and $u_{val}$. These quantities give an accuracy of the model used.

From $u_{model} = \sqrt[2]{u_E^2 - u_{val}^2}$ one can draw the following conclusions:

- If $u_{val}$ is relatively small, the comparison of the code prediction with experimental data can provide useful and precise information on the quality of the physical model since $u_{model} \cong u_E$.
- If an a priori model uncertainty $u_{model}$ is evaluated or expected, one can calculate the impact of this model uncertainty on any sensitive parameter of interest (or figure of merit, FoM) by sensitivity tests and compare with the impact of $u_{val}$.
- If $u_{model} < u_{val}$ the experiment is not very informative.
- If $u_{model} > u_{val}$ the experiment is capable of showing if the expected model uncertainty is reached.
- If $|E| >> u_{val}$ the model used induced more error than the validation uncertainty so the model can be improved or calibrated on the experiment in order to have less uncertainty on the result.
- If $|E| < u_{val}$ the larger uncertainty is on the validation uncertainty, which implies that the model accuracy cannot be improved if this uncertainty cannot be reduced. The standard indicates that in one or the other case, this is not proof that the model is of good or bad quality, but it gives an indication on it.

A CFD-grade experiment is an experiment that can be used to validate the physical model, which means that it provides a relatively low uncertainty of validation $u_{val}$ and allows a good determination of the model uncertainty $u_{model}$. Then, using the values of $\delta_{model}$ for many measured flow parameters, inverse uncertainty quantification methods may, in principle, be used to obtain the uncertainty of several model parameters such as C1, C2, Cμ, $Pr_k$ and Prε of the k-ε model. Inverse uncertainty quantification is currently used for system codes, but is not yet so common in CFD application. Reported applications may limit the analysis to one dominant model parameter (e.g. a turbulent Prandtl number for temperature mixing problems or a turbulent Schmidt number for a boron dilution problem).

Therefore, an experiment that minimises both $\delta_{input}$ and $\delta_D$ also minimises $u_{val}$ and provides more information on the accuracy of the model. One can consider that:

***A CFD-grade experiment should provide the lowest values of $\delta_{input}$ and $\delta_D$.***

However, the capability for an experiment to provide information on the uncertainty of model parameters may not be the concern of a reactor thermal-hydraulic safety analysis. This is the case by application of uncertainty extrapolation method. Here, the total uncertainty of all models together is the target. The final goal is often to compare a parameter of interest to a safety criterion to assess if the reactor is safe in the situation of interest. Very often, combined effect tests (CETs) or integral effect tests (IETs) are built to represent a part of a reactor circuit (e.g. the ROCOM test facility) at reduced scale trying to simulate the reactor situation of interest by respecting the non-dimensional numbers characteristic of the dominant phenomena. Due to the large dimensions and the complexity of the reactor components, it is much more difficult than in SETs to measure all of the necessary boundary and initial conditions and all flow field variables in the region of interest with a low uncertainty. Then $\delta_{input}$ and $u_{input}$ may be rather large. Such experiments should at least provide sufficient information to allow quantifying the accuracy of CFD code predictions for the relevant FoMs (the parameters of interest in the safety analysis such as some local temperatures, some boron concentrations, thermal stresses, etc.) and assessing whether such accuracy can support reliable conclusions for the safety case. In this case, the experiment should target a predetermined code uncertainty for the selected FoMs. Instead of providing data to allow quantifying the uncertainty on some specific model parameters, it should help in the determination of the uncertainties on FoMs prediction, which result from various sources of uncertainty. Minimising $\delta_{input}$ and $\delta_D$ remains the objective, but it is applied to any specified FoM. Therefore, one will consider first the requirements for CFD-grade SET, which may be used in the context of an uncertainty propagation methodology for the reactor application, then one will add some specific comments for CFD-grade CET or IET, which may be used in the context of an accuracy extrapolation methodology for the reactor application.

Another important requirement is that the design of the experiment should be done in collaboration with the code user from the beginning of the experimental project. Code users or safety analysts can then expose the goal of the experiment in terms of model validation (for example, what type of turbulence model is targeted), of target parameters necessary in the validation process, of uncertainties targeted, etc. On the other hand, CFD code users can perform pre-calculations to help design the mock-up, in terms of geometrical design, range of pressure and/or temperature reached during the future tests, choice of boundary conditions, etc.

***A CFD-grade experiment should first be characterised by a fruitful exchange between experimentalists and code users, from the beginning of the design of the mock-up to the end of the analysis of its results.***

When designing a CFD-grade experiment, it is expected that the domain of interest is clearly defined by:

- A fluid volume where phenomena are to be investigated: it is bound by solid boundaries and fluid boundaries. This fluid volume is the volume that will be simulated by the CFD.
- Inlet fluid surfaces are defined as surfaces where the fluid enters the fluid volume of interest and where inlet boundary conditions will be defined for the CFD simulation.
- Outlet fluid surfaces are defined as surfaces where the fluid leaves the fluid volume of interest and where outlet boundary conditions will be defined for the CFD simulation.
- Solids may be partly integrated to the domain of interest and domain of simulation. Depending on this, some boundaries of the solid are within the simulation domain (using conjugate heat transfer) and other boundaries will become external boundaries.

The preliminary specification of fluid and solid volumes of interest and of inlet and outlet fluid surfaces is of prime importance to select where initial and boundary conditions have to be known.

***A CFD-grade experiment should specify the fluid and solid volume of interest, the inlet and outlet fluid surfaces, the solid fluid boundaries and the external solid boundaries in a way that they can be used as input data with the required accuracy.***

A general requirement may be to define a priori acceptance criteria before designing an experiment.

If the only objective is to validate a CFD code on a specific flow configuration, the acceptance criterion may be to minimise the validation uncertainty on specific FoMs. Examples may include:

- The objective is to validate a CFD code for singular pressure losses prediction, the acceptance criterion may be that the validation uncertainty related to some predetermined pressure difference ΔP between two locations in the test section should not exceed a given percentage X%.
- If the objective is to predict the fluid temperature and wall heat transfer in a pressure vessel with a predetermined space and time resolution (e.g. for pressurised thermal shock investigation), the acceptance criterion may be that the validation uncertainty related to a predetermined temperature difference ΔT between emergency core cooling system injection and a region of the annular downcomer should not exceed a given percentage Y%.

If the objective is to determine a CFD code model parameter uncertainty, the acceptance criteria will be:

- measured flow parameters are sufficiently sensitive to the model parameter;
- measured flow parameters have a minimum validation uncertainty.

There may be reactor safety issues where the safety criterion is in a reactor component that will not be treated by the CFD tool. For example, boron dilution problems and steam line break transients are usually investigated with a coupling of a CFD tool – used from intermediate leg of a pressurised water reactor up to entrance of the core – a component code using a porous 3D model or a sub-channel analysis code for the core, and a system code for the rest of the reactor. The objective being to determine the core reactivity change, a requirement may be defined on the accuracy of the predicted temperature field or boron concentration field at inlet of the core, which will affect the reactivity. In such a case, preliminary simulations should define the requirement on the accuracy of T° or $X_{boron}$ to get the required accuracy on the reactivity. Acceptance criteria may then be defined for an experiment that simulates the mixing in the domain treated by CFD.

# 4. Scope of the analysis

CFD stands for computational fluid dynamics. This term could be used for any kind of fluid dynamic equations solved by a computer. However, in the current practice, CFD is usually applied for 3D (or 2D when some symmetry may be assumed) simulations only. CFD can be used for 1-phase, 2-phase, multiphase and multicomponent flows. Computational multi-fluid dynamics was also introduced for multi-fluid approaches.

Here our analysis will be limited to 1-phase possibly multicomponent (water-boron, air-steam-$H_2$, etc.) flow with possible heat and mass transfers within the fluid and with walls, at first. No chemical reactions are considered here.

Newtonian fluids are considered only.

In components with a lot of solid structures, the porous body approach may sometimes be used; this approach is not considered here. Only CFD in open medium with walls at the boundaries of the simulation domain are considered here, including conjugate heat transfer with a possible coupling of solid and fluid domains

CFD codes may include various approaches, such as:

- RANS-URANS approaches: time or ensemble averaging of equations for steady or slowly varying flows; turbulence is modelled over the entire range of scales.
- LES-VLES approaches: space filtered equations: necessarily 3D and transient in turbulent flows; turbulence is partly resolved (large scales) and partly modelled (small scales).

CFD-grade experiments are considered here for validation of all these approaches that are used for nuclear reactor design and safety assessment. One may list the main applications of CFD to reactors.

## Application of single-phase CFD to reactor design:

- prediction of pressure losses: regular and singular pressure losses in any geometry;
- prediction of thermal stratification/mixing;
- prediction of solid-fluid heat transfer coefficient in nominal condition (prediction of fuel temperature);
- prediction of fluid-solid interaction with mechanical efforts on solid structures: vibration, fretting;
- optimisation of temperature mixing in a core for critical heat flux investigations;
- prediction of flowrate distribution in a multichannel geometry (e.g. lower plenum).

## Application of single-phase CFD to reactor safety

Most issues are related to turbulent mixing problems, including temperature mixing or mixing of components in a mixture (boron in water, hydrogen in air, etc.):

- boron dilution;
- main steam line break;
- pressurised thermal shock;
- hot-leg temperature heterogeneities;
- induced break;
- thermal fatigue;
- hydrogen distribution in containment;
- temperature distributions in a spent fuel pool during a loss-of-coolant accident;
- special considerations for advanced (including gas-cooled) reactors.

In some mixing problems, density differences induce buoyancy effects, which have a significant influence on the mixing process.

These problems may be simulated with either RANS or LES models of turbulence or with both. For steady-state or quasi steady-state flows, one may use RANS. For rather slow and long transients (boron dilution, pressurised thermal shock, hydrogen distribution, etc.) one may use URANS. Situations where phenomena of interest are at a small timescale (e.g. thermal fatigue) may require LES, although URANS may be acceptable.

# 5. Requirements for boundary and initial conditions and physical properties of fluids and solids

Experimentally minimising $\delta_{input}$ requires accurate knowledge of:

- fluid and solid material properties;
- initial conditions in solid and fluids in transient problems;
- boundary conditions in both steady and transient problems (e.g. heat losses).

## Solid properties:

| | |
|---|---|
| Density: | ρ(P,T) |
| Specific heat | Cp(P,T) |
| Heat conductivity | λ(P,T) |
| Emissivity (if radiation is playing a role) | ε |
| Surface roughness | Ra |

Properties of most solids are known. However, in some cases, a specific measurement of properties may be needed. Also, the thermal expansion may be taken into account in some problems with significant boundary deformations.

## Fluid properties:

| | |
|---|---|
| Density (possibly) function of mass concentration: | ρ(P,T) or ρ(P,T, Xj) |
| Specific heat | Cp(P,T) or Cp(P,T, Xj) |
| Specific enthalpy or specific internal energy | h(P,T) or h(P,T, Xj) e(P,T) or e(P,T, Xj) |
| Heat conductivity | λ(P,T) or λ (P,T, Xj) |
| Dynamic viscosity | μ(P,T) or μ(P,T, Xj) |
| Mass diffusivity | Dj (P,T, Xj) |

Fluid properties of most single-component fluids are known. However, multicomponent fluids may require thermodynamic models to predict all mixture properties.

## Initial conditions in solids:

- Temperature field T(x,y,z) in the whole solid domain.

### Initial conditions in fluids:

- Temperature field T(x,y,z) in the whole fluid domain;
- Pressure field P(x,y,z) in the whole fluid domain;
- Mass concentration fields Xj(x,y,z) in the whole fluid domain;
- Velocity field $\vec{V}(x, y, z)$ in the whole fluid domain;
- Turbulent parameters in the fluid domain: k and ε, turbulent intensity.

Knowledge of initial conditions is necessary in transient problems. However, complete knowledge of all instantaneous variables in the whole domain of interest is never possible and limited information may be sufficient. One may first compare the transit timescale (or convective timescale defined as the time between fluid inlet and fluid outlet in the domain of interest) Ttr with the duration of the transient Tend-T0. If the transit timescale is very short compared to Tend-T0, precise knowledge of the initial state is usually not so important.

A pressure has to be prescribed in at least one point of the domain.

### Fluid boundary conditions on solid walls

Usually these conditions are:

- heat transfer-related: surface temperature or heat flux normal to surface or heat transfer coefficient and wall temperature;
- momentum related: wall-fluid slip conditions (no slip, free slip or imposed wall tangential velocity) and zero normal velocity or imposed velocity in case of porous wall;
- surface roughness.

### Inlet and outlet fluid boundary conditions

The type of boundary conditions in fluids depends on fluid velocity. Some general rules are:

- Transported scalars (temperature, mass concentrations, turbulent quantities, etc.) have to be given at all inlet boundaries where the transporting fluid is entering the volume of interest.
- In subsonic flow conditions (subsonic in the whole domain of interest), the velocity should be given at inlet and a pressure condition is usually given at outlet. Pressure at inlet and outlet is also an option. Since pressure is often measured only at walls, simple assumptions on the pressure field in the outlet surface may be necessary, such as uniform pressure, simple pressure profile or hydrostatic pressure field.

### Inlet fluid boundary conditions

Knowledge of mean quantities is, in principle, required in the whole surface of fluid inlet with a sufficient space resolution. In some cases, the upstream flow is designed so that the inlet velocity field is very simple:

- grids tend to homogenise the mean velocity;
- a damping chamber followed by a convergent geometry tends to decrease the turbulence intensity.

A symmetry may also decrease the need of measurements:

- axi-symmetry reduces the measurement location to a radius;
- plane symmetry reduces the measurement location to a transverse chord.

The type of averaging should be adapted to the type of turbulence models that are to be used. Ensemble averaging is very difficult to obtain in experiments and a time averaging is often used. In steady boundary conditions, the time averaging duration should be sufficient to obtain converged results. In transient flow conditions, the time averaging duration should be sufficiently small to follow the time evolution and sufficiently large to get precise results.

The velocity profile fixed by the CFD user at the inlet boundary condition cannot take into account the near wall region profile. In order to allow representative simulations of the experimental flow at inlet boundary condition, the issue of the hydraulic and thermal development of the flow must be considered when designing an experimental facility for CFD validation purposes.

The following quantities have to be known:

- local mean velocity vector (time or ensemble averaging);
- local mean temperature (if necessary);
- local mean mass concentration (if not uniform);
- fluctuations:
  - root mean square (rms) values of velocity components, of temperature and mass concentrations;
  - Reynolds stress tensor $\overline{v'_i v'_j}$;
  - turbulent heat flux $\overline{v'_i \theta'}$;
  - turbulent mass flux $\overline{v'_i X_j'}$.
- power spectra of fluctuations of velocity components, of temperature and mass concentrations (may be particularly important for LES application);
- turbulent dissipation ε is a variable of many RANS models, but is practically impossible to measure. ε may be evaluated from the turbulent kinetic energy and the spectra or from the turbulence intensity and a specified length scale;
- quasi 2D flows may need only 1D distribution of all principal variables, but a limited 2D exploration of inlet field is recommended.

The measurement of fluctuations may include rms values, correlations between fluctuations ($\overline{v'_i v'_j}, \overline{v'_i \theta'}, \overline{v'_i X_j'}$) and power spectra. If limited to rms values, it is still possible to provide boundary conditions to some RANS turbulence models such as k-ε. When Reynolds stresses are available, they may provide accurate boundary conditions to Rij-ε models. If spectra are available, they may be used to build instantaneous boundary conditions to LES models.

## Outlet fluid boundary conditions

In subsonic flow conditions, a pressure condition is usually given at outlet. Since pressure is often measured only at walls, simple assumptions on the pressure field in the outlet surface may be necessary, such as uniform pressure or hydrostatic pressure field. The pressure boundary condition may be a condition on the pressure, on the pressure axial gradient $\partial P/\partial n$ or even on a double derivative of pressure $(\partial^2 P)/\partial n \partial t$. If assumptions on the pressure field at outlet are necessary, the assumptions should be justified or even checked with some measurements.

"Opening" conditions exist in CFD codes, which authorise backflow at the outlet boundary

Backflow at the outlet condition can be a source of uncertainty due to additional parameters to be known (backflow temperature and other scalar, etc.). Such backflow may be influenced by external flow processes that are not simulated and, in general, such boundary conditions are not recommended.

If backflow at the outlet condition is expected, preliminary CFD calculations can be useful in order to check if a possible geometrical configuration can avoid the backflow issue. If it is not possible (for example in case of vortices exiting the fluid domain), precise information is needed on temperature, mass concentration and velocity of fluid backflow at the outlet condition and specific conditions that authorise fluid backflow has to be used ("opening" type).

In some cases, the outlet condition can be a mass flow rate imposed (pump imposing the mass flow rate after the test section).

## Recommendations

Preliminary sensitivity calculations to uncertainty of inlet conditions are recommended before selecting the measurement technique. Most sensitive fields should be determined with special care.

Preliminary sensitivity calculations to outlet conditions are recommended, including the outlet locations to find the best location that makes boundary conditions easier to handle.

# 6. Requirements for flow parameters measurement

Flow parameters have to be measured in the domain of interest particularly where important phenomena take place. All regions of the flow with shear layers such as boundary layers, mixing layers, jets, should be well instrumented. The measurements will allow the validation of some models of the computational fluid dynamics (CFD) tools that will later simulate the tests. A large number of measured parameters and a high number of measurement locations will provide better validation capabilities. However, measuring all principal variables everywhere is never possible or would be too long and expensive. Moreover, measurement devices are often intrusive, and could modify the downstream flow. Compromises are necessary following some general principles:

- An equation model may be precisely validated when all n principal variables are known. This does not necessarily mean that all variables are measured with the same density of measuring points. For example, the knowledge of pressure in a few locations may be sufficient.
- If pressure losses are investigated, more detailed pressure measurements are necessary.
- Even if pressure losses are not particularly investigated, measuring irreversible ΔP losses reflects the turbulent dissipation and contributes to turbulence model validation.
- The mean velocity field in shear layers is of prime importance and should be the first priority, since the velocity field strongly influences the mixing of all scalars and momentum turbulent diffusion is also coupled to scalar turbulent diffusion.
- For models other than LES, lack of velocity fluctuation measurement still enables the global efficiency of a turbulence model to be validated, but the closure laws of the additional transport equations for k, ε, $\overline{v'_i v'_j}$, used in some models will not be validated.
- For the LES model, the lack of velocity fluctuation measurement does not enable accurate model validation.
- The mean temperature and/or mass concentration fields in shear layers are also of prime importance when the mixing of all scalars is investigated.
- The lack of temperature and/or mass concentration fluctuation measurement still enables the global efficiency of a turbulence model to be validated, but closure laws of the additional transport equations for $\overline{\theta'^2}$ , $\overline{v'_i \theta'}$, $\overline{v'_i X_j'}$ used in some models will not be validated.
- The lack of frequency spectrum of fluctuations does not enable the LES to be fully validated.

- Turbulent dissipation ε is a variable of many RANS models, but is practically impossible to measure. When both the turbulence intensity and the velocity spectra or turbulent kinetic energy are available, ε may be derived from them.
- When investigating momentum, energy or mass diffusion processes, the measurement of the evolution of transverse profiles of mean and fluctuating quantities along the flow is necessary.
- Quasi 2D flows may need only 1D distribution of all principal variables, but a limited 2D exploration is recommended.
- Application of invasive measurement techniques has to be carefully analysed. The intrusive nature of each measurement device has to be evaluated to determine where each of them has to be placed in co-ordination with the other measurement devices. In some cases, the intrusive nature of the devices may require performing several identical experimental tests with only a variation of the location of the device. Even if the measured quantity is not disturbed, other measurements can be influenced.
- Near-wall measurements of velocity, temperature and fluctuations.

The near-wall region is mainly treated with models (single-phase law of the wall with corrections for roughness) in CFD codes. More precise measurements of the flow parameters in the near-wall region can validate and help improve these models. In particular, investigation of the effect of roughness can be useful.

## Recommendations

It is recommended to give an objective to the experiment by identifying:

- the main physical processes of interest;
- the target in terms of type of turbulence models that may be validated.

The choice of the measured parameters should be made after the objectives are clearly defined.

The measurement of fluctuations may include root mean square (rms) values, correlations between fluctuations ($\overline{v'_i v'_j}, \overline{v'_i \theta'}, \overline{v'_i X_j'}$) and power spectra:

- If limited to rms values, it is still possible to validate some RANS turbulence models such as k-ε. It can also provide a partial validation of a LES model.
- When Reynolds stresses are available, they may provide accurate boundary conditions to Rij-ε models.
- If spectra are available, they may provide information to build boundary conditions to LES models.
- The knowledge of spectra may help validate the turbulent dissipation equation when it is used.

It is also highly recommended to run preliminary CFD calculations to define the best measurement locations, taking into account the intrusive nature of the measurement devices.

# 7. Requirements for measurement uncertainty

Providing reliable evaluation of measurement uncertainty is a very difficult task, but is mandatory in a computational fluid dynamics (CFD) code validation perspective and for determining the model uncertainty. As mentioned above, an experiment that minimises $\delta_{input}$ and $\delta_D$ also minimises $u_{val}$ and provides more information on the accuracy of the model.

## Recommendations

- All measured variables should have a careful uncertainty determination, including uncertainty linked to the repeatability.
- In case of the intrusive measurement method, the impact on the measured flow parameter should be at least estimated.
- Comparison between several local methods measuring the same flow parameter is recommended.
- Repeatability tests should be performed in both steady and transient tests. The goal is to evaluate uncertainties on the target parameters (if the boundary conditions are not sufficiently well known), to detect a significant sensitivity to initial conditions and to identify possible chaotic behaviour.
- Local methods (velocity) confronted to integral methods (flowrate) is recommended. In the presence of heat transfers, integral energy conservation should be checked to verify the consistency of available measured parameters (velocity, temperature, heat flux).
- Preliminary sensitivity calculations of measured variables to uncertainty of a model parameter of interest (e.g. a turbulent Prandtl number) of field variables within the CFD domain are recommended to be compared to $u_D$. If $u_D$ is larger than an *a priori* or expected model uncertainty $u_{model}$, the experiment will not be very informative.
- A systematic analysis of all possible sources of errors or uncertainty should be made that may include:
    - errors due to space resolution that filters space variations;
    - errors due to imperfect knowledge of the locations of the sensors;
    - errors due to time resolution that filters time variations (inertia of the sensor);
    - errors due to non-fully converged time averaging;
    - error from imperfect signal treatment;
    - uncertainty due to the limited sensitivity of the sensor;
    - bias due to statistical treatment of a sample of discrete measurements;
    - any other source.

This is a very difficult and heavy task and very few experimental data are provided with a full evaluation of uncertainties. Some uncertainties may also be provided which are not fully reliable. Therefore, there is a clear need for a guide for experimentalists that gathers all the available knowledge on sources of uncertainty for every type of sensor used in CFD-grade experiments.

# 8. Feedback from some computational fluid dynamics experiments and benchmarks

Looking at validation experiments for computational fluid dynamics (CFD), it appears that some existing data suffer from some weaknesses:

- lack of local measurements;
- insufficient number of measured flow variables;
- lack of well-defined initial and boundary conditions;
- lack of information about experimental uncertainty.

This may be related to insufficient preliminary collaboration between CFD code users and experimentalists and insufficient specification of the requirements.

Experience gathered in past exercises, benchmarks and any CFD validation may be useful to avoid errors or limitations in future CFD-grade experiments.

The PSBT (PWR subchannel and bundle tests) and BFBT (BWR full-size fine-mesh bundle test) benchmarks offered a unique possibility of code validation against void fraction repartition in a pressurised water reactor (PWR) and boiling water reactor (BWR) rod bundle in high velocity flow. However, a deformed geometry was suspected (not proved), and consequently the boundary and initial conditions were not very accurate. More attention should be paid to the exact knowledge of the solid boundaries in future experiments.

Several Tee-junction experiments were designed for thermal fatigue investigations. In this case, the prediction of large-scale fluctuations is necessary. It appears that this requires very good knowledge of inlet conditions, not only the mean velocity field, but also the fluctuations. It was suspected that specific eddies created in a tube bend rather far upstream could influence the characteristics of the large eddies of interest in the mixing zone.

The MATIS-H rod bundle benchmark offered very detailed information of flow in a rod bundle downstream a spacer grid. Some simulations found a rather high sensitivity to the outlet boundary conditions and to the position of the outlet boundary. This illustrates the need to also properly characterise the outlet boundary conditions.

The PANDA test facility was used for a benchmark on stratification of $H_2$ layer erosion by a jet. Some sensitivity to inlet conditions in jet pipe and to initial conditions was found, which illustrates the need of preliminary CFD calculations before a test specification.

GEMIX mixing tests were envisaged for a CFD benchmark including uncertainty quantification. It was first found that measurements in inlet conditions were not sufficient, although the flow was carefully homogenised by grids. Additional velocity (mean and root mean square [rms] values) measurements were added. After comparing the calculations with data in a blind benchmark, a measured peak of turbulence intensity was never predicted by any code. After analysis, a possible effect of density and refraction index fluctuations on the measurement was suspected. Difficulties arose from the use of brine together with laser measurement techniques.

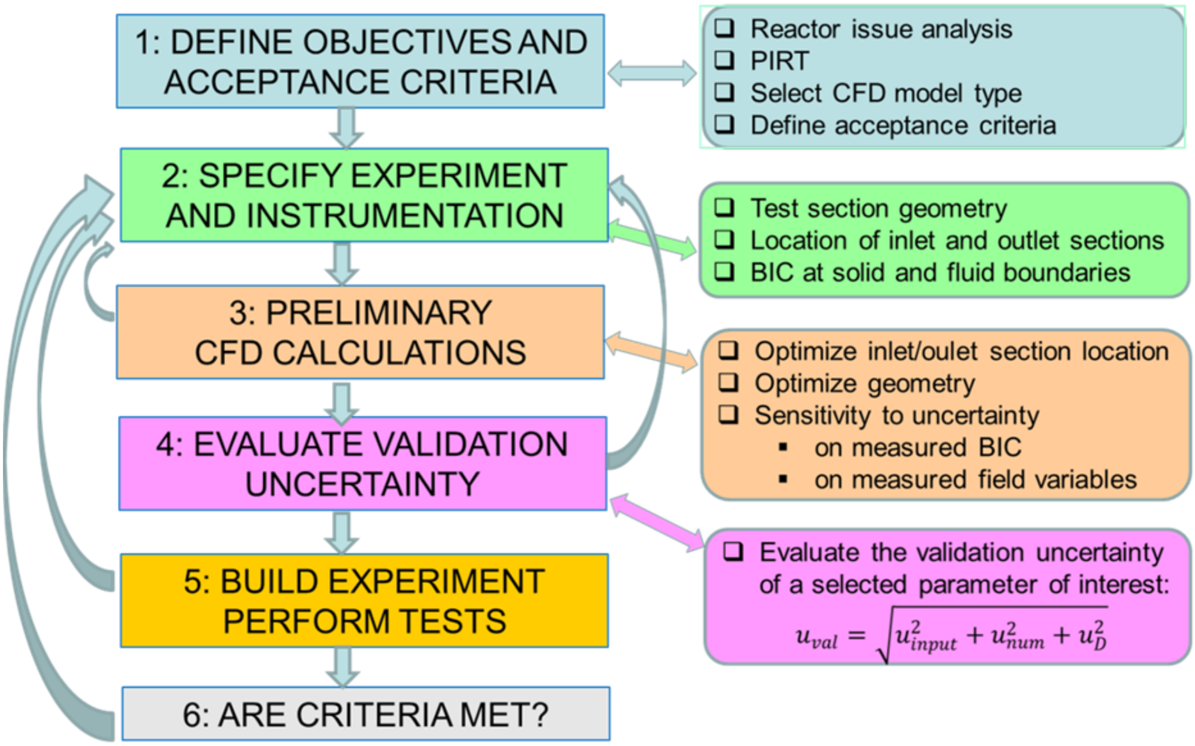
A generic problem is encountered when a part of a closed reactor circuit is simulated by CFD. Boundary conditions of this CFD part are not well known and can be approximated only by a macroscopic model (1D) or from established flow assumption whereas no established flow exists in a reactor. For such reactor applications of CFD, strategies to reduce the uncertainty of the boundary and initial conditions should be established: choice of the domain of CFD, preliminary CFD on a large domain compared to a smaller domain, etc.

# 9. Recommended roadmap for the design of computational fluid dynamics-grade experiments

A computational fluid dynamics (CFD)-grade experiment should first be characterised by a fruitful exchange between experimentalists and code users, from the beginning of the design of the mock-up to the end of the analysis of its results.

A multi-step method can be proposed to design a CFD-grade experiment as illustrated in Figure 3.

**Figure 3. Roadmap for designing and performing a computational fluid dynamics-grade experiment**




Note: PIRT: phenomena identification and ranking table; CFD: computational fluid dynamics; BIC: boundary and initial conditions.

## Step 1: Objectives

The first step is to assign clear objectives to the experiment:

- Identify the main physical processes of interest. Processes of interest may be generic processes, like temperature mixing, mixing of a mass concentration in case of a multicomponent flow, buoyancy driven natural circulation, pressure losses, heat transfers with solid structures, large-scale flow fluctuations and associated time fluctuations of velocities, temperatures and wall heat transfers.

- Identify the type of turbulence models that may be validated.
- If the experiment is devoted to nuclear reactor safety, identify the safety demonstration methodology that may need the use of this experiment. In particular, attention must focus on the uncertainty quantification method that may be used in a best estimate plus uncertainty methodology. The planned experiment should also be put in the framework of a general validation matrix.
- Define the figures of merit (FoMs) and acceptance criteria for the experiment.

### Step 2: Specifications

At this step, discussions between experimentalists and CFD code users are recommended to make the basic design of the facility, define the test conditions and select the measurement techniques. The needs have to be confronted to the experimental potentialities.

The geometry of the test section and general conditions of the tests to perform are first defined to answer the needs and to address the physical processes of interest.

The choice of the measured parameters should be made to meet the objectives and to investigate the processes of interest.

Then detailed test conditions are to be defined by the following:

- specify the fluid and solid volume of interest that will be later simulated by CFD;
- specify the inlet and outlet fluid surfaces;
- specify the solid fluid boundaries and the external solid boundaries;
- define requirements on boundary and initial conditions (BIC), physical properties;
- define requirements on measurement uncertainty;
- target some type of CFD model, either RANS (eddy viscosity based or Reynolds stress based) or LES or even hybrid model and define requirements on what to measure and where depending on the targeted type of CFD model.

### Step 3: Preliminary CFD calculations

When the test section is designed to address the physical processes of interest, preliminary calculations may be useful:

- Sensitivity calculations to uncertainty of inlet boundary conditions are recommended before selecting the measurement technique. Most sensitive fields should be determined with special care.
- Sensitivity calculations to outlet boundary conditions are recommended varying the outlet locations and possibly the type of outlet conditions.
- Calculations to define the best measurement locations in the test section.

Feedback on the specification step is possible if necessary, possibly including the test section geometry.

### Step 4: Evaluation of expected validation uncertainty

A CFD-grade experiment should provide the lowest values of $\delta_{\mathrm{input}}$ and $\delta_{\mathrm{D}}$ related to the exhaustive BIC specification, to the physical properties and to the measurement accuracy. After having defined the FoM based on available measurements, the global validation uncertainty on this FoM is evaluated.

- all measured field variables should have a careful evaluation to determine $\delta_{\mathrm{D}}$ on the field variable;
- all BIC variables should have a careful evaluation to determine $u_{input}$;
- preliminary calculations are used to evaluate the numerical uncertainty $u_{num}^2$;
- the resulting validation uncertainty on the FoM is determined by:

$$u_{val} = \sqrt{u_{input}^2 + u_{num}^2 + u_D^2}$$

If the acceptance criterion (criteria) is (are) met, one can go to the next step. If it/they is/are not met, feedback on Step 2 is possible to change the measurement technique, or to add measurements in the inlet and outlet fluid boundaries, or even to improve the measurement technique.

### Step 5: Building of the test facility and performing the tests

The test facility is built according to specifications and tests are carried out following the specified test conditions. Repeatability tests are mandatory to check and evaluate uncertainties on FoM. Then a posteriori verifications may be done after a comparison to the code simulations if unexplained differences are observed.

### Step 6: Final check of experiment suitability

Normally, the defined test conditions are not exactly the same as those observed during the experiments. Sometimes the differences are significant. The check of actual experimental uncertainties and a new evaluation of validation uncertainty allows proving the quality of the experimental work and eventually gives an indication what can (or needs to) be improved. Finally, it would provide information, if the experiment met the acceptance criteria and is suitable for the purpose of validation.

# 10. Specific comments for computational fluid dynamics-grade combined effect tests or integral effect tests

Due to the specific difficulties related to combined effect tests (CETs) and integral effect tests (IETs), there cannot be the same density of instrumentation in all parts of the test facility as in separate effect tests (SETs). The general principles applicable to CFD-grade SET experiments also have to be followed in CETs or IETs as far as possible and the same roadmap must be followed.

## Step 1: Define objectives and acceptance criteria

The general objective of the experiment must be clearly identified together with the reference reactor, the scenario and the figures of merit (FoMs) with the expected accuracy (see Chapter 2). The type of CFD model that will be used for the validation and for the reactor application is selected in order to select the appropriate quantities to be measured in initial conditions and boundary conditions.

## Step 2: Specify experimentation and instrumentation

Preliminary CFD calculations have to be performed during the specification step at both the reactor scale and at the experiment scale of the planned test in order to:

- Identify the regions of interest where important phenomena affecting the FoM are taking place. Check that the same phenomena may take place qualitatively and quantitatively in the experiment as in the reactor.
- The selection of the nature and the locations of the measured parameters should be made to make the validation of the models that control the processes of interest possible.
- A sufficient number of measured parameters has to be chosen to avoid compensation errors.
- Attention should be paid to geometrical details that may have an influence, such as sharp edge or rounded edge connections, obstacles, etc. Check that simplification of the geometry does not significantly affect the process of interest, as far as the code model is able to see this effect. This is an a priori verification that may be complemented by *a posteriori* verifications (see below).

## Step 3: Preliminary calculations

CET also needs preliminary calculations at the experiment scale:

- Sensitivity tests to the assumed uncertainty on boundary and initial conditions (BIC) corresponding to the planned instrumentation are necessary to check that the impact on the uncertainty of the FoMs is not too high.

- An estimation of the total uncertainty of the predicted FoM coming from all sources of uncertainty other than physical modelling is necessary to determine if the test will be useful for the safety analysis. If necessary, some sources of uncertainties (BIC, measurement uncertainty) have to be reduced by additional efforts on the instrumentation.

### Step 4: Evaluate validation uncertainty

- If CFD code users intend to use an uncertainty evaluation of the code models for uncertainty quantification (UQ) of the CFD simulation in a general UQ method, a preliminary estimation of the total uncertainty of the predicted FoM coming from all sources of uncertainty including physical modelling is necessary to determine if the test will be useful for the safety analysis.

### Step 5: Build the test facility and perform the tests

When the test facility is built and the tests are started, some recommendations are:

- An *a posteriori* check of the physical behaviour in the regions where important phenomena affecting the FoMs were expected is recommended to confirm the preliminary analysis. If necessary, more precise experimental investigations in other regions of the test facility may be added.
- Possible sensitivity tests by changing some geometrical details that may have an influence – such as sharp edge or rounded edge connections, obstacles, etc. – may provide valuable information on the real influence of these details.
- Repeatability tests are mandatory.

# 11. Conclusions

The design of validation experiments for computational fluid dynamics (CFD) application to reactor simulation still requires some guidelines to check that they will be able to provide the expected information on the accuracy of reactor simulations. In an attempt to establish requirements for CFD-grade experiments, a multi-step roadmap is proposed and recommendations and guidelines provided. Collaboration between code users and experimentalists at the beginning of the design is required to lay out clear objectives and define the specifications of the test facility and the instrumentation. This is placed in the general framework of a best estimate plus uncertainty approach for safety analysis of some reactor transients. Preliminary calculations are necessary in the design process and the uncertainty of validation must be evaluated to check that the experiment will be informative enough on some predetermined figure of merit.

This document is expected to help build more useful future experimental programmes, although the proposed guidelines and recommendations still need to be complemented and improved.

A significant effort should be made in the future to establish practical guidelines for estimating the experimental uncertainty, which seems to be the weak point in the current roadmap. This could justify a future joint activity between the NEA Working Group on the Analysis and Management of Accidents' CFD Task Group and the SILENCE network to write a guide for experimentalists that gathers all the available knowledge on sources of uncertainty for every type of sensor used in CFD-grade experiments.

# *References*


ASME (2009), *Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer*, VV 20-2009(R2016), American Society of Mechanical Engineers, New York, NY, www.asme.org/codes-standards/find-codes-standards/v-v-20-standard-verification-computational-fluid-dynamics-heat-transfer.

ASN and IRSN (2017), "Qualification of scientific computing tools used in the nuclear safety case – 1st barrier", Guide No. 28 (version of 25/07/2017), Autorité de Sûreté Nucléaire, Montrouge, www.asn.fr/professionnels/installations-nucleaires/centrales-nucleaires/guides-de-l-asn-dans-le-domaine-des-installations-nucleaires/guide-de-l-asn-n-28-qualification-des-outils-de-calcul-scientifique-utilises-dans-la-demonstration-de-surete-nucleaire.

Bestion, D. (2010), "Extension of CFD code application to two-phase flow safety problems", *Nuclear Engineering and Technology*, Vol. 42/4, http://dx.doi.org/10.5516/NET.2010.42.4.365.

Höhne, T. and S. Kliem, (2020), "Detailed Simulation of the Nominal Flow and Temperature Conditions in a Pre-Konvoi PWR Using Coupled CFD and Neutron Kinetics", *Fluids* 2020, 5, 161, https://doi.org/10.3390/fluids5030161.

NEA (2016a), "Review of Uncertainty Methods for Computaional Fluid Dynamics Application to Nuclear Reactor Thermal Hydraulics", CSNI/R(2016)4, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_19700.

NEA (2016b), "The Nuclear Energy Agency-Paul Scherrer Institut Computation Fluid Dynamics Benchmark Exercise", 9-11 September 2014, Zurich, Switzerland, NEA/CSNI/R(2016)2, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_19696.

NEA (2016c)," Computational Fluid Dynamics for Nuclear Reactor Safety-5 (CFD4NRS-5) Workshop proceedings", NEA/CSCI/R(2016)1, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_19694.

NEA (2015), "Best Practice Guidelines for the Use of CFD in Nuclear Reactor Safety Applications – Revision", NEA/CSNI/R(2014)11, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_19548.

NEA (2014a), "Assessment of CFD codes for nuclear reactor safety problems – Revision 2", NEA/CSNI/R(2014)12, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_19550.

NEA (2014b), "Extension of CFD codes application to two-phase safety problems – Phase 3", CSNI/R(2014)13, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_19560.

NEA (2014c), "Proceedings of the OECD/NEA & IAEA Workshop CFD4NRS-4", 10-12 September 2012, DaeJeon, Korea, NEA/CSNI/R(2014)4, OECD Publishing, Paris, www.oecd-nea.org/nsd/docs/2014/csni-r2014-4.pdf.

NEA (2013), "Report of the OECD/NEA KAERI rod bundle CFD benchmark exercise", NEA/CSNI/R(2013)5, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_19286.

NEA (2011a), "Report of the OECD/NEA-Vattenfall T-junction benchmark exercise", NEA/CSNI/R(2011)5, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_19022.

NEA (2011b), “Proceedings of the CFD for Nuclear Reactor Safety Applications (CFD4NRS-3) Workshop”, NEA/CSNI/R(2011)14, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_19112.

NEA (2010), “Extension of CFD codes to two-phase flow safety problems”, NEA/CSNI/R(2010)2, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_18898.

NEA (2008a), “Assessment of Computational Fluid Dynamics (CFD) for Nuclear Reactor Safety Problems”, NEA/CSNI/R(2007)13, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_18504

NEA (2008b), “Proceedings of the OECD/NEA & IAEA Workshop: Experiments and CFD code applications to nuclear reactor safety”, Joint OECD/NEA and IAEA Workshop, 10-12 September 2008, NEA/CSNI/R(2009)12, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_18864.

NEA (2007a) “Best Practice Guidelines for the use of CFD in Nuclear Reactor Safety Applications”, NEA/CSNI/R(2007)5, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_18444.

NEA (2007b), “Workshop on Benchmarking of CFD Codes for Application to Nuclear Reactor Safety (CFD4NRS)”, Garching (Munich), Germany, 5-7 September 2006, NEA/CSNI/R(2007)3, OECD Publishing, Paris, www.oecd-nea.org/jcms/pl_18440.

NEA (2006), “Extension of CFD codes to two-phase flow safety problems”, NEA/SEN/SIN/AMA(2006)2, OECD Publishing, Paris.