

AN OVERVIEW OF PAST AND PRESENT CFD ACTIVITIES WITHIN THE FRAMEWORK OF WGAMA

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Abstract

In 2003, three *Writing Groups* (WG1, WG2, WG3) were established within the Working Group on Analysis and Management of Accidents (WGAMA) of the OECD Nuclear Energy Agency. The groups had the responsibility of summarising the state-of-the-art in the application of Computational Fluid Dynamics (CFD) to items of concern in nuclear reactor safety. The Best Practice Guidelines (BPGs) drawn up by the WG1 group defined the procedures which need to be followed to produce trustworthy results from a CFD simulation. The WG2 group itemised the assessment base which underpins single-phase CFD as an established technology. The WG3 group focused on the challenges that still need to be faced before two-phase CFD may be regarded as a mature science. The background to the activity, method of approach, documented evidence, status and current activities are described under appropriate section headings in this paper.

Introduction

The spectacular growth in computer hardware over the last 30 years, accompanied by the development of stable and efficient numerical algorithms, has created a situation in which the use of computational methods has reduced the reliance on scale-model tests in the safety analysis of reactor systems. During this time, very reliable system codes, such as RELAP-5 [1], TRACE [2] and CATHARE [3] for example, have been used in the analysis of primary circuit transients. Other programs, such as GOTHIC [4] and GASFLOW [5] are used for containment analyses, and MAAP [6] and MELCOR [7] for severe accidents. The application of CFD methods to problems relating to Nuclear Reactor Safety (NRS) is less well developed, but is accelerating.

One of the reasons why the application of CFD methods in the NRS area has been slow to establish itself is that transient, two-phase events associated with accident analyses are extremely complex. Traditional approaches using system codes have been successful because of the very large database of phasic exchange correlations on which they are based. The correlations have been formulated from essentially 1-D special-effects experiments, and their range of validity has been very well scrutinised. Data on the exchange of mass, momentum and energy between phases for 3-D flows is very sparse in comparison. Thus, although 1-D formulations may restrict the use of system codes in simulations in which there is complex geometry, the physical models are well-established and reliable, provided they are used within their specified ranges of validity. The trend has therefore been to continue with such approaches, and live within their geometric limitations. However, fluid flow situations arise which are strongly 3-D in character. A model approach involving networks of

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1-D or even 0-D elements may then be not only a gross oversimplification, but misleading, and erroneous conclusions could be drawn from the results. Typical situations of this type are flows in the upper/lower plena, downcomer and core of a reactor vessel, and circulation, mixing and stratification in the pipe network and containment volumes. CFD codes, with full 3-D capability, are the most appropriate numerical tools to use in these circumstances, provided the physical models within them can be substantiated.

With a growing awareness of the emerging role for CFD analyses in nuclear reactor technology, a CSNI^{*} action plan was drawn up on the recommendations of the OECD/NEA[%] and IAEA[±] to create three Writing Groups, with mandates to perform the following tasks:

- WG1 Provide a set of Best Practice Guidelines for the use of CFD in NRS problems;
- WG2 Evaluate the existing CFD assessment bases, and identify gaps that need to be filled;
- WG3 Summarize the extensions needed to these codes for two-phase NRS applications.

Work began early in 2003. Teams of experts were assigned to the groups representing the following OECD member countries: the Czech Republic, France, Germany, Italy, Japan, S. Korea, the Netherlands, Norway, Sweden, Switzerland and the USA. Each of the groups prepared preliminary reports which scoped the work needed to be carried out to fulfil the mandate, and which made recommendations on how to achieve their defined objectives. In January 2005, all three groups were reformed to carry out their tasks. Each group issued a CSNI report [8,9,10], which can be considered a state-of-the-art on the respective subject area at the time of issue.

The present paper summarises the work undertaken by the Writing Groups, as described in detail in the CSNI reports, and some follow-up activities that have been initiated since their issue. The Best Practice Guidelines (BPGs) drawn up by WG1 define the procedures which need to be followed to produce trustworthy results from a CFD simulation. The WG2 document focuses on the verification and validation procedures that have been carried out to ensure that single-phase CFD is an established technology. The assessment is based on material assembled in both nuclear and non-nuclear areas, since often the flow situations are similar. The WG3 document itemises the challenges that still need to be faced before two-phase CFD may be regarded as a mature science. These are mainly in establishing appropriate 3-D closure laws governing inter-phase transfer of mass, momentum and heat, wall-to-fluid heat transfer, and generalising single-phase turbulence models for two-phase application.

Though the responsibilities of the Writing Groups formally ended with the issue of the CSNI reports, many tasks remain ongoing due to the creation of new initiatives. First is the establishment of a web portal to act as a dynamic basis for the material collected and collated by the groups. The portal has been constructed using Wiki software to enable users to find information they need via appropriate web links, and to actively participate in the maintenance and updating of the site. A special WGAMA *CFD Task Group* has been set up to this purpose. A smaller core group, the *CFD Special Group*, also operating within the framework of WGAMA, organises, on a biennial basis, a series of international workshops under the title CFD4NRS, which are aimed at providing suitable

^{*} Committee on the Safety of Nuclear Installations

[%] Organisation for Economic Co-operation and Development/Nuclear Energy Agency

[±] International Atomic Energy Agency

forums in which experimenters and CFD practitioners can exchange topical information dedicated to the application of CFD in nuclear reactor safety. This group also provides the organisational basis for launching international CFD benchmarking exercises. All these activities are also described in this paper.

1. WG1: Best Practice Guidelines

1.1 Background

Twelve WGAMA member organizations participated in writing the BPG document. Their representatives, who acted as co-authors of the report, are listed in Table 1. The group met twice per year for summary discussions, starting in May 2003 and concluding in September 2006 with formal submission of the report [8], approved by WGAMA, to the CSNI for approval. All other exchanges were undertaken remotely. The primary purpose of the document was to provide practical guidance for the application of single-phase CFD to the analysis of nuclear reactor safety (NRS) issues. Initially, it was intended to also include guidance on two-phase CFD applications to NRS, but this was later considered too ambitious, and anyway such a task should only be undertaken after preparation of the WG3 document, which deals with the model extensions needed for this.

Table 1. Contributors to the BPG document.

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B. Chung	KAERI	KO	P. Mühlbauer	NRI	CZ
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One of the main focus points for the use of single-phase CFD in industrial flows is the appropriate choice of turbulence model. Reynolds Average Navier-Stokes (RANS), Large Eddy Simulation (LES) and Detached Eddy Simulation (DES) models were all considered in this context. The inclusion of Direct Numerical Simulation (DNS) was considered premature for practical NRS applications. The full range of issues associated with a high quality CFD analysis was covered by the group. This begins with proper definition of the problem to be solved, and the selection of an appropriate simulation tool. For the probable range of tools, generic guidance was provided on the selection of physical models and numerical issues, including creation of a suitable spatial grid. Both structured and unstructured meshing strategies were discussed. To complete the process of analysis, guidance was also provided for verification of the input model, validation of results, and documentation of the project application.

Although the primary target audience could be considered to be the less experienced CFD practitioners, the document should also be valuable to a wider audience. High-quality CFD analysis is a complex process, with many steps, and many opportunities to forget important details. More experienced CFD users should find value in the checklist of steps and considerations provided at the end of the document, and summarized here in the Subsection 1.4 below. Project managers should

find the discussion useful in establishing the level of effort needed for a new analysis, and regulators should find the document to be a valuable source of questions to ask those using CFD in support of licensing requests.

The WG1 BPG document is built on, and extends, other sources of guidelines for the use of CFD, both of the generic and specialized type. The European Research Community On Flow, Turbulence And Combustion (ERCOFTAC) produced a general set of guidelines for the creation of CFD input models [11,12], though the main application area in this case was turbo-machinery. In the area of reactor safety analysis, a set of guidelines was produced within the ECORA project [13]. Similar guidelines were produced specifically for marine applications by MARNET [14], and the AIAA had previously produced a short guidelines document on verification and validation [15].

The BPG document produced by WGI was intended to be as internally complete as possible. Specific guidance, that might also be available in the above publications, is provided in the context of NRS and the experience of the group in using CFD. However, “internally complete” does not imply that the document is exhaustive. No attempt is made, for example, to cover the full history of turbulence theory and modelling, nor the full range of turbulence models available today in CFD software. For more details on these subjects, the reader is referred to specialist papers on the subject, such as the recent work of Wilcox [16].

1.2 Modelling Guidelines

The BPG document begins with a summary of NRS-related CFD analyses being carried out in the countries represented by the WG1 members, to provide a scope for the existing range of experience. Examples cited in the summary date back as far as the late 1970s, but most analyses discussed were performed after 2000. In parallel, the WG2 group (see Section 2) were compiling a list of safety issues for which (single-phase) CFD is considered to bring benefits in terms of better insights, understanding and quantification. This material also points to the application areas in which the BPGs were concentrated. These included all aspects of 3-D single-phase mixing, and in addition there is an extended discussion of special modelling needs within single-phase CFD for: containment wall condensation; pipe wall erosion; thermal cycling; hydrogen deflagration and detonation; fire analysis; water hammer; liquid-metal systems; and natural convection. Some specific areas are listed here by way of illustration.

1. Turbulent flows in various rod bundle geometries;
2. Pressurized thermal shock;
3. Boron dilution transients;
4. Flow mixing and stratification in plant loops;
5. Natural circulation in the reactor primary circuit;
6. Thermal fatigue in a mixing tee;
7. Hydrogen distribution in a containment during a severe accident;
8. Flows induced by hydrogen recombiners in containments;
9. Breaks induced by high temperature steam during a severe accident;
10. Detailed analyses to improve understanding of boiling heat transfer;
11. Natural circulation in pools;
12. Steam-jet-driven circulation in pools;
13. Strainer clogging in a containment sump;
14. Fluid/structure interactions (particularly at the start of a large pipe-break);

15. Cooling issues associated with spent fuel storage casks.

Given such a diverse application area, it was not possible to give case-specific instructions on the procedures to follow to produce quality CFD predictions for each item on the list. Instead, four items (2,3,7,15) were discussed in extended form by way of illustration of the general BPG approach. The compilation of precise guidelines for other entries on the list is then left as a follow-up exercise. The interested reader is referred to the full CSNI report [8] for more details.

1.3 Overall Strategic Approach

Computer simulation is much more than generating input and plotting results. In an NRS project producing trusted results, these activities do not even occupy the majority of the staff time expended. A project must begin with a clear written statement of the problem, including identification of the specific system and scenario to be analysed. Figure 1 graphically depicts the procedural steps to be followed. Ideally, things start with a PIRT, a *Phenomena Identification and Ranking Table* [17].

The PIRT approach originated as part of the US NRC's methodology for the use of best-estimate simulation codes in the licensing of nuclear power plants. Phenomena and processes are ranked in the PIRT based on their influence on primary safety criteria, and subsequent efforts are focused on the most important of these. This process has broadened over the years, and is now used outside the nuclear community as well, and now represents an important component of any assessment process.

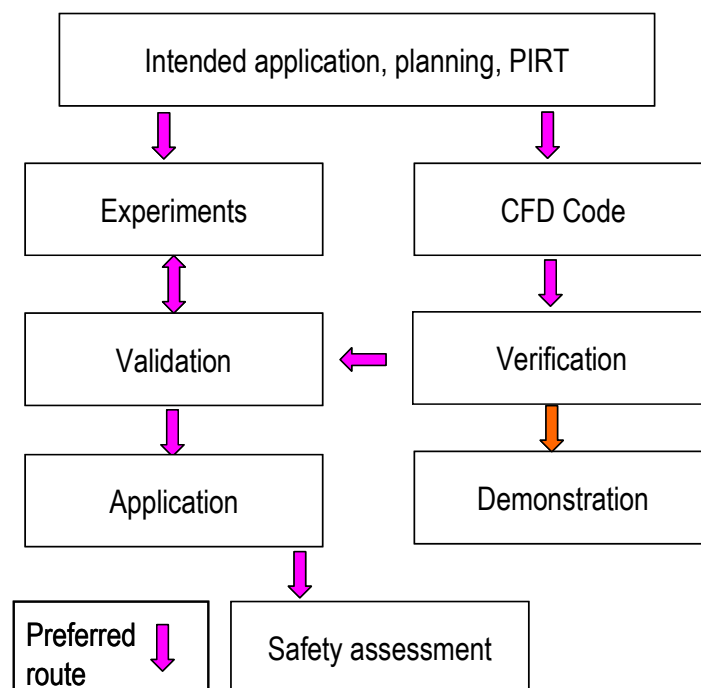


Figure 1. An assessment procedure from conception to final product.

Step #1 of the PIRT is a careful definition of the objectives of the exercise. It is often more effective to define a series of specific PIRT exercises (e.g. boron dilution) rather than trying to cover everything with a very general exercise (e.g. Small-Break Loss of Coolant Accident SB-LOCA). At

Step #2, a panel of experts is appointed. The panel should have both technical and managerial expertise. At least one member should have a primary focus in each of the following areas, relevant to the scenario being studied:

- Experimental programs and facilities;
- Simulation code development (numerical implementation of physical models)
- Application of relevant simulation codes to this and similar scenarios;
- Configuration and operation of the system under study.

At Step #3, the panel reviews the defined objectives, system and scenario to identify parameters of interest (e.g. boron concentration at core inlet for the boron-dilution problem). Step #4 consists of identifying existing information that can be used to verify the coding, and to validate the physical models in the code over the range of conditions in the specified scenario. This step relies heavily on the knowledge and experience of the panel members, but can be broadened. Step #5 involves identification of the key physical phenomena involved in the specified scenario (e.g. turbulent mixing). This is followed by Step #6 in which these phenomena are ranked in terms of importance. Perhaps initially this can be in terms of a low/medium/high categorization, but with subdivisions if necessary. The process is often iterative. The result is the ranking table containing all the phenomena of importance, and the priorities given to them. The identification and hierarchy ultimately guides the analyst in the selection of an appropriate CFD code, and in selecting optional physical models within that code.

As exemplified in Fig. 1, *Verification* and *Validation*, or V&V, are essential components of the assessment process. Verification is the process that confirms that accurate and reliable results can be obtained from the models programmed into the code. The verification process entails comparing code predictions against exact analytical results, manufactured solutions [18], or previously verified higher accuracy simulations. The question of whether the models represent physical reality in the context of the given application is not part of code verification. This issue is taken up within the validation procedure. Roache [19] sums up the difference concisely as:

Verification	—	solving the equations right;
Validation	—	solving the right equations.

As part of verification, analysts must always be aware of their ability to introduce errors into input models, and developers' ability to leave errors in a code that can be very difficult to detect. It is extremely important to have some quality assurance (QA) procedure in place for any CFD project, part of which is a review of existing code verification relevant to all the models being exercised. Although rigorous adherence to international standards for a QA program is not recommended, since this entails a very large overhead in terms of documentation, what is recommended is the development of a programme specifying requirements for the four primary components of QA: documentation of the work; development procedures for input models and the code; testing; and review of all the work done. Documentation is the least appreciated, but perhaps the most important, of these. Writing a clear description of, and justification for, all aspects of an input model is an excellent way to expose errors, and is a necessary prerequisite for a good review process. The BPG document [8] contains extended discussion of all these QA aspects.

As part of the verification process, minimisation of numerical error needs to be demonstrated. This can only be done by comparing solutions obtained using different mesh sizes (and different time steps for transient simulations), and/or comparing solutions obtained using different orders in spatial

and temporal discretization schemes. Frequently, available time and computer resources restrict the rigour in estimation of the discretization errors. However, analysts must not use these restrictions as an excuse to abandon quantitative error estimation. Error analysis using portions of the mesh and/or intervals in a transient can also be very productive.

Figure 2 illustrates the principle of how mesh independence of the solution may be demonstrated by performing multiple simulations for different mesh sizes. First, a *Target Variable* (or set of target variables) is selected. The target variable is usually a scalar quantity. It should be representative of the goal(s) of the simulation (e.g. peak cladding temperature in a core bundle calculation), and one expected to be sensitive to numerical treatment and grid resolution. Thus, overall heat balance or flow rate, for example, would be poor choices for a target variable. Optimal, though not essential, is that the target variable be monitored continuously during run-time. Otherwise, the converged value can be found using post-processing.

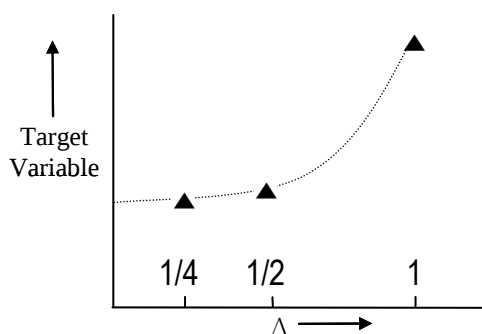


Figure 2. Testing for mesh independence.

For the example given in Fig. 2, the coarse-mesh variant ($\Delta = 1$) is far from the converged value and would thus be considered unacceptable. There is a dramatic approach to the asymptotic value if the mesh size is halved, and only slight improvement with further refinement. The practitioner then would need to decide whether a fine-mesh ($\Delta = 1/4$) calculation is really necessary, given the additional computational overhead, or whether the error associated with the $\Delta = 1/2$ option can be tolerated. The error analysis can be placed on a firm mathematical footing using the concept of Richardson extrapolation [19], and the BPG document strongly recommends following this procedure.

Validation is the process of determining whether the basic code models chosen for the simulation represent physical reality for the scenario being investigated, and can only be established by comparing numerical predictions against measured data. If new validation calculations are required, a verification process is necessary to estimate errors associated with discretization before any comparison with real data. This may result in an iterative adjustment of discretization until quantitative assurance is available that errors associated with selection of the spatial mesh, and for transient analyses the time step also, and the associated discretization schemes for both, do not contaminate conclusions of the validation exercise. Errors introduced by numerical errors can result in incorrect choices being made for specific physical process models. For more details regarding V&V procedures, the interested reader is referred to the work of Oberkampf and his co-workers [20, 21].

1.4 Steps to be Followed in Performing Quality CFD

The need for Best Practice Guidelines and their systematic use by analysts became very clear during the assembly of the BPG document. With the exception of individuals working within the ECORA project [22], in which guidelines on the use of CFD in nuclear engineering had already been produced, most CFD practitioners in the nuclear safety community worked from personal experience, advice from co-workers, and at times code manuals. For those with experience in development and use of classic thermal-hydraulic safety codes, the procedures to follow were in the most part somewhat familiar. Even if the BPG document is not used on a regular basis for CFD projects, it should have significant value as a repository of expertise for training inexperienced CFD users. As a set of step-by-step instructions, the list reproduced below would be the recommended path to follow in performing a safety assessment using CFD, as illustrated in Fig. 1.

1. Initial Preparation

- Produce a clearly written problem description, specifying the system and scenario requiring analysis, and clearly listing study objectives.
- Assemble a panel of experts and go through a PIRT process based upon the problem description.
- Decide whether the problem requires full CFD or whether a classical system code would be adequate.
- With knowledge of the problem and the physical processes, select an appropriate CFD code.
- If necessary, develop enhancements (e.g. interface tracking) in addition to the standard models in the code.
- Decide whether coupling is required between the CFD code and a system code to supply the boundary conditions to the CFD calculation. That is, are there important system feed-back effects that need to be taken into account?

2. Geometry Preparation

- Ensure the coordinate system is appropriate, and the units correct.
- Examine any modifications/simplifications that have been made to the geometry.
- Confirm that the geometric domain is complete.
- Assess the adequacy of any simplifications made; e.g. due to symmetry.
- Check that inlet, outlet, symmetry and cyclic boundary condition regions are located correctly.

3. Selection of Physical Models

- Establish a basic understanding of the prevailing physical phenomena and flow fields (part of the PIRT process).
- Select the appropriate level of turbulence representation (RANS, LES, VLES, DES, etc.).
- For RANS or URANS, select the most appropriate statistical model for turbulence (k - ϵ , k - ω , SST, RSM, etc.).
- For LES or DES, select an appropriate sub-grid scale (SGS) model (Smagorinsky, WALE, etc.).
- Either resolve the wall boundary layer explicitly or choose a wall-function model.
- Set boundary conditions consistent with the choice of turbulence model.

4. Grid Generation

- Check the grid quality. A good grid generation software package will generate internal statistics on grid quality in terms of skewness, aspect ratio, mesh size distribution, etc.
- Ensure the grid been appropriately scaled.
- Ensure grid nodes are concentrated in areas in which sharp gradients in physical variables occur.
- Avoid non-matching grid interfaces in critical regions of the flow.
- Ensure the grid is compatible with the physical models and flow conditions (turbulence model, wall treatment, etc.).

5. Numerical Method

- Avoid use of first-order upwind spatial discretization, and first-order time differencing (often defaults) where possible, to reduce numerical diffusion.
- If first-order methods are used, compare the numerical diffusion coefficient against an estimate of the turbulent diffusion coefficient at a number of locations.
- When using LES, employ central differencing in space and 2nd-order time differencing, if possible.

6. Verification

- Check for round-off errors. Generally, try to run on a 64-bit machine.
- Monitor target variables (these should have been set during the PIRT).
- Check for errors associated with the selection of the iteration convergence criteria. Ensure that residuals/tolerances of internal code iteration loops have been set low enough.
- Demonstrate mesh/time-step independence of results using target variables.
- Follow quality-assurance procedures to limit and locate user errors.

If the CFD simulation is part of an exercise to validate models against experimental data, see Fig. 1, then the following additional guidelines should also be followed.

7. Validation

- Follow a tiered approach, comparing first to separate-effect experiments and working up to complete system experiments.
- Where possible, use repeat experiments to help quantify experimental error.
- Using guidance from the PIRT process, select appropriate target variables for comparison between calculation and experiment.

8. Application

- If sufficient computer resources are available, perform an uncertainty analysis. This will help to place bounds on the numerical predictions, to cross-check the initial PIRT assumptions concerning the relative importance of the different physical phenomena, and to quantify sensitivity of results to uncertainties in input parameters, e.g. lack of measured data on inlet velocity profiles and turbulence statistics.

Note that without the validation step, it is only possible to *demonstrate* the capability of the CFD code to perform the required task, not to perform a genuine *safety assessment* (see Fig.1). As reflected in the procedural steps listed above, computer simulation is much more than generating

input and examining results. The initial PIRT process guides the analyst in the selection of (i) an appropriate CFD code, (ii) the appropriate physical models to be selected within that code, and (iii) validation tests relevant to the final analysis. A well-designed QA process is necessary to minimize unintended errors in the input model, and verification through use of target variables is needed to bring discretization errors within acceptable bounds.

When the original 2007 BPG document [8] was finalized, the group realized that it could only act as a starting point. Expansion of the document was envisaged as more experience was accumulated through WGAMA benchmarking activities (see Section 4.4) and from increased activity within the NRS community. The group was also convinced of the need for additional guidance for specific applications: such as containment analysis, thermal fatigue in piping systems, or pressurized thermal shock. Such application-specific guidelines would contain more detailed recommendations on appropriate selection of discretization and physical models, and identification of appropriate experimental data for validation. Such guidance could be defined as part of new International Standard Problems (ISPs) sponsored by the OECD/NEA.

Since the appearance of the BPGs [8], the CSNI has decided to promote further development of the Writing Group documents through the creation of Wiki-type pages at the NEA website. At the time of writing, the original document has been converted to MediaWiki format, and is open for review by a limited number of individuals associated with CSNI programmes. A project is in progress at CEA and EDF to improve the guidelines in respect to turbulence modelling, while another project is planned to include lessons learned from the OECD/NEA–Vattenfall T-junction benchmark [23]. It is anticipated that the BPG Wiki pages will be publicly available as a link from the NEA webpages during 2011. The archival version of the BPGs [8] is currently available from a link on this webpage.

2. WG2: Assessment Database

2.1 Background

The group's activities began in May 2003 and ended with formal endorsement of the final document [9] by the CSNI in December 2007. The group was then disbanded. During the time in which the group sat, the following objectives were fulfilled:

- Provide a classification of NRS problems requiring CFD analysis;
- Identify and catalogue existing CFD assessment bases, both nuclear and non-nuclear;
- Identify any gaps in the CFD assessment bases;
- Give recommendations how the CFD assessment databases may be extended.

Table 2. Contributors to the WG2 document.

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F. Ducros	CEA	FR	P. Mühlbauer	NRI	CZ
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M. Heitsch	GRS	DE	M. Scheuerer	GRS	DE
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T. Höhne	FZD	DE	T. Watanabe	JAERI	JP
D. Lucas	FZD	DE	G. Zigh	US NRC	US

The contributors to the Writing Group 2 activity are listed in Table 2. The group's first task was to identify the NRS issues for which it was considered the use of CFD would bring real benefits. Both single-phase and two-phase safety issues were considered, though in the latter case the information was simply passed over to WG3 for closer attention. It was recognized that, unlike the situation with system and containment codes, the nuclear community was not the primary driving force for the development of commercial CFD software, but could benefit from the validation programmes originating in non-nuclear areas, since often the thermal-hydraulic phenomena were similar. This is why it was thought relevant to include non-nuclear assessment bases in the survey.

Table 3: NRS problems requiring the application of CFD.

	NRS problem	System classification	Incident classification	Single- or two-phase
1	Erosion, corrosion and deposition	Core, primary and secondary circuits	Operational	Single/Multi
2	Core instability in BWRs	Core	Operational	Multi
3	Transition boiling in BWR/determination of MCPR	Core	Operational	Multi
4	Recriticality in BWRs	Core	BDBA	Multi
5	Reflooding	Core	DBA	Multi
6	Lower plenum debris coolability/melt distribution	Core	BDBA	Multi
7	Boron dilution	Primary circuit	DBA	Single
8	Mixing: stratification/hot-leg heterogeneities	Primary circuit	Operational	Single/Multi
9	Heterogeneous flow distribution (e.g. in SG inlet plenum causing vibrations, HDR expts., etc.)	Primary circuit	Operational	Single
10	BWR/ABWR lower plenum flow	Primary circuit	Operational	Single/Multi
11	Waterhammer condensation	Primary circuit	Operational	Multi
12	PTS (pressurised thermal shock)	Primary circuit	DBA	Single/Multi
13	Pipe break – in-vessel mechanical load	Primary circuit	DBA	Multi
14	Induced break	Primary circuit	DBA	Single
15	Thermal fatigue (e.g. T-junction)	Primary circuit	Operational	Single
16	Hydrogen distribution	Containment	BDBA	Single/Multi
17	Chemical reactions/combustion/detonation	Containment	BDBA	Single/Multi
18	Aerosol deposition/atmospheric transport (source term)	Containment	BDBA	Multi
19	Direct-contact condensation	Containment/ Primary circuit	DBA	Multi
20	Bubble dynamics in suppression pools	Containment	DBA	Multi
21	Behaviour of gas/liquid surfaces	Containment/ Primary circuit	Operational	Multi
22	Special considerations for advanced (including Gas-Cooled) reactors	Containment/ Primary circuit	DBA/BDBA	Single/Multi

DBA – Design Basis Accident; BDBA – Beyond Design Basis (or Severe) Accident;
MCPR – Minimum Critical Power Ratio

The entries on the list, with some overlaps, are grouped into problems concerning the reactor core, the primary circuit or the containment, listed in this order. Full details are given in [9], where each of the entries in Table 3 is discussed in terms of (i) relevance to nuclear reactor safety; (ii) description of the issue; (iii) why CFD is needed; and (iv) what has been attempted to date. For example, in the case of boron dilution, mechanisms have been identified [24], such as SB-LOCA or steam generator tube rupture (SGTR), which could lead to a slug of low-borated water being injected through one of the coolant loops into the reactor pressure vessel (RPV) of a Pressurized Water Reactor (PWR). If the slug arrives at the core without mixing significantly with the streams from the other cold legs, a

(local) criticality excursion could ensue. The complete phenomenological model requires two steps: (i) knowledge of the concentration of boron at the core entrance, and (ii) coupled thermal-hydraulics/neutronics calculations for the core region. The first step (covered by state-of-the-art CFD) thus provides the initial and boundary conditions for the second. Main CFD inputs to this problem concern the description of the transportation mechanisms to the core: namely, pump start-up, or natural circulation after restoration of the water inventory. Relevant parts of the reactor for flow modelling concern at least the downcomer, the lower plenum, and possibly the pipework related to the initial transportation of the slug to the RPV. Given the intrinsic multi-dimensionality of the flow, the geometrical complexity of the computational domain, and the requirement of accurately representing the mixing of the different flow streams, CFD analysis is needed.

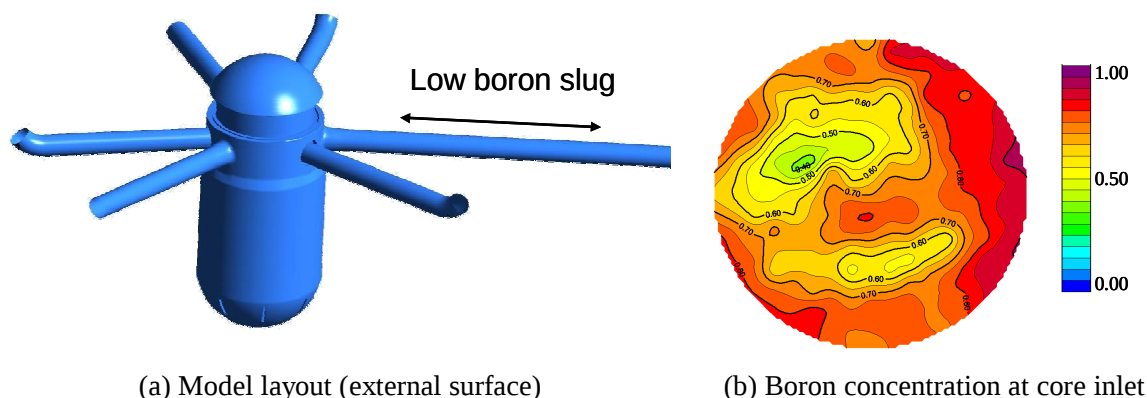


Figure 3. CFD simulation of a three-loop PWR to study the boron dilution issue.

Figure 3a shows the outer surface of a CFD model (gridlines removed) for a 3-loop PWR [25]. The mesh is constructed in this case of 6.7 million hexahedral cells. At the start of the transient, a low-boron water slug occupies the region indicated in one of the cold-legs. The flow in all three cold legs is started simultaneously. Profiles of the boron concentration at the entrance to the core at the instant the slug arrives are shown in Fig. 3b. As can be seen, there remains a heterogeneous distribution of boron, indicating that incomplete mixing of the cold-leg streams in the downcomer and lower plenum is predicted for this case.

The assessment database underpinning CFD analysis of the boron dilution issue at plant scale consists of a series of scaled experiments performed principally in Europe and the US. For example, very careful tests have been performed at the University of Maryland [26], the ROCOM facility at FZD Rossendorf [27], and the Vattenfall 1:5 scale test in Sweden [28]. In addition, boron dilution and general in-vessel mixing has been the subject of the EU-funded programmes EUBORA [29] and FLOWMIX-R [30]. In all cases, measured data from model tests have been made available for validation of CFD code predictions. In this example, and for the other safety issues listed in Table 3, relevant information has been catalogued and documented by the WG2 group.

2.2 Assessment Databases (Non-Nuclear)

As remarked above, until perhaps very recently, the nuclear industry could not be considered a primary driving force for the development of the physical models embodied in CFD software. Consequently, the major sources of validation data exist in the non-nuclear areas. Nonetheless, if the flow characteristics are similar to those encountered for the safety items identified in Table 3, the

information can still be of relevance in the nuclear context. Consequently, major sources of non-nuclear validation data were identified by the WG2 group.

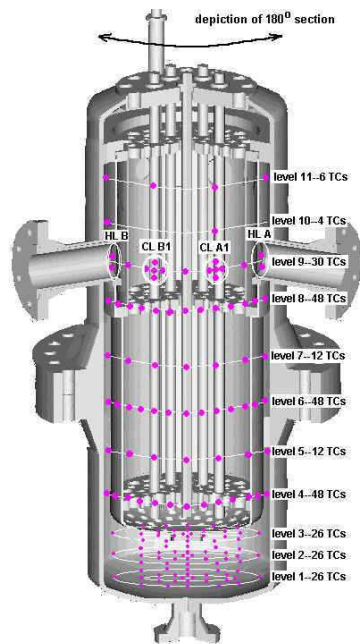
The principal commercial CFD software vendors, namely ANSYS-CFX [31], STAR-CCM+ [32], FLUENT [33] and (to a lesser extent these days) PHOENICS [34], promote general-purpose CFD, but increasingly have customers in the nuclear industry. Each code has an extended validation data base to which their customers have access. The best source of specific information is through their respective websites. Here, one finds documentation, access to the workshops organised by the company, and to the conferences and journals where customers and/or staff have published validation material, and details of the company's active participation in international benchmarking exercises. It should also be noted that even codes explicitly written for the nuclear applications, such as TRIO-U [35] and SATURNE-NEPTUNE-CFD [36] also include basic (often academic) validation cases, just like the codes from which focus on customers within the general industrial (commercial) area.

The European Research Community on Flow, Turbulence and Combustion (ERCOFTAC) is an association of research, educational and industrial groups [37] operating within Europe. The ERCOFTAC BPGs have already been referenced in Section 1.1 of this paper. The ERCOFTAC database was started in 1995, and is actively maintained by the University of Manchester, UK. It contains experimental as well as high-quality numerical data relevant to both academic and applied CFD applications. Regular Workshops on Refined Turbulence Modelling are held around Europe, information from which is used to update and refine the database. The Classic Data Base is open to the public. There are more than 80 documented cases, either containing experimental data, or with highly accurate DNS (Direct Numerical Simulation) data available. Each case contains at least a brief description, some data to download, and references to published work. Some of the cases could be used also in NRS applications, such as flow in curved channels, mixing layers, separated flows, impinging jets and flows through tube bundles.

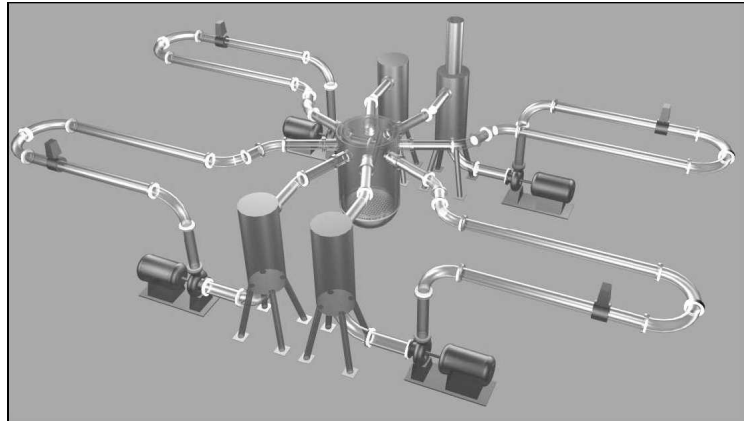
QNET-CFD KB developed from the QNET-CFD web-based thematic network, which was a part-funded European project to promote quality and trust in the industrial application of CFD [38]. Between 2000 and 2004, a knowledge base containing 43 *Application Challenges* was compiled, expanded, and finally brought online by means of a Wiki-based website developed from the prototype pioneered by the QNET-CFD network. The Wiki pages now come under the administration of the ERCOFTAC organization [37]. For each Application Challenge, its description, test data, CFD simulations, evaluation, best practice advice, and information on related underlying flow regimes are all available.

Other databases worth exploring are NPARC and AIAA. NPARC is principally directed towards the aerodynamics community, but there is a link to the data archive of NASA, which is particularly useful. High quality data are available in many flow configurations relevant to NRS analyses at a fundamental level [39]. The American Institute of Aeronautics and Astronautics (AIAA) participates to the definition of standards for CFD in its *Verification and Validation Guide*, and has important links to websites containing lists of references (papers, books, author coordinates) related to CFD verification and validation [40]. With the information from these and the European sites, there exist extensive validation data for CFD simulations in terms of basic, generic flow configurations. By this means, the nuclear community can benefit from the quality and trust in CFD established in non-nuclear areas in which there are similar flow and heat transfer situations. Of course, situation-

specific data are also needed for nuclear safety analyses, and such data bases were also catalogued by the WG2 group. Highlights are given in the next subsection



(a) Maryland (ISP-43 Benchmark)



(b) ROCOM (FLOWMIX-R Project)

Figure 4. Two boron dilution experiments for which measured data were released.

2.3 Assessment Databases (Nuclear)

Of the NRS items requiring CFD analysis identified by the WG2 group and listed in Table 3, the most comprehensive programmes to create a CFD assessment database have been made for boron dilution, pressurized thermal shock, thermal fatigue and hydrogen distribution in containments. Concertive efforts have been made in terms of experiments, benchmark exercises, and nationally and internationally supported study programmes. The work is fully documented in the WG2 report [9], and only some highlights are given here.

Experiments focusing on the boron dilution event generally try to reproduce the mixing in the reactor downcomer and lower plenum, upstream of the reactor core inlets. Data from two sets of experiments performed at the University of Maryland UM2x4 Loop were made available for numerical analysis under the terms of OECD/NEA International Standard Problem ISP-43 [26]. Sixteen redundant Test A experiments (front mixing test, with an infinite slug of cold water entering the RPV) and six redundant Test B experiments (slug mixing test, with a finite-volume slug of cold water entering the RPV) were performed. The model of the RPV, with positions of thermocouples marked, is shown in Fig. 4a. Time histories of temperatures at nearly 300 positions at 11 elevations within the downcomer and lower plenum were ultimately released. Ten participants from eight countries submitted numerical results to the blind-calculation phase of the benchmark before release of the measured data. Large discrepancies were observed between results from the blind calculation and measured data, even for participants using the same CFD tool [41]. At the time the simulations were carried out (before 2000), the use of BPGs was not widespread, and the disparities of the

predictions reiterate the message that reliable numerical predictions can only be expected if very precise guidelines are followed.

The ROCOM [27] facility (Fig. 4b) consists of four loops, with fully controllable coolant pumps in each. In contrast to the Maryland tests, demineralised water was used in these tests, supplemented by the injection of slugs of a tracer solution (diluted salt) into one loop. The salt concentration was measured by means of wire-mesh sensors [42]. Laser Doppler Anemometry (LDA) was applied for the velocity measurements. Data from selected tests were made available for CFD analysis within the European FLOWMIX-R [30] project.

Pressurized Thermal Shock (PTS) has become a safety issue of concern following plant-life extension plans in many countries. During a Small-Break Loss of Cooling Accident (SB-LOCA) in a PWR, Emergency Core Cooling (ECC) water is injected into the cold-leg pipe, and mixes with any hot water remaining there. The combined streams flow towards the downcomer, where further mixing takes place. In the case of incomplete mixing of the streams, the cold water from the ECC line may come into direct contact with the RPV wall, generating high thermal stresses. Knowledge of such thermal loads is important, since during its service life the RPV will have become subject to radiation-embrittlement and the stress may accentuate crack growth in the vessel wall.

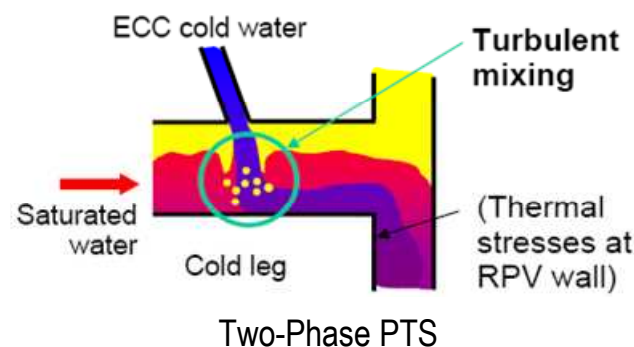


Figure 5. Schematic of the two-phase PTS event.

Most attention has been paid to the two-phase PTS event (Fig. 5), with high pressure injection from the top into a partially filled cold-leg pipe (a scenario of relevance to French PWR designs), though there remain thermal shock issues associated with the single-phase event too, in which either the pipe is full, or the injection is below the water surface (as in the German Konvoi and Russian VVER designs). An extensive experimental database for single-phase fluid mixing relevant to the PTS issue was compiled in the 1980s [43]. Since that time, the major PTS test facilities have concentrated on the two-phase PTS issue, which is described in detail in Section 3 below.

Flow-induced failures of parts of structural components of NPPs caused by high-cycle thermal fatigue include Genkai Unit 1 (Japan), Tihange Unit 1 (Belgium), Farley Unit 2 (USA), PFR (UK), Phénix (France), Tsuruga Unit 2 (Japan) and Loviisa (Finland). As a result of these incidents, considerable research effort has been devoted to the phenomenon. Thermal fatigue is studied mainly for two geometric configurations: T-junctions, and for two or more parallel jets in contact with a neighbouring structure. In the case of T-junctions, the work of the group is described in a companion paper at this conference [23], and no further comments will be made here. An example of a study of thermal stripping is the series of experiments carried out at the O-arai Engineering Center in Japan

[44]. The tests were carried out using liquid sodium as the fluid medium. The test section (Fig. 6a) consists of three rectangular slots sandwiched between two vertical plates through which alternate hot-cold-hot sodium jets are discharged. Thermocouples on a movable rake measure the temperature fluctuations at and near the plate surface. A typical power spectrum of the temperature fluctuations (Fig. 6b) shows a low-frequency peak, which is often is an indication of potential for high-cycle thermal fatigue [45].

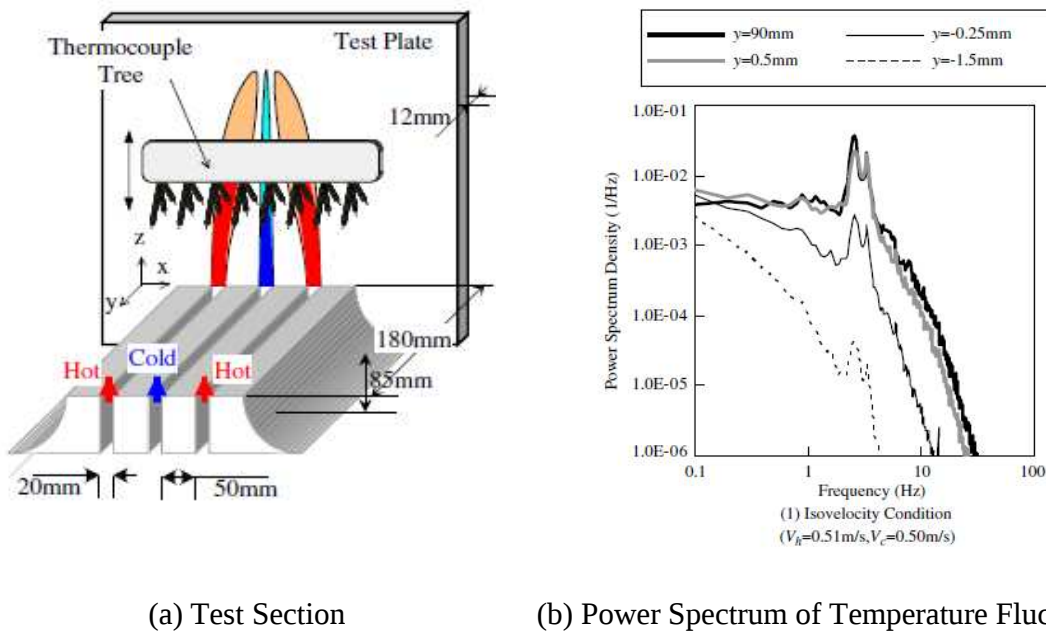


Figure 6. Thermal Stripping Experiment

The WG2 group endeavoured to assemble all assessment bases relating to the nuclear safety issues requiring CFD analyses, as listed in Table 3. In some cases, restricted data had been made available to the nuclear community, either through participation in benchmarking activities or by the involvement of the owners of the data in international research projects. It was recognized that integral data would be of limited value in validating models in a CFD code, so special attention was made to *CFD-grade data*, i.e. where localized measurements of temperatures, velocities or concentrations. Most valuable were experiments in which measurements of upstream conditions had also been made, to precisely defines inlet boundary conditions for the subsequent CFD simulations.

2.4 Gaps in the Assessment and Technology Databases

The essential role of validation in the pathway to a safety assessment using CFD has already been shown in schematic form in Fig.1. Of the 22 safety issues for which the WG2 Writing Group considered CFD could bring substantial benefits, and listed in Table 3, not all have appropriate validation data associated with them. These represent gaps in the assessment databases. In addition, in some instances, the need for CFD is accepted, but the current stage of development of CFD software prevents the recommended analysis from being undertaken. One might refer to this as the CFD technology gap. Some typical examples are given here by way of illustration.

CFD simulations are computationally very demanding, both in terms of memory and CPU time. Traditional system codes, such as RELAP-5, TRACE and CATHARE are much less demanding,

and the models are well developed and reliable within their proven ranges of validity. Coupling of the two approaches then becomes attractive, using the 1-D system code to provide boundary conditions for the 3-D CFD part of the calculation performed using the CFD code. A recent example is the coupling of TRACE to ANSYS-CFX [42]. Though progress is being made in the area, the validation database is not yet comprehensive for the coupled code concept.

Precise prediction of the thermal loads to fuel rods, and of core behaviour, result from a balance between the thermal hydraulics and neutronics. Only the nuclear community has an interest in these phenomena. The current state-of-the-art is a coupling between a sub-channel description of the thermal hydraulics and neutron diffusion at the sub-channel level. However, some progress is being made in the direct coupling of CFD codes with existing neutronics packages. An example is the coupling between MCNP and STAR-CD [47], and between MCNP and FLUENT [48]. Several benchmark exercises have been set up in the framework of OECD/NEA activities, including a PWR Main Steam Line Break (MSLB), a BWR turbine trip, and for a VVER-1000 coolant transient (for which fine-mesh CFD models were used). However, a concerted effort is needed to bring together all appropriate data to place the assessment process on a sound basis.

In a recent PIRT-type exercise conducted within the framework of the WGAMA activities [49], aerosol deposition in containments following a severe accident was ranked ahead of thermal fatigue in terms of generic interest. However, in comparison with the multitude of CFD-grade data available from experiments based on flow mixing in T-junctions, there are virtually no data from the nuclear area useful for validation of CFD aerosol deposition models. All experiments are of the integral type, with no local data measurements. More suitable data are available from experiments performed in generic configurations, such as a straight pipe or pipe elbow, and in specific non-nuclear application areas [50].

2.5 Perspectives

The activities of the WG2 Writing Group were concluded at the end of 2007 with the completion of the final CSNI report [9]. The group had provided evidence to show that CFD is a tried-and-tested technology, and that the main industrial-level CFD software vendors were themselves taking active steps to quality-assure their software products, by testing their codes against standard test data, and through active participation in international benchmarking exercises. However, at present, the primary driving forces for the development of CFD technology remain in non-nuclear areas, such as in the aerospace, automotive, marine, turbo-machinery, chemical and process industries, and to a lesser extent the environmental and biomedical industries. In the power-generation arena, the principal applications are again non-nuclear: combustion dynamics for fossil-fuel burning, gas turbine optimization, design of vanes for wind turbines, etc. However, application of CFD to nuclear power generation is growing.

It was recognized that like any state-of-the-art report, the WG2 document could only represent a state-of-the-art at the time of writing, and, given the rapidly expanding use of CFD generally, and in nuclear technology specifically, the information it contained would soon become outdated. To preserve topicality, improvements and extensions to the document are foreseen. This viewpoint is also applicable to the WG3 document, since there is increased use of two-phase CFD in nuclear reactor safety, and to a lesser extent the WG1 document dealing with BPGs also. Consequently, there was a common initiative to build on the information already collected by the groups. The consequent actions taken are discussed in Section 4 of this paper.

3. WG3: Extension to Two-Phase Flow Applications

3.1 Background

The focus of the third of the Writing Groups, WG3, was to establish some requirements for extending CFD codes to two-phase flow safety problems. Most of the work was accomplished during the period 2003-2007, in parallel with that of the other groups, of which there was some synergy. The group produced a final report [10], which was endorsed by the CSNI in December 2009. The contributors to the report are listed in Table 4.

Table 4. Contributors to the WG3 document.

D. Bestion	CEA	FR	F. Moretti	UniPisa	IT
M. Andreani	PSI	CH	T. Morii	JNES	JP
H. Anglart	KTH	SE	P. Mühlbauer	NRI	CZ
M. Heitsch	GRS	DE	M. Scheuerer	GRS	DE
E. Graffard	IRSN	FR	B. L. Smith	PSI	CH
F. Kasahara	JNES	JP	C.-H. Song	KAERI	KO
D. Lucas	FZD	DE	T. Watanabe	JAERI	JP
J. H. Mahaffy	PSU	US	G. Zigh	US NRC	US

Extending CFD codes for application to two-phase flow problems enables safety investigations to access smaller scale processes masked by traditional system codes. Using such tools as part of a safety demonstration may bring a better understanding of the physical situations, which would ultimately result in more confidence in the results, and thereby an improved estimation of safety margins. Increased computer performance allows a more extensive use of 3D modelling of two-phase thermal hydraulics to be undertaken with fine nodalization. However, the two-phase flow models are not as mature as those for single-phase CFD, and much work still needs to be done on the physical modelling and numerical schemes used in such codes.

The WG3 group first identified and classified those NRS problems for which extending CFD to two-phase flow may bring real benefits, and classified the different modelling approaches. A general multi-step methodology was proposed, including a preliminary identification of the important flow processes, model selection, and verification and validation processes. Of these, and given the resources available to the group, six NRS problems were then selected to be analysed in greater detail. These problems are dryout, Departure from Nucleate Boiling (DNB), Pressurised Thermal Shock (PTS), pool heat exchangers, steam discharge into a pool, and fire protection. These are issues where some effort was already ongoing, and where investigations using CFD had a chance of gaining some level of success in a reasonable period of time. The selected items address all flow regimes, so may, to some extent, envelop many other safety issues.

A general multi-step methodology was applied to each issue to identify the gaps in the existing approaches. Basic processes were identified, and modelling options discussed, including closure relations for interfacial transfers, turbulent transfers, and wall transfers. Available data for validation were reviewed and the need for additional data identified. Verification tests were also listed, and a few benchmarks proposed as future activities. A preliminary state-of-the-art report was prepared, which identified the remaining gaps in the existing approaches. Although two-phase CFD is still not very mature, a provisional set of BPGs was created, which would need to be expanded and updated in the future. The proposed multi-step methodology allows users to formulate and justify their

choice of models, including listing of some necessary consistency checks. Some methods for controlling the numerical errors were also given as a part of the BPGs.

3.2 Review of Safety Issues that may Benefit from Two-Phase CFD

A list of 26 NRS problems for which two-phase CFD may bring real benefits was compiled. Each issue was examined in turn, and classified with respect to the degree of maturity of present CFD tools to resolve it in the short or medium term. Three maturity ratings (Low, Medium and High) were assigned according to the following definitions.

- ‘High’ maturity was applied to the case in which sufficient information was available, all related phenomena were well identified, and models had been developed for each physical phenomenon, even though improvements may be necessary for some of them.
- “Medium” maturity was applied if a published background already existed, most basic phenomena had been well identified, but where some models still required improvement and validation.
- ‘Low’ maturity was applied to the case in which no trusted information was available on the validity of the existing models.

The results of the classification procedure are shown in Table 5. Some NRS problems require two-phase CFD in an open medium, and others in a porous medium approach. For some problems, investigations with a two-phase CFD tool for an open medium were used for a better understanding of the flow phenomena, and for developing appropriate closure relations for a 3-D model of the porous medium type. These trends are marked in the 4th column of the Table.

Table 5: Two-Phase NRS Issues that may benefit from Investigations at CFD Scale.

	NRS problem	Level of Maturity of CFD Tools	Open/Porous Medium
1	DNB, dryout and CHF investigations	M	O; O $\Rightarrow$ P
2	Subcooled boiling	M	O; O $\Rightarrow$ P
3	Two-phase Pressurized Thermal Shock (PTS)	M	O
4	Thermal fatigue in stratified flows with gas/liquid interface	L	O
5	Direct contact condensation: steam discharge in a pool	M	O
6	Pool heat exchangers: thermal stratification and mixing	H	O; P
7	Corrosion, erosion deposition	L	O
8	Containment thermal hydraulics	H	O
9	Two-phase flow in valves, safety valves	L	O
10	ECC bypass and downcomer penetration during refill	L	O; O $\Rightarrow$ P
11	Two phase flow features in BWR cores	M	P; O $\Rightarrow$ P
12	Atmospheric transport of aerosols outside containment	M	O
13	DBA reflooding	M	P; O $\Rightarrow$ P
14	Reflooding of a debris bed	L	P; O $\Rightarrow$ P
15	Steam generator tube vibration	L	O $\Rightarrow$ P
16	Upper plenum injection	L	P
17	Local 3-D effects in complex geometries	L	O
18	Phase distribution in inlet and outlet headers of steam generators	L	O; O $\Rightarrow$ P
19	Condensation induced waterhammer	L	O
20	Components with complex geometry	L	O $\Rightarrow$ P
21	Pipe Flow with cavitation	M	O
22	External reactor pressure vessel cooling	M	O
23	Behaviour of gas-liquid interfaces	M	O

24	Two-phase pump behaviour	L	O
25	Pipe break causing in-vessel mechanical load	M	O; P
26	Specific features in passively cooled reactors	M	O

3.3 Classification of CFD Modelling Approaches

The traditional thermal-hydraulics system codes, such as RELAP-5, CATHARE or TRACE, have an extensively validated “frozen” model – usually the two-fluid model [51] – and one choice of numerical algorithm available (backward Euler for time differencing and 1st-order upwind for spatial differencing). In contrast, CFD codes offer a multitude of numerical modelling options, but the two-phase models have only a very limited validation database in more than 1-D. If two-phase CFD codes are to be used in NRS, some requirements need to be applied to the code, and to its verification and validation procedures, which take into account the versatility of the options available.

Consequently, the WG3 group proposed a classification of modelling options. These are listed here, followed by some brief explanations.

1. Open medium or porous medium approach.
2. Phase-averaging or field-averaging option.
 - (i) homogeneous model (both phases have equal velocities and temperatures);
 - (ii) two-fluid model (phases have different velocities and temperatures);
 - (iii) multi-field model (i.e. to distinguish between droplets and continuous liquid, or between bubbles and continuous vapour).
3. Filtering of turbulent scales and two-phase intermittency scales.
 - (i) all turbulence scales are modelled (RANS-type models);
 - (ii) large scales are calculated, small scales are modelled (LES-type models);
 - (iii) all turbulence scales are calculated directly (DNS-type models).
4. Interface treatment.
 - (i) use of an explicit interface tracking/capturing technique;
 - (ii) use of a purely statistical treatment of interfaces (i.e. in terms of void fraction);
 - (iii) use of Identification of the Local Interface Structure (ILIS);
 - (iv) characterization through Interfacial Area Density (IAD), or by other quantities.

The choice between open medium or porous medium approach depends ultimately on whether the boundaries of the flow domain are exactly captured by the mesh (open medium) or not (porous medium). For example, in a CFD simulation involving a reactor core, it may not be possible to model explicitly all the flow channels surrounding the fuel elements, due to the associated computational overhead. In this case, representative sections of the core are “homogenized” to reduce the number of meshes. Clearly, in an open medium, the cell size – and by implication the region over which the basic equations are time-averaged, and possibly space-averaged – is much smaller than a typical hydraulic diameter: the porosity $\Theta = 1$ everywhere. In a porous medium, the equations are space-averaged over a scale larger than the hydraulic diameter: each cell contains solid as well as fluid, and $\Theta < 1$.

Unless one is performing DNS and explicitly resolving all liquid/gas interfaces, some averaging (or filtering) procedure will need to be applied to the basic conservation equations of mass, momentum and energy in order to distil from them a workable set for computation. The averaging process simplifies the equations, but at the expense of losing information concerning the interplay between

physical processes. Already for single-phase turbulent flows, time or ensemble averaging is a common way to derive equations for the mean flow field in the Reynolds Average Navier-Stokes (RANS) approach that can subsequently be used under steady, or quasi-steady, flow conditions. For two-phase flows, the situation is vastly more complex, since one is not just averaging over the turbulence scales, but over the phase-exchange scales too. For example, time-averaging does not allow for the prediction of the positions of the interfaces of dispersed droplets and dispersed bubbles. There is also a smearing or diffusive effect of the large interfaces between continuous liquid and continuous gas, such as a free surface, or the surface of a liquid film along a wall.

Space-averaging, or filtering, is the basis of the Large Eddy Simulation (LES) approach to turbulence modelling in the open medium context. The technique has become increasingly applied in single-phase CFD in order to predict large-scale, coherent turbulence structures. The filter scale defines that part of the turbulence spectrum which is to be simulated and the part that is to be modelled. Space-averaging in two-phase flow filters not only the small eddies, but also the interfaces. Only statistical or averaged information on interfaces of dispersed fields (bubbles and droplets) can be predicted through averaged quantities, such as void fraction or interfacial area density. Statistical treatment may result from time-averaging or from space-averaging. An interface is a filtered interface if its position in space, and evolution in time, is predicted with some filtering due to either a space filter or time-averaging. Based on this classification, the various time and space resolution options possible in two-phase CFD are summarized in Table 6.

Table 6: Time and Space Resolution in the Various Modelling Approaches in Two-Phase CFD

	Open Medium					Porous Medium
Time and space filtering	No filter and no averaging	Space filtering			Time averaging	Time averaging
Turbulence model	DNS	LES	LES VLES	LES VLES	RANS URANS	RANS URANS
Interfaces	Calculated	Calculated	Filtered plus statistical	Statistical	Statistical	Statistical
No. of fields	1	1	1, 2, n	1, 2, n	1, 2, n	1, 2, n
Types of model	Pseudo-DNS	LES with calculated interfaces	Hybrid LES with filtered and statistical interfaces	LES with statistical interfaces	RANS, URANS with statistical interfaces	Statistical interfaces

Three different sub-classes exist in the case of space-filtering:

- The filter scale is much smaller than the scales of the interfaces (bubble size, droplet size, wavelength at a free surface), and all interfaces are calculated explicitly (3rd column).
- The filter scale is larger than the scales of the interfaces (bubble/droplet size) and no interfaces are calculated explicitly (5th column in Table 6). All interfaces are then treated statistically.
- The filter scale is larger than some interface scales (small bubble/droplet sizes) but smaller than other interface scales (free surface, film interface, interfaces of large bubble/droplet sizes). No interface is explicitly calculated, some interfaces are filtered, and some interfaces are treated statistically (4th column).

3.4 Multi-Step Methodology

The WG3 group proposed the general method illustrated in Fig. 7 for using two-phase CFD for NRS problems. The first step is to identify all the important flow processes. This is followed by the selection of the main modelling options, including choosing a basic model (1-fluid, 2-fluid, multi-field), choosing a turbulence model, and deciding on the way to treat the interface(s). Next, the choice of closure laws has to be made, involving how to model the interfacial, turbulent and wall transfers. Finally, there are the verification and validation procedures to follow, as discussed earlier in Section 2. Ideally, if the CFD tool is to be used in the context of a nuclear reactor safety demonstration that uses a best-estimate methodology, one should add a final step: uncertainty evaluation. This may be difficult to fulfil without access to high-performance computing facilities.

Multi-step methodology for applying two-phase CFD to NRS

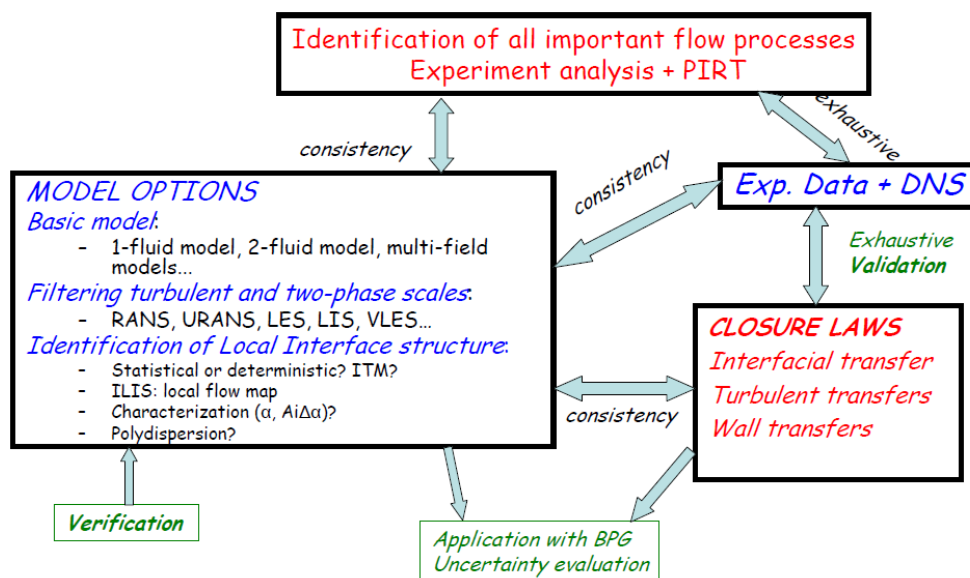


Figure 7. General Methodology for Two-Phase CFD Applications to NRS

Most issues with reactors involve complex, two-phase phenomena in complex geometries, and many basic flow phenomena may play a role. The user must identify all these basic thermal hydraulic phenomena before selecting the various modelling options. None of the available CFD codes can be used as a black box in this regard, and the use of a PIRT procedure [17], or something similar, may be the best way to proceed. Here also, a preliminary analysis of experiments simulating the problem (or part of the problem) may be of great help in identifying the phenomena. Given the inherent complexity of any two-phase flow situation, this step may need to be revisited several times during the successive steps of the general methodology. Also, analysing experimental data from the validation matrix may highlight some sensitive phenomena that had not been previously identified. The methodology route may then become iterative, as Fig. 7 indicates.

Three choices are necessary to select the set of balance equations to be used to solve the problem, and they must be consistent with each other. These choices are related to separation into fields, time and space filtering, and the treatment of interfaces (calculated, filtered or statistical). Any two-phase flow situation may be seen as a juxtaposition of several fields and/or phases. The separation into

fields is particularly necessary if each field has a velocity and/or temperature significantly different from the others. In some cases, it may be necessary to separate droplets (or bubbles) into several classes of different sizes, especially if their behaviour significantly depends on their size.

The second important choice is the type of time or space averaging, or filtering, to be employed. Pseudo-DNS techniques are still too time-consuming computationally for pragmatic application, and currently can only be used as support to the modelling carried out at more macroscopic scales. Filtered approaches (LES) are also CPU-intensive, but are now within the realms of possibility. RANS-type models are more affordable, and remain the industrial standard for most applications.

Depending on the averaging, the interfaces are either tracked directly (i.e. deterministic), filtered, or treated statistically. Two-phase flows have interfaces with a wide range of geometrical configurations. There are locally *closed* for dispersed fields, e.g. bubbles and droplets, and locally *open* for free surfaces, a falling film, or a jet. Tracked or filtered interfaces are more appropriate for large interfaces, such as free surfaces or films. A purely statistical treatment is more appropriate for dispersed flows, such as bubbly or droplet flows. In a RANS context, one may need an Identification of the Local Interface Structure (ILIS) to select the appropriate closure laws for the interfacial transfers. Such an ILIS is equivalent to the flow regime map used in 1-D two-fluid models in system codes. A local interfacial structure is defined by three items:

1. the presence of a dispersed gas field (i.e. bubbles)
2. the presence of a dispersed liquid field (i.e. droplets)
3. the presence (and orientation) of a large interface.

In some cases, one may combine a deterministic treatment of large interfaces with a statistical description of the dispersed fields. In a statistical description of interfaces, the interfaces are characterized at least by volume fraction, but very often further information, provided by additional equations, is required for particle number density, interfacial area density, multi-group volume fractions (e.g. the MUSIG model), or any other parameters relating to the particle population.

Any kind of interface may be subject to mass, momentum, and energy interfacial transfer. The formulation of these transfer processes depends on the modelling choices made at previous steps, as described above. If a large interface (such as a free surface) is present, the model may require knowledge of the precise position of this interface, either by using an Interface Tracking Method (ITM) or some other approach. If an ILIS has been used to define the interface structure, the choice of the most appropriate closure laws is then possible. All mass, momentum and energy interfacial transfers have had to have been previously validated on available Separate Effect Tests (SETs). This is also true for the turbulent and wall transfers.

The importance of the verification and validation steps has already been exemplified in Fig. 1. The verification step is very difficult to achieve for actual 2-phase flow situations, though the use of numerical benchmarks may be useful to check the viability of the numerical schemes and to measure the accuracy of the solution. A matrix of validation tests (and possibly also demonstration tests) has to be defined and employed. Scoping tests may be necessary to demonstrate the capability of the modelling approach to capture all the important flow processes, at least qualitatively. Validation tests are then necessary to evaluate the models for interfacial, turbulent, and wall transfer, as far as possible by using SETs.

3.5 Analysis of Pressurized Thermal Shock

As mentioned previously, six NRS problems for which two-phase CFD may bring significantly more information than possible from traditional lumped-parameter or 1-D system code approaches were selected by the WG3 group for detailed analysis. By way of illustration, one of these – the 2-phase PTS event – is described here, since this typifies many of the modelling difficulties described above.

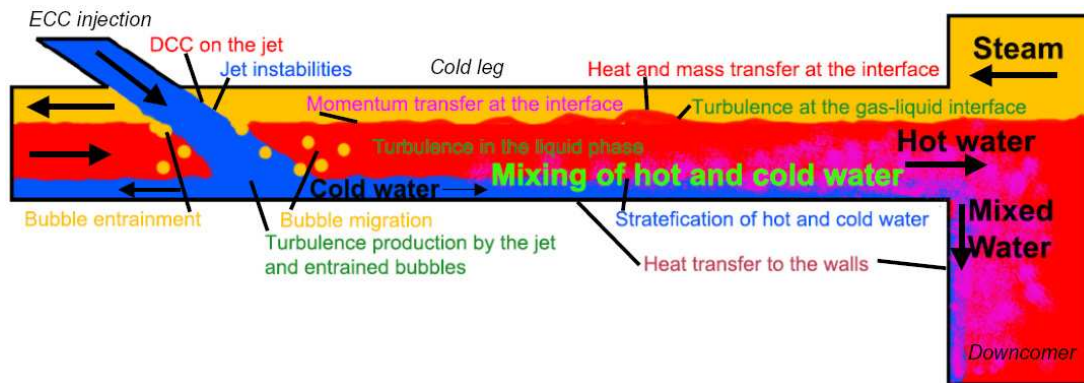


Figure 8. Schematic of the 2-Phase PTS Event

The Pressurized Thermal Shock (PTS) event has become an issue of concern in many countries as a consequence of plant-life extension programmes. Following a Small Break Loss of Coolant Accident (SB-LOCA) in a PWR, cold water is injected via the Emergency Core Cooling System (ECCS) and mixes with the hot water in the primary circuit. A typical situation is shown schematically in Fig. 8 in which the ECCS water enters a cold leg partially filled with saturated water. If insufficient mixing occurs, cold water could enter the downcomer and directly contact the Reactor Pressure Vessel (RPV) wall. There is concern that for ageing plants, for which there is radiation-induced lack of ductility of the RPV material, the sudden overcooling, coupled with a high internal pressure, could lead to vessel failure.

The main fluid flow and heat transfer processes are also indicated in Fig. 8. Though analysis of PTS events have been carried out using traditional 1-D system codes [52] the rapid progress in computing power now enables use of fine-resolution CFD tools for PTS investigations using a 3-D nodalization of the cold legs and part of the downcomer region. The main heat source of the liquid is due to steam condensation in the cold leg and in the top of the downcomer. Condensation is mainly dependent on the interfacial structure and turbulent mixing in the liquid phase, and a rather simple interfacial structure is that of the stratified flow conditions existing in the cold leg. The use of CFD enables the liquid temperature field to be predicted, this depending mainly on interfacial heat and mass transfer related to direct contact condensation of steam on a sub-cooled liquid, and on turbulent diffusion of heat within the liquid.

Many previous studies have supported the belief that turbulence behaviour near the interface plays a dominant role in interfacial transfers. For ECC injection cases, the turbulence mainly comes from the impact of the water jet, as well as the shears created at the wall and gas-liquid interface. Thus, as a first step to simulate such scenarios, separate effects tests in simple geometries need to be set up in order to develop and validate the physical models.

The identification of all basic flow processes has recently been made in the context of the NURESIM [53] project. Many of the phenomena indicated in Fig. 8 were identified. In the ECCS jet area, these are:

- Instabilities of the ECC injection jet;
- Condensation on the jet surface before impact with the liquid surface;
- Entrainment and migration of steam bubbles below the water level;
- Turbulence production in the liquid below the jet.

For the stratified flow in the cold leg, consideration has to be given to:

- Interfacial transfer of momentum at the free surface;
- Interfacial transfer of heat and mass at the free surface;
- Turbulence production due to wall shear, and in the interfacial shear layers;
- Heat transfer with the cold leg pipe and RPV wall;
- Effects of turbulent diffusion on condensation;
- Interactions between interfacial waves, interfacial turbulence production and condensation;
- Effects of temperature stratification upon turbulent diffusion;
- Influence of non-condensable gases on condensation.

And in the downcomer:

- Flow separation (or not) in the downcomer at the cold leg nozzle exit;
- Heat transfer with the downcomer and vessel walls.

The free surface of the liquid in the cold leg pipe may be flat or wavy as a consequence of the passage of the steam over it. Though the entrainment of bubbles below the surface due to the impact of the ECCS jet may produce a somewhat complex interface structure, it is at least limited to a small region. The question of whether to treat the free surface very precisely, using an interface tracking method, remains open, and several options have been explored [54] within the NURESIM project.

The flow occurring during a PTS event is quasi-steady, and generally averaging over all turbulent scales (i.e. a RANS approach) would then seem to be appropriate. However, it is recognized that this modelling approach may affect the interfacial wave patterns. If the interfacial waves play an important role in the condensation process, the best CFD modelling approach remains unclear. Turbulent diffusion within the liquid controls the condensation efficiency, and mixing and entrainment due to the ECCS jet impingement are certainly the main sources of turbulence. The k- ϵ turbulence model seems to be a reasonable first approach for this situation, but a sufficiently fine meshing is required for the turbulence levels to be correctly predicted. Interfacial transfer of heat and momentum (friction force) on the free surface require a specific modelling that takes into account the space filter scale imposed by the meshing (i.e. the transfer coefficients may depend on the distance to the interface in the same way as the distance to the wall is used in wall functions for a solid surface). Nonetheless, modelling turbulence and heat transfer at the free surface in the case of a high interfacial shear and the presence of waves using a RANS model requires additional modelling. Yao *et al.* [55] and Coste *et al.* [56] have used a two-fluid approach for this, with a k- ϵ model in each phase. The interface position is determined using the void fraction. Momentum and heat transfer in those meshes containing the free surface are treated using an extrapolation of the wall function approach. The model was found to be satisfactory for the momentum transfer and

turbulence intensity, but further development is needed to improve the heat and mass transfer predictions.

More recently, the LES turbulence modelling has been employed in combination with an interface-tracking method (ITM) to investigate stratified counter-current air-water flow with high interfacial shear [57,58]. Such fine-scale simulations may be of great interest in understanding the complex interactions taking place at the free surface during a PTS event. Close investigation of the processes at a fundamental level can yield closure models for more macroscopic (RANS) approaches, and be complementary to experiments aimed at developing similar models. All this illustrates the benefits of having a multi-scale approach to two-phase CFD.

Several experimental data sources have been identified with NURESIM [53] and used for the development and partial validation of physical models to be used in PTS studies. Most feature free-surface flows without mass transfer, but with smooth or wavy interfaces, including wave breaking [59]. Two experiments provide information on plunging jets with entrainment of air bubbles and production of turbulence below a free surface. The turbulence induced by a plunging jet was found to be the main source of turbulence, dramatically influencing condensation. The k - ϵ turbulence model was found to be generally inaccurate, but was able to predict the turbulence intensity reasonably well [59]. Condensation at the free surface of a stratified steam/water flow in a rectangular channel was the subject of two experimental investigations [56, 60] and condensation driven Kelvin-Helmholtz instability in a horizontal pipe was also investigated in the PMK test facility [61]. Finally, the COSI tests are combined-effects tests with several phenomena representative of those occurring during PTS scenarios, and a UPTF-TRAM test could simulate at a reactor scale many phenomena, but without condensation.

3.6 Guidelines for using Two-Phase CFD

As remarked earlier, two-phase CFD models remain rather immature in comparison with those formulated for single-phase CFD. Nonetheless, as the above example demonstrates, two-phase CFD is being used actively to bring insights into NRS issues for which there is a strong 3-D component to the flow and when a rather fine space resolution is required. Other two-phase safety issues are listed in Table 3. Many of these are currently being analysed using CFD, and it is anticipated more will follow in the near future. The WG3 group thought it important that some guidance be made available to any potential two-phase CFD analyst, even though the physical models were still under development. Certainly, all the major CFD codes now have two-phase modelling capability, and some help in choosing the most appropriate models is needed.

A general multi-step method of working for using two-phase CFD for safety issues is recommended, as explained below. Following these steps, and being able to justify what is being done at each step, is a good way to demonstrate that the users actually control the whole process and do not simply rely on simulation tools which are still relatively immature. The first step just states that the user should not expect that the CFD code will tell him/her which flow processes will take place in the problem that needs to be studied. The user must himself identify these flow processes, and then check that the simulation tool is able to describe them, either as it is, or after some additional developments are made. The second and third steps will exist as long as precise guidelines lack options for selecting the main model and closure relations. The user must elaborate the rationale for these choices for

each application. Feedback from many users, in many varied applications, will eventually provide more guidance to users for this step in the future.

A number of consistency checks must also be made as elaborated below, .

1. The basic choice of the number of fields needed to be adapted to the physical situation, or to an acceptable degree of simplification of it. In particular, if two fields are mechanically and/or thermally uncoupled, and have very different behaviour, they must be treated separately.
2. The averaging procedure needs to give a clear definition of the principal variables, and of the closure terms in the equations. The filtering of the turbulent scales and the two-phase intermittency must be fully consistent.
3. A deterministic treatment of an interface using an Interface Tracking Method (ITM) can be chosen, but only if all phenomena having an influence on the interface are also deterministically treated.
4. The choice of an adequate interfacial transfer formulation must be consistent with the selected interface treatment, and with the Identification of the Local Interfacial Structure (ILIS).
5. The SET validation matrix should be exhaustive with respect to all flow processes identified in Step 1, and should be able to validate all the interfacial, turbulent and wall transfers regarded as playing an important role according to Step 1.
6. The number of measured flow parameters in the validation experiments should be consistent with the complexity of the selected model they aim to validate. A model defined by a set of n equations having a set of n principal variables X_i ($i = 1, n$) can be said to be clearly “validatable” when one can measure n parameters giving the n principal variables.
7. The averaging of measured variables must be consistent with the averaging of the equations.

The proposed multi-step methodology and classification of modelling approaches represent a first approach to producing Best Practice Guidelines for two-phase CFD by inviting users to formulate and justify all their modelling choices, and by conforming to some necessary consistency checks. The work performed by the WG3 group confirms that two-phase CFD is developing into a useful tool in safety investigations, one that is complementary to those carried out using system codes. An estimation of safety margins for any of the selected issues has not yet been provided, but the work has given access to small-scale flow processes, thereby providing a better understanding of the physical situations. CFD is already a useful tool for safety analysis, and may become one for safety demonstration too once all the steps in the methodology have been correctly addressed, including uncertainty evaluation.

4. New Initiatives

4.1 Background

During the time the Writing Groups were still meeting regularly, there was already discussion among the groups of how better to make use of the material collected. These thoughts manifested themselves in a proposal to the WGAMA committee to extend and broaden the work beyond just the production of the three archival documents. The following ideas were put forward:

- To organise a new series of international workshops to provide a forum for experimenters and numerical analysts to exchange information;

- To establish a Wiki-type web portal to give online access to the information collected and documented by the groups, and to provide a means for updating and extending the information by inviting reader participation; and
- To encourage nuclear departments at universities and research organisations to release previously restricted test data by initiating a series of international benchmarking exercises.

The first of these activities was organised directly by the WG2 group, while the remaining two were accomplished by a smaller *Special CFD Group* formed later, consisting of the chairmen of the three Writing Groups together with the NEA secretariat.

4.2 The CFD4NRS Workshops

The first of the workshops, which are all specifically focused on the application of CFD to nuclear reactor safety (NRS) issues, took place in 2006 under the acronym CFD4NRS [62], sponsored jointly by the OECD/NEA and the IAEA. The workshop provided a forum for both numerical analysts and experimenters to exchange information in the field of NRS-related activities relevant to CFD validation: there were 79 attendees. Papers describing CFD simulations were accepted only if there was a strong validation component. In total, 39 technical and 5 invited papers were presented. 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 appeared in a special issue of Nuclear Engineering and Design [63]. The workshop flyer is reproduced in Fig. 9a.

The second workshop in the series, XCFD4NRS [64], took place in Grenoble, France in September 2008. Here, the emphasis was more on new experimental techniques and two-phase CFD, addressing many of the NRS issues identified in Tables 3,5. The workshop attracted 147 participants. There were 5 invited speakers, 3 keynote talks, 44 technical papers and 15 posters. Again, selected papers have been collected in a special issue of the journal Nuclear Engineering and Design [65]. The workshop flyer is reproduced in Fig. 9b.

The third workshop, CFD4NRS-3, took place in Washington DC in September 2010. The workshop proceedings will appear during 2011, and selected papers in a Topical Issue of Nuclear Engineering and Design in 2012. Plans are in place for a fourth workshop in the series, to take place in Daejeon, Korea in 2012.

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 special-effects validation experiments which qualify them. There is a strict review process for all papers. For the numerical analyses, the use of BPGs is mandatory, and the papers reporting experimental findings must contain data from local measurements, suitable for CFD validation, and the use of error bounds on the data are strongly encouraged.



(a) CFD4NRS



(b) XCFD4NRS

Figure 9. Pictures taken from the flyers announcing the first two OECD/NEA-IAEA workshops.

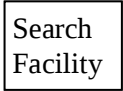
4.3 Moving the Writing Group Documents to the Web

The activities of the three OECD/NEA Writing Groups on CFD were concluded at the end of 2007 with the completion, or near completion, of their respective CSNI reports. It was recognized, like any state-of-the-art report, these documents would only be up-to-date at the time of writing, and, given the rapidly expanding use of CFD in the nuclear technology field, the information they contained would soon become outdated, though perhaps less so for the WG1 document dealing with BPGs. To preserve their topicality, improvements and extensions to the documents are foreseen. It was decided that the most efficient vehicle for regular updating would be to create a Wiki-type web portal. Consequently, in a pilot study, a dedicated webpage has been created on the NEA website using Wikimedia software [66]. In a first step, the WG2 document in the form in which it appears as an archival document [9] has been uploaded to provide on-line access. (The WG1 document [8] has since also been uploaded and the webpages for the WG3 document [10] are currently under construction.)

The current version of the main page is shown in Fig. 10; a customized version is being prepared. There is unrestricted access to the webpages, which can be reached via the NEA website (www.nea.fr) by following successively the links Work Areas: Nuclear Safety, CSNI, WGAMA. Listed are the main chapter headings as they appear in the archival WG2 document [9], the blue colour signifying an active internal link to the detailed information. There is also an active scroll bar, and a hierarchical search facility for finding text strings in the pages. Navigation can be via the Navigation Bar or by use of the Browser functions.

However, the most useful feature of the web portal will be the opportunity to modify, correct, update and extend the information contained there, the Wiki software being the vehicle for this. The aim is to have a static site, with unrestricted access. Readers will not be able to directly edit or change the information, since this requires CSNI endorsement, but can communicate their suggestions to the website editors (the authors of this paper). In parallel, a beta version of the webpage will be maintained for installing updates prior to transfer to the static site. It will be the editor's responsibility to review all new submissions, and implement them into the open-access version of the site. A special *CFD Task Group* has been set up within WGAMA (currently 30 members) to

organize and coordinate the regular updating the websites. This group is chaired by one of the authors of this paper (DB).



4.4 Benchmark Exercises

Experiments to study mixing in T-junctions had been conducted at a number of facilities in France, Germany, Sweden, Japan and Switzerland, but previously unreleased test data became available from tests carried out in November 2008 at the Älvkarleby laboratory of Vattenfall Research and Development in Sweden. These became the basis of the first blind CFD benchmarking exercise organized within WGAMA. Interest in mixing in T-junctions arose following the incident at the Civaux-1 plant in France in 1998 in which both circumferential and longitudinal cracks appeared near a T-junction in the Residual Heat Removal (RHR) system of the N4-type PWR [67]. The

Vattenfall experiment was an ideal test basis for launching a blind CFD benchmarking exercise based on this safety issue. The reasoning is listed here.

- There was widespread interest in the context of high-cycle thermal fatigue [49];
- Downstream data from the test had previously not been released;
- Temperatures, velocities and turbulence data upstream had been carefully measured to provide precise boundary conditions for a CFD simulation;
- Uncertainty estimates were available for all measurements;
- Vattenfall R&D agreed to release measured data to all those who submitted blind calculations in this benchmark.

More details of the benchmarking exercise are contained in a companion paper at this conference [23], and a full CSNI report is due to be circulated during 2011.

5. Final Summary

Since their creation in 2003, the three CFD Writing Groups of the OECD/NEA were very productive in their respective areas. A set of Best Practice Guidelines (BPGs) for performing high quality CFD simulations for nuclear reactor safety analyses have been produced for single-phase applications. These give guidance on preparation for the (safety assessment) task in terms of proper tool selection, geometry, mesh construction, physical modelling options, error control, and verification and validation procedures to follow. The initial work needs to be followed up by application-specific BPGs for the safety issues being currently addressed by the nuclear CFD community, and placing all the information on a Wiki-type web portal is a vital first step in this process. Already, improved guidelines have been submitted to the newly formed *WGAMA CFD Task Group* for updating and extending the material.

The assessment databases for single-phase NRS applications have been collated by the WG2 group, binging together information from the nuclear and non-nuclear domains. The work started with identifying those NRS issues for which the application of CFD tools is needed. These are all characterized by recognition of a strong 3-D component to the flow. Many of the thermal hydraulic situations arising in nuclear technology are mirrored in other industries, and the quality assurance of CFD simulations directly relating to NRS issues inherits the verification and validation efforts made elsewhere. In addition, NRS-specific validation data are also available, and much has been circulated in the context of common projects and benchmarking exercises. Some gaps remain, however. A notable example is the lack of CFD-grade validation data in support of deterministic studies of aerosol deposition in containments within a severe accident scenario.

Many of the safety issues for which CFD can bring better modelling capability involve two-phase flow situations. Two-phase CFD used for safety investigations are able to predict small-scale flow processes not amenable to the classical system thermal-hydraulic codes. However, the two-phase CFD models are not as mature as those developed for single-phase CFD, and the assessment databases available are mostly restricted to 1-D situations. Nonetheless, two-phase CFD is being practised, both within and outside the nuclear area, and potential users need proper guidance to ensure meaningful results. The WG3 group made a large step forward in producing a classification of the various modelling approaches to be used in given NRS situations. A general-purpose, multi-step methodology for performing two-phase CFD was composed, which included a preliminary identification of the different flow processes, a model selection procedure, and listing the necessary

verification and validation steps. A list of 26 nuclear reactor safety issues that could benefit from investigations at the CFD scale was identified by the group. Then, some issues were analysed in more detail, and a preliminary state-of-the-art assessment proposed for each. The outstanding gaps in the existing approaches were also identified. Finally, guidelines for users performing two-phase CFD simulations were proposed. Highlights of the work are described in the preceding sections.

The work of the WGAMA Writing Groups did not only entail the writing of the respective archival documents. A small core group was formed, consisting of the chairmen of the three groups plus the NEA secretariat. This group took up three new initiatives. The first was to organize a series of international workshops under the acronym CFD4NRS to provide a forum for numerical analysts and experimentalists to exchange information in the field of NRS-related activities relevant to CFD analysis. The workshops include single-phase and two-phase CFD applications, and experiments producing CFD-grade data; i.e. detailed local measurements.

The second initiative was to promote a series of blind benchmarking exercises to test the analysts' ability to perform trustworthy CFD simulations without guidance in advance from the experimental data. Such exercises would also encourage universities and research institutions to release previously unpublished test data, and so contribute to the CFD assessment database. The first such benchmark addressed thermal mixing in a T-junction, and has just been completed. The second will be launched during 2011, and will focus on turbulent flow generated by spacer grids in a rod bundle geometry.

Finally, a web portal has been established based on the information gathered by the Writing Groups. Online access will not only provide a more coordinated framework for the material, but the Wiki-type format will give readers an opportunity to modify, upgrade and extend the information, and ensure it remains topical and dynamic. A special *CFD Task Group* has been formed within WGAMA to oversee and coordinate this work.

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