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NUCLEAR ENERGY AGENCY
COMMITTEE ON THE SAFETY OF NUCLEAR INSTALLATIONS

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Working Group on the Analysis and Management of Accidents

(TECHNICAL NOTE)

RECOMMENDATIONS ON GUIDELINES FOR THE USE OF CFD IN NUCLEAR REACTOR SAFETY APPLICATIONS

J. Mahaffy (PSU), M. Scheuerer (GRS), P. Dietrich (IRSN), F. Ducros (CEA), M. Henriksson (Vattenfall), P. Fantoni (Halden), T. Morii (JNES), P. Mühlbauer (NRI), J. Royen (OECD-NEA), B. L. Smith (PSI), T. Watanabe (JAERI)

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COMMITTEE ON THE SAFETY OF NUCLEAR INSTALLATIONS

WORKING GROUP ON THE ANALYSIS AND MANAGEMENT OF ACCIDENTS

The Working Group on the Analysis and Management of Accidents (GAMA) is mainly composed of technical specialists in the areas of thermal-hydraulics of the reactor coolant system and related safety and auxiliary systems, in-vessel behaviour of degraded cores and in-vessel protection, containment behaviour and containment protection, and fission product release, transport, deposition and retention. Its general functions include the exchange of information on national and international activities in these areas, the exchange of detailed technical information, and the discussion of progress achieved in respect of specific technical issues. Severe accident management is one of the important tasks of the group.

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Requests for additional copies of this report should be addressed to:

Nuclear Safety Division
OECD Nuclear Energy Agency
Le Seine St-Germain
12 boulevard des Îles
92130 Issy-les-Moulineaux
France

EXECUTIVE SUMMARY

Background

In May 2002, an “Exploratory Meeting of Experts to Define an Action Plan on the Application of Computational Fluid Dynamics (CFD) Codes to Nuclear Reactor Safety Problems” was held at Aix-en-Provence, France. One of three recommended actions was the formation of this writing group to report on the need for guidelines for use of CFD in single phase Nuclear Reactor Safety (NRS) applications. The second writing group focused on assessment of CFD codes for NRS problems. The report of the second group provides many detailed examples of NRS applications requiring single phase CFD analysis. The third writing group was tasked with recommending extensions to CFD codes to meet the needs of two-phase problems in NRS. Current CFD codes are incapable of analyzing the full range of two-phase flow conditions in the most common transients considered during the licensing of nuclear plants.

Objective of the work

This writing group had three primary objectives:

1. read and summarize existing best practice guidelines for single phase CFD analysis;
2. review and summarize flows in NRS applications for which understanding requires or is significantly enhanced by single phase CFD analysis; and
3. analyze the adequacy of existing guidelines and completeness for NRS applications, and make a recommendation on the need for NRS specific guidelines.

Results and their significance

At the highest level Best Practices Guidelines (BPGs) address two aspects of CFD analysis. The first is practices for construction of an input model for a CFD calculation. These include selection of a CFD method (RANS, LES), specification of the computational mesh, implementation of boundary conditions, selection of an appropriate turbulence model, appropriate use of wall functions, recommended user training, and general quality assurance practices. The second class of guidelines are associated with Verification and Validation (V&V) of CFD results. These include guidance on grid convergence studies, quantification of uncertainty (verification), and comparison against experiments (validation). Roughly half of the BPGs that we reviewed covered both of the areas, generally with more emphasis on guidelines for input specification. The other half focused almost exclusively on V&V of codes and results. A need exists for documents with depth in both input construction and V&V.

Our review of existing guidelines was restricted to those published in the open literature, or produced by an organization to which one of us belongs. We are aware that such documents exist within industries using CFD for design, but in such cases the documentation is proprietary. Some discussions with General Motors indicated a corporate view that general BPGs are inadequate. General Motors creates specific BPGs for each subsystem modelled with CFD.

The report includes reviews of seven specific documents found to be relevant to NRS. The European Research Community on Flow, Turbulence and Combustion (ERCOFTAC), Special Interest Group on “Quality and Trust in Industrial CFD” provided a good general set of guidelines for creation of a CFD input model, including considerations of physical models, and the computational mesh. Other documents, particularly those written by William Oberkampf and by Patrick Roach, provided more comprehensive coverage of verification and validation of CFD calculations. The only NRS specific guidelines for CFD have been created by the EU project Evaluation of Computational Fluid Dynamic Methods for Reactor Safety Analysis (ECORA).

Reviews of specific documents contain detailed comments on their:

- discussion of calculation errors;
- recommended procedures;
- examples provided;
- guidance on physical and numerical models; and
- applicability to NRS.

Although the ECORA document is a particularly good start, we have concluded that none of the available documents provides the full range of information needed for NRS applications of single phase CFD.

Conclusions and recommendations

Our writing group sees a strong need for an OECD/NEA sponsored set of guidelines for use of Computational Fluid Dynamics in Nuclear Reactor Safety analyses. Although we consider ECORA guidelines to be an excellent starting point, there are enough necessary extensions beyond ECORA to justify another document. In addition we feel that Best Practice Guidelines documents should be issued by OECD/NEA to provide maximum international participation in writing and circulation of the documents. We have considered options of documents that are internally complete versus those that rely heavily on references to other works. To maximize the benefit to analysts, we recommend creation of an internally complete document. This approach was used successfully by MARNET, building on the ERCOFTAC guidelines, to create a comprehensive set of guidelines for Marine applications.

We also recommend creation of more than one document. A general best practices guide at the level of the ECORA or ERCOFTAC would follow the outline provided in the Section 5.1 of our report. With this as a template, organizations with direct experience in a specific analysis would contribute information to the OECD/NEA for inclusion in an application specific document. The process of creating and exercising international standard problems would be a particularly good venue for creation of these specific BPGs.

A writing group should be formed within the auspices of OECD/NEA to create the general Best Practices Guidelines document. The group could also be responsible for assembling the application specific guidelines documents, based on input provided by organizations directly involved in the specific CFD analysis. In addition the group would have responsibility for setting up a Web-based format for this document and related application specific guidelines. However, we do not envision the BPG writing group continuing as an independent entity beyond June 2006. Given overlapping membership and responsibilities, any work related to application specific guidelines should be picked up as part of follow-on efforts by the groups on assessment and two-phase needs as they deal with benchmark activities.

A recommended schedule for the writing group and estimated resources are reflected in Annex 1 of our report. If approval is given by the Working Group on the Analysis and Management of Accidents GAMA and CSNI before the end of this year, initial writing will begin in January 2005. A first meeting in March 2005 will discuss introductory sections and general organization of the remaining tasks. A second meeting in September 2005 will review contributions to Chapters 5 through seven of the document and discuss remaining contributions. In March 2006 contributions to the remaining Chapters (8 through 12) will be reviewed and tasks assigned to complete a final draft. A meeting will be held in June 2006 to review the final draft and agree on any last minute changes before submittal to GAMA.

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FOREWORD

Following recommendations made by a group of experts in the field of Computational Fluid Dynamics (CFD) and the Working Group on the Analysis and Management of Accidents (GAMA) at the end of 2002, the NEA Committee on the Safety of Nuclear Installations (CSNI) set up an action plan on CFD issues. The initial phase of the action plan consists of the preparation, by three Writing Groups, of reports in the following areas:

- Guidelines for Use of CFD in Nuclear Reactor Safety Applications
- Assessment of CFD Codes for Nuclear Reactor Safety Problems
- Extension of CFD Codes to Two-Phase Flow Safety Problems

This phase will be followed by a second phase devoted to the performance of CFD computational benchmark exercises.

This report is the result of the preliminary work of the first Writing Group. It summarizes existing CFD Best Practice Guidelines (BPG), discusses specific needs for CFD in Nuclear Reactor Safety (NRS) applications, and recommends a structure for a general guidance document on BPGs for NRS applications. The Writing Group considers the preparation of such a guidance document, as well as the drafting of specific application documents, absolutely necessary.

1. Introduction

CFD has become an accepted tool for design and analysis in a number of industries (*e.g.* aircraft, automotive, marine). However, reliability of these calculations is not based so much on improvements in technology of the codes as it is on improvement in user understanding of nodalization techniques, proper selection of turbulence models, wall functions, and other modelling options. Formal guidelines have been produced by the American Institute of Aeronautics and Astronautics (AIAA) [0], ERCOFTAC [0, 0], ECORA [0] and other studies. In addition general requirements for acceptable publications in the area of CFD have been established by various editorial boards. A number of these have been collected in an Appendix to Patrick Roache's book "Verification and Validation in Computational Science and Engineering [0].

There is a need to sort through all existing user guidance and check its applicability to the range of geometries and transient conditions where single phase CFD is useful to NRS. Guidance for this activity must come from a survey of reactor subsystems and flow conditions in which use of CFD is necessary or highly desirable. Most of this work is being done by the Writing Group on Assessment of CFD Codes for Nuclear Reactor Safety Problems. We have supplemented their effort with a summary of special needs for some specific reactor types.

Our work has focused on guidelines for application to single phase flow, because two-phase CFD is still in its infancy. The Writing Group on the Extension of CFD Codes to Two-Phase Flow Safety Problems is developing recommendations on the path to a mature two-phase CFD capability. As more mature tools become available, usage guidelines can be extended, from those suggested in this report.

2. Objectives of the work

Objectives for this activity were first established in a May 2002 exploratory meeting of experts on the application of Computational Fluid Dynamics (CFD) to Nuclear Reactor Safety (NRS) problems [0], held in Aix-en-Provence, France . The meeting examined current use of CFD for NRS problems and future needs for CFD. Papers covered applications in both the primary coolant system, and containment. Lists were developed of specific problems for which CFD is or should be used; reliable CFD models and nodalization techniques; needs with respect to application methodology and practice; needs for an assessment base; and needs for continued development of CFD codes.

The experts at this meeting reached a consensus on an action plan containing three near term action items:

1. Formation of a writing group to review existing CFD guidelines, analyze their completeness for single phase NRS applications, and make recommendations on the need to write a new guidance manual devoted to NRS.
2. Formation of a writing group to list NRS problems requiring CFD use, identify existing and needed assessment actions, and define a methodology to develop NRS specific assessment matrices.
3. Formation of a writing group to explore extension of CFD to two-phase problems, including classification of two-phase NRS problems requiring CFD, classification of different modelling approaches, specification and analysis of needs for physical assessment, specification and analysis of needs for numerical assessment.

In addition the experts recommended establishing benchmarks on turbulent and stratified flows, jet impingement, and CFD coupling to 0-D/1-D thermal-hydraulic codes.

This writing group has addressed the first action item recommended in Aix-en-Provence, and approved by CSNI. This report summarizes existing guidance for application of single phase Computational Fluid Dynamics (CFD), and analyzes its adequacy and completeness for Nuclear Reactor Safety (NRS) applications. Our writing group noted that Best Practice Guidelines (BPGs) for NRS are already being developed by the ECORA project and has specifically tried to identify what is needed beyond ECORA's work.

The ECORA BPGs contain a general outline on grid generation, model selection, error analysis, quantification of uncertainties, and assessment of experimental data. The BPGs are general procedures. Within ECORA, they are applied to PTS-relevant flows in the primary system of pressurized water reactors and to near-wall and free plumes in the containment.

The ECORA BPGs are focussed on quality improvement of CFD results. The validation of these results requires experimental data of equivalent high quality. In order to obtain the required quality, comparable BPGs should be produced for the experimental side. Among other things, they should comprise standard procedures for quantifying measurement uncertainties and systematic errors, and guidelines for the validation of CFD codes against such data. In addition, the general BPGs should be supplemented by typical flow examples (for instance International Standard Problems) relating to the following reactor types: PWR, VVER, BWR, ADS, HTGR, GCFR, LMFBR, with emphasis on PWR and BWR, as outlined in Chapter 4. The findings of these test cases should be stored in a relational database allowing searches for specific reactors and flow phenomena, and producing recommendations for physical and numerical models, as well as references to available sample applications.

3. Summary of existing guidelines

At the highest level BPGs address two aspects of CFD analysis. The first is practices for construction of an input model for a CFD calculation. These include selection of a CFD method (RANS, LES), specification of the computational mesh, implementation of boundary conditions, selection of an appropriate turbulence model, appropriate use of wall functions, recommended user training, and general quality assurance practices. The second class of guidelines are associated with Verification and Validation (V&V) of CFD results. These include guidance on grid convergence studies, quantification of uncertainty (verification), and comparison against experiments (validation). Roughly half of the BPGs that we reviewed covered both of the areas, generally with more emphasis on guidelines for input specification. The other half focused almost exclusively on V&V of codes and results. A need exists for documents with depth in both input construction and V&V.

Our review of existing guidelines was restricted to those published in the open literature, or produced by an organization to which one of us belongs. We are aware that such documents exist within industries using CFD for design, but in such cases the documentation is proprietary. Some discussions with General Motors summarized at the end of this chapter, indicated a corporate view that general BPGs are inadequate. General Motors creates specific BPGs for each subsystem modelled with CFD.

3.1 ECORA

The EU project Evaluation of Computational Fluid Dynamic Methods for Reactor Safety Analysis (ECORA) is still in progress, but has issued a draft BPG document [0]. Their primary area of application is thermal-hydraulics in the primary system and containment of pressurized water reactors. The document addresses the following issues:

- Definition of errors in CFD simulations. These are numerical errors, user errors, software errors, and application uncertainties, for instance missing boundary condition information.

- Guidelines on avoiding user errors, on minimising numerical errors, on geometry and grid generation, on model selection and application.
- Guidelines for the evaluation of CFD simulations.
- Guidelines for the selection and evaluation of experimental data. A distinction is made between:
    - verification test cases; Simple single-effect tests to check the correct implementation of models;
    - validation test cases: Single-effect, NRS-relevant experiments to as-sure the implementation of the correct models to represent reality;
    - demonstration test cases: Multi-effect experiments to demonstrate the applicability of models and methods for NRS-relevant flows.

3.1.1 Discussion of calculation errors

An error hierarchy is proposed. At first, all numerical errors have to be quantified and reduced to an acceptable level before a comparison with certified experimental data is made. Thus, numerical errors and model errors are separated and valid conclusions on model performance can be made.

The quality assessment of CFD simulations is based on target variables which are either fields or integral values like forces, heat transfer rates, maximum or minimum temperatures. The target quantities must be representative of the goals of the simulation and sensitive enough to detect local changes in the solution when numerical methods or physical models are changed.

3.1.2 Recommended procedures

The following steps in performing a CFD calculation are proposed:

- Definition of representative and solution sensitive target variables to monitor numerical errors.
- Minimisation of iteration errors: Monitoring target variables as function of convergence criteria.
- Minimisation of solution error:
    - Discretization error of spatial derivatives by systematic grid refinement studies using a single discretization scheme and/or comparison of target variables obtained on a single grid using discretization schemes with different truncation error order.
    - Discretization error of time derivatives by systematic time step refinement studies using a single discretization scheme and/or comparison of target variables obtained with a single time step and discretization schemes with different truncation error order.
- Identification of uncertainties arising from insufficient information on the problem by performing a sensitivity study or an uncertainty analysis on the unknown parameters.

Most software programming errors should show up in the calculations when the above steps are performed systematically. ECORA guidelines suggest that these steps be taken in close cooperation with the software developers.

3.1.3 Examples provided

The BPG document contains templates for reports on test case selection and on documenting CFD results. Selected test cases are described in a separate EC-report, EVOL-ECORA-D05a. The ECORA project is still in progress until October 2004. Reports on the CFD computations for verification, validation and demonstration test cases will be summarized in EVOL-ECORA-D06, D07, and D08. These test cases are focused on the investigation of pressurized thermal shock phenomena in the primary system of pressurized water reactors.

In addition, test calculations following the ECORA BPGs will be performed for selected SETH PANDA experiments. These relate to the simulation of near-wall plumes in the containment of pressurized water reactors. A preliminary report on a scoping exercise with simplified geometry and boundary conditions is being prepared by M. Andreani (PSI).

The ECORA BPGs have been adopted for CFD calculations performed in the frame of other European projects like ASTAR [0] and FLOMIX-R [0]. In the ASTAR project, the main emphasis is on the verification of numerical methods. The ASTAR test cases include “Oscillations in a U-Tube Manometer”, “Phase Separation” and “Flow in a Uniformly Heated Vertical Boiling Channel”. The FLOMIX-R project investigates three-dimensional mixing in the primary system of PWRs with emphasis on Boron dilution scenarios. The CFD codes CFX-5 and FLUENT are validated for these conditions by comparison with experimental results from the ROCOM and Vattenfall test facilities. Advanced measurement techniques are applied with enhanced resolution in space and time providing more insight into the details of the turbulent flow phenomena.

3.1.4 Guidance on physical and numerical models

General guidance is given on avoiding user errors, on model selection (turbulence, heat transfer and multi-phase models), and on the reduction of application uncertainties.

In geometry generation, attention should be given to:

- the correct use of a valid coordinate system;
- the correct use of units;
- the use of geometrical simplification, especially on the validity of symmetry planes; and
- local details, in general, geometrical features with dimensions below the local mesh size are not included in the geometrical model, *e.g.* wall roughness or porous elements. These should be incorporated via a suitable model.

Recommendations on grid generation are:

- Avoid high grid stretching ratios.
  - Aspect ratios should not be larger than 20 to 50 in regions away from the boundary
  - Aspect ratios may be larger than that in unimportant regions
  - Aspect ratios may be larger than that in boundary layers
- Avoid jumps in grid density: Growth factors should be smaller than 1.4.
- Avoid small grid angles (< 10º).
- Avoid non-scalable grid topologies. Non-scalable topologies can occur in block-structured grids and are characterised by a deterioration of grid quality under grid refinement.

- Avoid non-orthogonal, *e.g.* unstructured tetrahedral meshes, in (thin) boundary layers.
- Use a finer and more regular grid in critical regions, *e.g.* regions with high gradients or large changes such as shocks.
- Avoid the presence of arbitrary grid interfaces, mesh refinements or changes in element types in critical regions. An arbitrary grid interface occurs when there is no one-to-one correspondence between the cell faces on both sides of a common interface between adjacent mesh parts.
- If possible, determine the size of the cells adjacent to wall boundaries where turbulence models are used before grid generation has started.
- Numerical diffusion is high when computational cells are created which are non-orthogonal to the fluid flow. When cells are large they should be aligned with the fluid flow.
- Judge the mesh quality by using the options offered by the mesh generator. Most modern mesh generators offer checks on geometric mesh parameters, such as aspect ratio, internal angle, face warpage, right-handedness, negative volumes, cracks, and tetrahedral quality.
- It should be demonstrated that the final result of the calculations is independent of the grid that is used. This is usually done by comparison of the results of calculations on grids with different grid sizes.

Modern CFD methods allow the application of adaptive grid procedures. In these methods, the grid is automatically refined in critical regions (high truncation errors, large solution gradients, etc.). The ECORA guidelines note that the selection of appropriate indicator functions for the adaptation is essential for the success of the simulations. They should be based on the most important flow features to be computed.

3.1.5 Applicability of this document

The ECORA BPGs are defined for quality assurance procedures for test case simulations relevant for NRS. In the first step, these guidelines give a fundamental approach to quality assurance of CFD calculations, as three-dimensional CFD applications are a novelty in the field of NRS. However, since the ECORA project is still in progress and the ECORA BPGs are intended as a living document, input from the partners is expected when using and applying the BPGs, in particular for transient two-phase flows.

The ECORA BPGs are a good starting point for discussing Guidelines for use of CFD in NRS applications. The quality procedure documented in the ECORA BPGs put a strong emphasis on the different roles of numerical and model errors and advocates a clear separation of these types of errors. There are rational and affordable methods given to quantify numerical errors which should be part of any CFD calculation in NRS.

Suggestions for extensions beyond ECORA include guidelines for:

- transients;
- steady-state and transient two-phase phenomena;
- evaluation of quality experimental data, including scaling problems;
- validation of CFD codes against such experimental data;
- application examples, International Standard Problems, construction of the database;
- which physical and numerical models to use for a specific NRS application;

- a reference table for specific flow phenomena containing recommended physical and numerical models as well as references to application examples; and
- documentation of special considerations for particular reactor types: PWR, BWR, ADS, HTGR, GCFR, LMFBR.

3.2 ERCOFTAC

The European Research Community on Flow, Turbulence and Combustion, Special Interest Group on "Quality and Trust in Industrial CFD" has published a general CFD BPGs document [0]. It covers a wide range of considerations for single phase CFD. However, emphasis is on creation of the input model. Verification and Validation activities are not described in a rigorous way.

3.2.1 Discussion of calculation errors

At the highest level the document's authors distinguish between error ("A recognizable deficiency that is not due to lack of knowledge"), and uncertainty ("A potential deficiency that is due to lack of knowledge"). They then define seven specific areas in which errors and uncertainty can occur:

1. Physical models, which may simply be uncertain due to underlying data, or in error due to an intentional approximation (*e.g.* incompressible flow, ideal gas).
2. Numerical discretization error (difference rather than differential equations are actually solved).
3. Iterative convergence error (the non-linear difference equations associated with CFD must be solved iteratively with a finite convergence criterion).
4. Round-off errors due to finite precision arithmetic.
5. Application uncertainties such as uncertainties in measurements of geometry, initial conditions, and boundary conditions.
6. User errors associated with input to the CFD program.
7. Code errors, including both bugs in the CFD program and in the compiler.

Three procedures for bounding and controlling errors are defined:

Verification:	Procedure to ensure that the program solves the equations correctly;
Validation:	Procedure to test the extent to which the model accurately represents reality;
Calibration:	Procedure to assess the ability of a CFD code to predict global quantities of interest for specific geometries of engineering design interest.

Most discussions of this subject by other authors lump this concept of calibration into validation, and define calibration differently.

3.2.2 Recommended procedures

The document provides lists of procedures for limiting errors in each of the seven categories listed above and as appropriate expands into subcategories. Specific procedures are provided for selection and proper use of turbulence models. Procedures and recommendations provided to limit user errors include problem definition, common code use errors, interpretation of results, documentation and training requirements. Procedures are also given for the process of validation and construction of sensitivity studies.

The document concludes with a very specific, thirteen page checklist of steps for best practice of an industrial CFD calculation. Contents of the checklist range from general training required for the CFD user to detailed considerations for the turbulence model and mesh construction.

3.2.3 Examples provided

The ERCOFTAC document includes thirty-five pages covering eight examples:

1. 2-D transient scalar bubble convecting at 45 degrees;
2. T-Junction between main and auxiliary pipe;
3. Natural convection flow in a square cavity;
4. Sudden pipe expansion;
5. Transonic airfoil RAE2822;
6. Engine Valve;
7. Low speed centrifugal compressor;
8. Turbulent flow in a model outlet plenum.

These examples do not illustrate all steps in their best practice checklist but are a useful introduction.

3.2.4 Guidance on physical and numerical models

Guidance on physical models is restricted to turbulence, as would be expected for single phase CFD. They cover linear eddy viscosity models, algebraic models, one and two equation models, Reynolds stress models, non-linear eddy viscosity models, and low Reynolds number models.

Guidance on Numerical Models focuses on grid design and time step selection. Guidance is also provided for use of wall functions, and proper implementation of other boundary conditions. In general guidelines apply to finite volume or finite difference based numerical methods. However, some specific guidelines are provided for use of finite element methods.

3.2.5 Applicability of this document

The examples and general guidelines in this document are very appropriate for Nuclear Reactor Safety applications. The checklist introduced at the end of this document is also very useful. A similar list should be considered for NRS BPGs. In addition to providing a summary of most important considerations when performing a CFD analysis, it serves as a reminder of the complexity of the process. All items are familiar to an experienced CFD analyst, but there are so many of them that without some form of checklist, even a very experienced analyst might forget one or more important items on a given project.

The major weakness of this document is that it does not address any formal approach to mesh sensitivity studies and quantification of numerical discretization errors. Fortunately this topic is addressed in detail in a number of other documents reviewed below.

3.3 MARNET

“Best Practices Guidelines for Marine Applications of CFD” was prepared by WS Atkins Consultants, see Ref. [0]. It takes the general ERCOFTAC document as a starting point, and provides specific advice on the application of CFD methods within the marine industry. These guidelines address common aspects of CFD such as:

- Overview of the CFD methods, with particular emphasis on marine applications;
- Sources of errors and uncertainties and their classification;
- Guidance on mesh generation methods;
- Guidance on turbulence modelling, with special considerations on the weakness of the standard k-ε model;
- Boundary conditions: definition, choice and applications;
- Analysis of results and sensitivity studies; and
- Application examples.

Problems related to specific phenomena like cavitation on propellers are not covered in this volume. Applications covered include:

- Vessel boundary layers and wakes;
- Seakeeping;
- Vessel manoeuvring;
- Propeller performance;
- Control surface performance;
- Fluid/structure interaction;
- Offshore fluid loading and platform response; and
- Free surface flow.

3.3.1 Discussion of calculation errors

These guidelines use the same categorisation of errors adopted by ERCOFTAC BPG (see Section 3.2.1 above). Guidelines on how to handle and reduce each of the classified sources of errors are provided.

3.3.2 Recommended procedures

Following the ERCOFTAC pattern, this document presents a checklist that the user should follow in order to take into consideration the guidelines written in the previous chapters. The lists are presented to follow the chronological sequence required to complete a general CFD project.

3.3.3 Examples provided

Four detailed examples are provided:

1. Wave pattern calculation for steady-state ship flow.
2. Viscous stern flow calculation.

3. Example of unsteady manoeuvring calculations.
4. Example of propeller flow calculations.

3.3.4 Guidance on physical and numerical models

The document deals with two different application conditions: potential flow (inviscid and irrotational) and viscous turbulent flow. Although separate and detailed guidelines are provided to address the two approaches, not much is said to help the user in the choice of the best model.

3.3.5 Applicability of this document

Although these guidelines were written for marine applications, most of their contents are very general and applicable to any CFD application, including Nuclear Safety. Guidelines related to the use of RANS (Reynolds Averaged Navier-Stokes). Their guidelines for turbulent flows containing unsteady eddies are very interesting. The MARNET guidelines could provide useful input to the development of NRS specific BPGs, because they contain many domain independent considerations. Obviously, high temperature and pressure effects and multi phase models are not addressed in the document. As with the ERCOFTAC document, the major weakness is that a formal approach to quantification of numerical errors is not addressed.

3.4 AIAA Guidelines

The American Institute of Aeronautics and Astronautics issued the “Guide for the Verification and Validation of Computational Fluid Dynamics Simulations” in January 1998 [0]. It was created for the specific area of CFD modelling in aerospace design and simulation. However, it has broader application in CFD.

This document addresses the process of verifying simulation codes and verifying and validating calculations, including design of validation experiments. It begins by carefully defining and explaining concepts and terminology, used by the AIAA in describing their view of the Verification and Validation processes. Not everyone will agree with all aspects of their definitions, but it is important that they have established some common meaning that can be used to describe internally consistent processes. Next the elements of Verification are described, including grid convergence studies, iteration convergence studies, consistency tests, and comparison against known highly accurate solutions. Finally an approach to Validation based on a tiered hierarchy of test cases is provided.

3.4.1 Discussion of calculation errors

At the highest level errors are delineated by two definitions:

Uncertainty: A potential deficiency in any phase or activity of the modelling process that is due to lack of knowledge.

Error: A recognizable deficiency in any phase or activity of modelling and simulation that is not due to lack of knowledge.

Sources of uncertainty include incomplete knowledge of a physical process or parameter, inadequate specification of boundary conditions (including boundary configuration), and complexity of a physical process (*e.g.* random nature of turbulence).

Four predominant sources of error in CFD simulations are listed as:

1. Insufficient spatial discretization convergence;
2. Insufficient temporal discretization convergence;
3. Lack of iterative Convergence; and
4. Computer Programming.

AIAA focuses its procedures for bounding and controlling errors in the categories of Verification and Validation, defining the terms as:

Verification: The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model

Validation: The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model

These definitions are very similar to those quoted in Section 0 from ERCOFTAC. However, a strong contrast with ERCOFTAC is seen in the AIAA definition of Calibration:

Calibration: The process of adjusting numerical or physical modelling parameters in the computational model for the purpose of improving agreement with experimental data.

AIAA regards V&V as an ongoing process with no clearly defined end. They discuss verification both in terms of verifying a computer code, and verifying an input model for that code. Validation is of models implemented in the simulation code, within the context of a specific set of experiments which have been simulated with the code.. Validation is qualified by the range of state variables tested, and a range of accepted uncertainty in the model output.

3.4.2 Recommended procedures

AIAA expands the discussion of V&V beyond basic definitions, making a number of specific recommendations on procedures. The guidelines suggest sensitivity analysis or Monte Carlo uncertainty analysis to characterise errors due to uncertainty. They suggest Richardson Extrapolation to quantify nodalization errors. Iteration convergence studies are also recommended as part of the verification process. They recommend comparison against known highly accurate solutions as one means to detect errors associated with computer programming.

The guidelines recommend application of a tiered validation hierarchy. Validation problems are defined for a complete system, subsystem cases, benchmark cases, and unit problems. The report emphasizes the importance of designing experiments specifically for use in code validation, and suggests six specific guidelines for designing and implementing validation experiments.

3.4.3 Applicability of this document

The general definitions and guidance for verification and validation are a starting point for determining the appropriate terminology and guidance in Nuclear Reactor Safety, Best Practice Guidelines. This document was meant only as an outline and starting point for a verification and validation process. Variations on the

AIAA choice of definitions and organization are possible. However, this is a good foundation for construction of internally consistent and useful procedures for verification and validation of CFD or other computational simulations.

3.5 Verification and validation in CFD (SAND2002-059)

This paper [0] by Oberkampf and Trucano of SANDIA National Laboratories repeats most of the material in the AIAA report, and expands on suggested procedures. It provides guidelines on terminology and steps in the verification and validation process for CFD. Verification and validation approaches are summarized, major error sources are identified and a hierarchical approach for validation is recommended. Specific topics include: code verification, software engineering, software testing, solution verification and validation, physical model validation and calibration, designing and conducting validation experiments, and estimating experimental uncertainty.

3.5.1 Discussion of calculation errors

The authors refine the AIAA definition of error to include “acknowledged error” (*e.g.* grid truncation error, machine round-off error, iteration convergence errors, known approximations to physical models), and “unacknowledged error” (*e.g.* programming errors, input data errors, compiler errors). They split quantifiable acknowledged errors into contributions when a calculation is performed with converged grid spacing and time step size and contributions due to lack of grid or time step convergence.

For solution verification the authors suggest that the sensitivity of iterative solutions to the convergence criteria should be quantified. For unsteady problems the convergence criteria should be at least one order of magnitude smaller than the global convergence criteria for related steady-state problems.

The authors suggest and demonstrate Richardson extrapolation for quantifying grid and time step related errors. They also reference a study by Roy et al. [0] that determines the extrapolated (converged) solution based on a fit to a polynomial with both first and second order terms. Adaptive grids and a grid convergence index, based on Richardson extrapolation for the estimation of grid convergence errors are mentioned.

This report contains an extended discussion of the Method of Manufactured Solutions (normally requires the ability to alter source code), and “strong sense” benchmarks as the major contributors to dynamic testing.

For errors associated with lack of knowledge of physical models, the report contains a long discussion and set of guidelines for the validation process (see below). The authors recommend construction of a tiered validation hierarchy as also discussed in the AIAA Guide. Using the example of the hypersonic cruise missile, they show how the validation hierarchy for a complex system is structured into subsystems, benchmarks and unit problems. For prioritizing the validation experiments the use of a Phenomena Identification Ranking Table (PIRT) is recommended. In a later invited paper that draws strongly from this report [0], the authors have a much longer discussion of the PIRT process, and give it a central role in validation.

Another section of the report covers the separate issue of uncertainty analysis. This relates to physical parameters, for instance initial or boundary conditions which are not precisely known or measured in an experiment. They believe that uncertainty of these parameters should be incorporated into the computational analysis by ‘ensemble computing.’ An assumed probability distribution of the uncertain parameters generates a set of calculations needed to estimate uncertainty The authors favour Monte Carlo and Latin Hypercube approaches.

After the set of calculations has been completed, an uncertainty quantification of the output is generated. Statistically determined estimates are useful for comparing computational and experimental results, (*e.g.* when comparing the mean value of multiple experimental realizations). Alternatively, a sensitivity analysis is recommended for determining the effect of varying model components (*e.g.* input parameters, model assumptions) on output quantities. This approach is computationally less demanding, but only limited information is obtained compared to an uncertainty analysis.

The report also contains guidance on verification of CFD codes. The authors strongly suggest testing for "static faults" [0] to aid detection of programming errors. This is part of a recommended procedure for Software Quality Testing. One recommended tool for "static testing" is a product named PureCoverage^{TM}.

The other contribution to detection of software errors is "dynamic testing". The authors break this into:

1. Regression Testing, rerunning a large, well chosen test suite with each change to the software, to insure existing capabilities are not damaged unexpectedly;
2. Black Box Testing, users run a code against test problems without knowledge of the code internals
3. Glass Box Testing, developers run tests with full knowledge of the code.

3.5.2 Recommended procedures

Oberkampf and Trucano give the following guidelines for validation of a code:

1. A validation experiment should be jointly designed by experimentalists, model developers, code developers, and code users working closely together throughout the program, from inception to documentation, with complete candour about the strengths and weaknesses of each approach.
2. A validation experiment should be designed to capture the essential physics of interest, including all relevant physical modelling data and initial and boundary conditions required by the code.
3. A validation experiment should strive to emphasize the inherent synergism between computational and experimental approaches.
4. Although the experimental design should be developed cooperatively, independence must be maintained in obtaining both the computational and experimental results.
5. A hierarchy of experimental measurements of increasing computational difficulty and specificity should be made, for example, from globally integrated quantities to local measurements.
6. The experimental design should be constructed to analyze and estimate the components of random (precision) and bias (systematic) experimental errors.

These validation guidelines evolved from earlier work by Oberkampf and others [0,0,0,0], and were adopted with only minor revisions for the official AIAA guidelines[0].

Oberkampf and Truncano also state that validation (*i.e.* the quantification of the level of agreement between computational results and experimental data) is not useful without a set of metrics. They provide general guidance on construction of a quantitative measure of the match between simulation results and experiments, indicating that such metrics should account for known error offsets in the model, uncertainties in the model and in the experiments, and level of confidence in the mean value of experimental results. However, development of one or more useful metrics containing all of these features is still an active research topic. It may be premature to make a specific recommendation on metrics in an initial draft of CFD Guidelines for NRS applications.

As part of verification, the authors define a “strong case benchmark” as containing the following four elements:

1. An exact, standardized, frozen, and promulgated definition of the benchmark.
2. An exact, standardized, and promulgated statement of the purpose of the benchmark. This statement addresses the benchmark's role and application in a comprehensive test plan for a code, for example.
3. Exact, standardized, frozen, and promulgated requirements for comparison of codes with the benchmark's results.
4. An exact, standardized, frozen, and promulgated definition of acceptance criteria for comparison of codes with the benchmark's results. The criteria can be phrased either in terms of success or failure.

3.5.3 Examples provided

This report contains an instructive example of validation associated with design calculations for a hypersonic cruise missile. Although the application is not related to NRS, the steps followed in the process are relevant, and similar to standard practice in the NRS community. The authors discuss a validation hierarchy ranging from full system experiments down to experiments capturing a single physical process. In NRS, we validate simulation codes against integral system tests, component tests, and separate effects tests. Specific guidelines on construction of a validation set for NRS-related CFD can be constructed from the long experience with validation in our discipline. However, it is worth reviewing Oberkamfp’s and Truncano’s general comments for a perspective from a different area of system simulation.

3.5.4 Applicability of this document

This is a very valuable report for anyone considering issues in Verification and Validation. Oberkampf and his colleagues have given the subject very careful thought over a number of years, and their work should be considered in any discipline requiring V&V. Specific procedures for V&V within the NRS community may not match those proposed by these authors. However, the issues raised in this document are generic and should be considered as part of any NRS BPGs.

3.6 Verification and Validation book by P. Roache

Roache’s book [0] provides guidelines and examples for Verification and Validation of codes and calculations. It does not provide many guidelines on construction of input models for CFD codes, best choice of physical models or numerical methods. The area covered in the most detail by the book is grid convergence studies for verification of codes and calculations. The book also covers basic terminology, quantification of uncertainty, use of experimental data for validation, code quality assurance, and journal policy statements on control of numerical accuracy.

3.6.1 Discussion of calculation errors

Roache first divides errors into those determined through the Verification process (errors associated with not solving the equations right) and the Validation process (errors associated with not solving the right equations). He further breaks down errors associated with Verification into the following five categories:

1. errors in code generation;

2. errors in code documentation (*e.g.* in a user manual or comment cards);
3. errors in problem set-up;
4. errors in defining and coding a test case (analytic solutions are often more difficult to code than numerical solutions); and
5. errors in the interpretation of code results.

He also provides and discusses the following taxonomy of errors based on a list provided by Oberkampf et al [0].

- Errors ordered in discretization measures Δ; these errors can be evaluated by grid convergence studies.
- Errors ordered in some numerical (rather than physical) parameter not associated with discretization (like distance to an outflow boundary);
- Errors ordered in some physical parameter.
- Non-ordered approximations (like $\partial\rho/\partial n=0$ at a boundary) that are conceptual modelling errors.
- Programming Errors; these can be detected by grid convergence studies for a problem with an exact solution.
- Computer round-off errors.

Roache suggests a combination of grid convergence studies and application of problems with known solutions (*e.g.* from the Method of Manufactured Solutions) for detecting programming errors, estimating round-off errors, and determining discretization errors. He discusses studies required for errors associated with location of boundaries, and boundary condition assumptions. These are just a question of being aware of assumptions at boundaries, and performing careful sensitivity studies to determine the impact of these assumptions. Roache does not have any easy answer on how to deal with physical modelling errors, but devotes two chapters on the validation process.

3.6.2 Recommended procedures

Roache makes recommendations for providing conservative bounds on mesh related errors, based on standard Richardson extrapolation methods. Given a result f_1 on a fine grid and a result f_2 on a coarser grid, the estimated fractional error on the fine grid is given by:

$$E_1 = \frac{\varepsilon}{r^p - 1} \text{ where } \varepsilon = \frac{f_2 - f_1}{f_1},$$

r is the grid refinement ratio, and p is the numerical method's order of accuracy. He notes that experience with a wide range of grid studies indicates that E_1 is not a conservative bound on the actual discretization error. He defines a Grid Convergence Index (GCI) as:

$$GCI = F_s E_{1},$$

where F_s is the "factor of safety". He recommends $F_s=3$ when only two grids have been used and $F_s=1.25$ for a good quality 3 grid study.

For 3 grid (or better) studies, Roache also recommends calculation of the effective order of the method from the expression:

$$p = \ln\left(\frac{f_3 - f_1}{f_2 - f_1}\right) / \ln(r).$$

He further recommends that consistency in predicted values of p should be checked if more than 3 grids are used.

As part of error analysis, and conclusions on utility of E_1, Roache recommends use of Cumulative Area Fraction Error (CAFÉ) curves. These plot the fraction of the total domain which exceeds a particular error level against that error level.

3.6.3 Examples provided

The book is a rich source of examples for V&V procedures, and references to sources of other examples. This is one reason that it is frequently referenced in other documents on V&V. Examples are mainly in the field of aerospace applications, and in the field of groundwater flows (author's field of interest). Nevertheless, some NRS relevant documents were found in the area of radionuclide transport. Work by Salri et. al. [0, 0] is mentioned on p. 170 of Roaches book in connection with the SECO_TRANSPORT code for groundwater flow, transport, and particle tracking. This work [0] is also mentioned on p. 83 in connection with the shift of a computational cell representing a point source during a grid refinement study. Solution accuracy was affected not only in the neighbourhood of the source as expected, but also at the boundaries far from the source. Pages 175 to 178 contain figures and tables taken over from this document. Roache references work on verification of a multiple species transport code against a problem with an analytical solution [0]. In addition, he illustrates the need for grid convergence studies (pp. 206 and 256) with results of the international project HYDROCOIN [0]. In this project, most of the contributors used only a single grid despite proven effect of grid refinement on important parameters of the flow.

3.6.4 Applicability of this document

This is an excellent reference work in the area of Verification and Validation. Roache is very careful to precisely define his terminology at the beginning of the book (a good model for any set of Guidelines), and to use these definitions to maintain the precision of his writing. This should be used as a source for any specific guidelines on grid convergence studies. Although examples used and cited in the book do not come from NRS applications, the points illustrated by these examples are relevant to NRS.

3.7 ASME publication guidelines for CFD

The American Society of Mechanical Engineers (ASME) has not issued general guidelines on use of CFD, but ASME journals have guidelines for papers reporting CFD methods and/or results from CFD calculations. The Journal of Fluids Engineering has the most detailed such statement on the control of numerical accuracy (see the Journal's web site or Appendix A of Roache's book [0]). These guidelines focus on quantification of numerical errors, and clarity in reporting results.

3.7.1 Discussion of calculation errors

The ASME guidelines specifically address truncation errors, iterative convergence errors, and errors in specification of boundary conditions. They require that numerical methods used must be at least second order in space, unless it can be demonstrated that numerical diffusion is controlled. They recommend demonstration of solution accuracy by using a range of different grid resolutions.

3.7.2 Recommended procedures

ASME publication guidelines require:

- Precise description of the numerical method used;
- Demonstration of mesh convergence;
- Demonstration of temporal accuracy for transient applications;
- Explanation of stopping criteria used in iterative solutions;
- Clear explanation of the implementation of boundary conditions;
- Establish uncertainty for any experimental results compared to calculations.

3.7.3 Applicability of this document

Publication guidelines are useful in constructing the high level outline for a document on best practice of CFD for NRS problems. They should also be adopted when setting requirements for documents relying on CFD to argue the safety of any aspect of a nuclear power plant.

3.8 Other BPGs

General Motors uses CFD for design processes ranging from body shape down through details of the windshield washer system. Because they believe that use of CFD contributes significantly to their competitive advantage, they were unwilling to discuss details of their BPGs. However, two important points were emphasized during conversations with a former employee and communication with a current manager of CFD analysis. GM has established a general outline for contents of BPG documents. However, they do not rely on a general document like the ERCOTFAC guidelines. They construct a specific BPG document for each subsystem modelled with CFD. This maintains very specific knowledge on such things as initial specification of a spatial grid, choice of an appropriate CFD code, and selection of a turbulence model. Given the diversity of flows and geometries associated with a nuclear power plant, this approach can serve as a useful model for BPG's used in NRS analysis.

4. Specific NRS needs for CFD

To provide a basis for our recommendations on needs for NRS specific guidelines we have surveyed a number of existing and planned reactor types. Regions and scenarios have been identified where single-phase CFD is necessary to adequately predict behaviour. This provides some basis for judging completeness of guidelines reviewed in Section 3, and a starting point for recommendations on guidelines for specific sub-systems.

Our charter is to make recommendations on creation of guidelines for existing **single phase** CFD codes for NRS applications. Situations permitting single phase analysis are most likely to occur in Pressurized Water Reactors, therefore, this discussion will primarily focus on applications in these plants. We leave discussion of needs for two-phase CFD to the writing group exploring extension of CFD to two-phase problems.

4.1 Western PWRs

Pressurized Water Reactors have a long history of intense scrutiny by regulatory agencies. The earliest CFD analyses associated with safety issues date back over 20 years to concerns about Pressurized Thermal Shock (PTS). Turbulence models were not as good in those days, but for this, like many of flows requiring

CFD, turbulence is just a part of the story. Complex flow patterns must be resolved involving such features as thermal stratification, impact of jets on structures, and recirculation zones. The special geometry and flow conditions at the cold leg to downcomer connection require an application specific set of guidelines on nodalization and choice of turbulence models.

The next application of CFD to PWRs both downstream and probably chronologically in the history of analysis is understanding of the core inlet flow distribution during normal operating conditions. Proper modelling of the cold leg connections is again required to establish the flow distribution in the downcomer. Guidelines here will differ from those for PTS because of the different character of the inlet flow. Flow patterns also become complex in the lower plenum. This relatively open region is a classic example where 3-D porous media codes such as CATHARE, RELAP-3D and TRACE have little hope of capturing the details of the flow. CFD is required for good results.

Another fairly old core application for CFD is in understanding of cross-flow. Some success was obtained with 3-D porous media codes by applying experimentally determined loss coefficients to flow perpendicular to the fuel rods. However, it has taken CFD with Large Eddy simulation (LES) to provide useful predictive capabilities for these flows. Guidelines will be needed for use of LES in these geometries and flow conditions.

CFD has also aided in the understanding of boron dilution transients. Although turbulent mixing plays a role, the spread in flow due to impingement on the core barrel has more influence on the boron concentration history in the core [0]. This is another situation where standard 3-D porous-media calculations should not be expected to give reasonable results without special intervention. In addition to proper modelling of geometry and flow within the vessel, a detailed understanding of a boron dilution transient might benefit from prediction of enhanced mixing by the main coolant pump. To be most useful, these flow calculations should be directly coupled to a 3-D neutron kinetics calculation, and might use a system safety code for boundary conditions.

Experience gained from prediction of inlet flow distribution and boron dilution transients could be applied to simulation of thermal transients such as a main steam line break. It can be extended with appropriate nodalization of the upper plenum to provide detailed information on temperature distribution in the hot leg during normal operation.

Two other common CFD analyses for PWRs are related to severe accidents. The first is an induced break. Superheated steam flowing from the core to the steam generator will cause failure of steam generator tubes and radioactive release outside the containment unless temperatures in the tubes are sufficiently lowered by mixing in the steam generator inlet plenum with a return flow of cooler steam. The second analysis is not of the PWR itself, but the associated Containment building. Here a CFD code is used to model hydrogen mixing in the containment and predict the threat of hydrogen explosion. This scenario contains jet and buoyancy driven flows, possible jet impingement, stratification due to thermal and species concentration gradients, questions of mixing efficiency, and complicated geometries.

In addition to such basic CFD analyses, two specific vibration analyses have been the subject of significant safety studies. Concerns arose over twenty years ago about flow induced core barrel oscillations and associated metal fatigue. These were explored with early CFD and structural mechanics codes. Flow induced vibrations of steam generator tubes have been a recent safety issue. Although some information can be obtained from single phase analysis, this is fundamentally a two-phase problem.

Additional details on all of these CFD applications are provided in the report by the writing group on Assessment of CFD Codes for NRS Problems.

Similar issues arise in advanced PWR designs, as well as some new potential applications for CFD. Major differences (improvements) between APWR and current PWR include the following:

- The improved core design, for an APWR rated at 1,420 MWe, where the reactor core consists of 257 fuel assemblies of the improved 17x17 type.
- Safety and reliability enhancement
    - Increase of redundancy and independency of the ECCS, 4 subsystems of 50% capacity (Figure 1)
    - Elimination of the switch-over operation of emergency water source during LOCA
    - The emergency water storage (refuelling water storage pit) located inside containment
    - Elimination of the switch-over of the safety injection system during LOCA. Both the large flow rate at early stage of LOCA and relatively low flow rate at later stage are obtained by the newly designed accumulator. Figure 2 and Figure 3 show the characteristics and basic principle of the accumulator.
    - Reducing a number of bolts in the baffle structure of a current PWR Radial reflector (Figure 4)

CFD is valuable in this design in several regions. The new accumulator tank has a vortex damper requiring CFD analysis in its design, and detailed simulations of tank behaviour. CFD also improves understanding of the behaviour of the tank’s free surface and the possible effects of cavitation at the tank outlet.

Within the vessel, CFD is used to evaluate the distribution of the coolant flow rate into the radial reflector. Special considerations are needed to correctly evaluate the flow rate through paths which are very small relative to the scale of a system calculation. As with standard PWRs, CFD is also used to evaluate the downcomer fluid pressure fluctuations. These are provided as the load conditions to the structural vibration code, which calculates the vibration of the radial reflector. Special guidelines are needed to apply the LES model to the large system calculation.

Outside the primary coolant system, containment analyses described for a standard PWR are important, but have different details in the containment layout. The new feature for APWR and other proposed advanced passive designs is the large in containment water storage tank. When the tank becomes a heat sink during accident conditions, CFD is required to understand the temperature distribution within the tank, how this is affected by mixing and stratification, and details of heat transfer to any heat exchangers immersed in the tank.

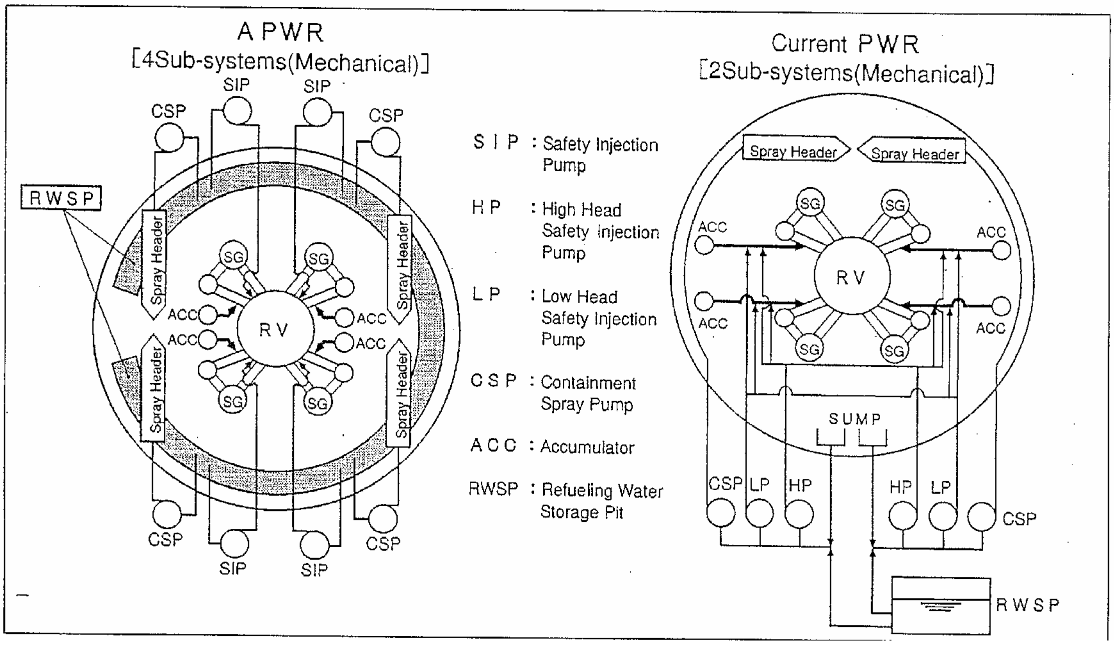


Figure 1. **Configuration of APWR Engineered Safeguard System**

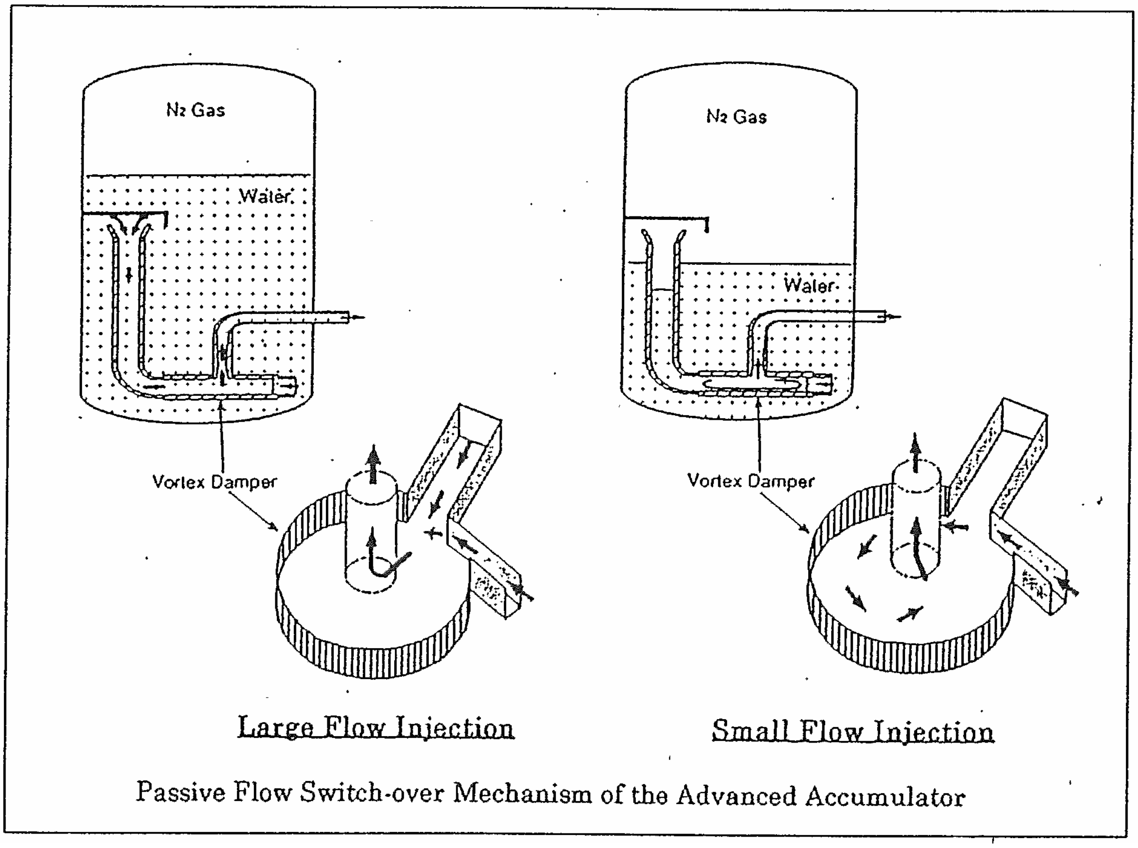


Figure 2. **Advanced Accumulator Diagram**

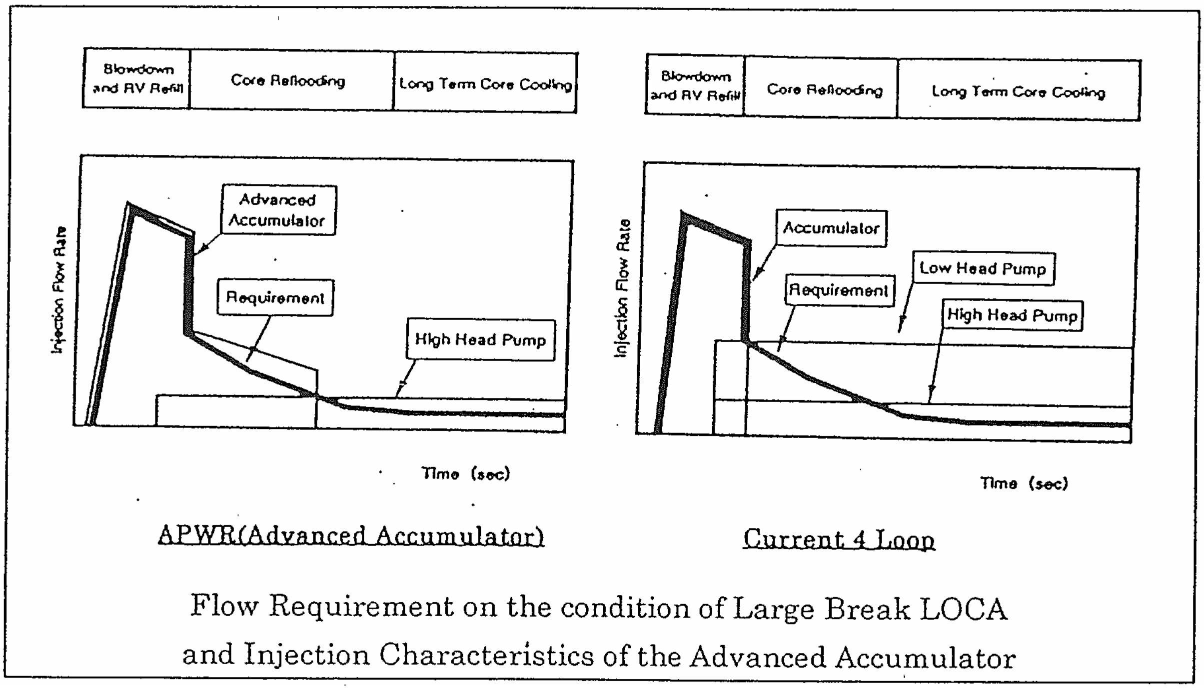


Figure 3. **Advanced Accumulator Flow Characteristics**

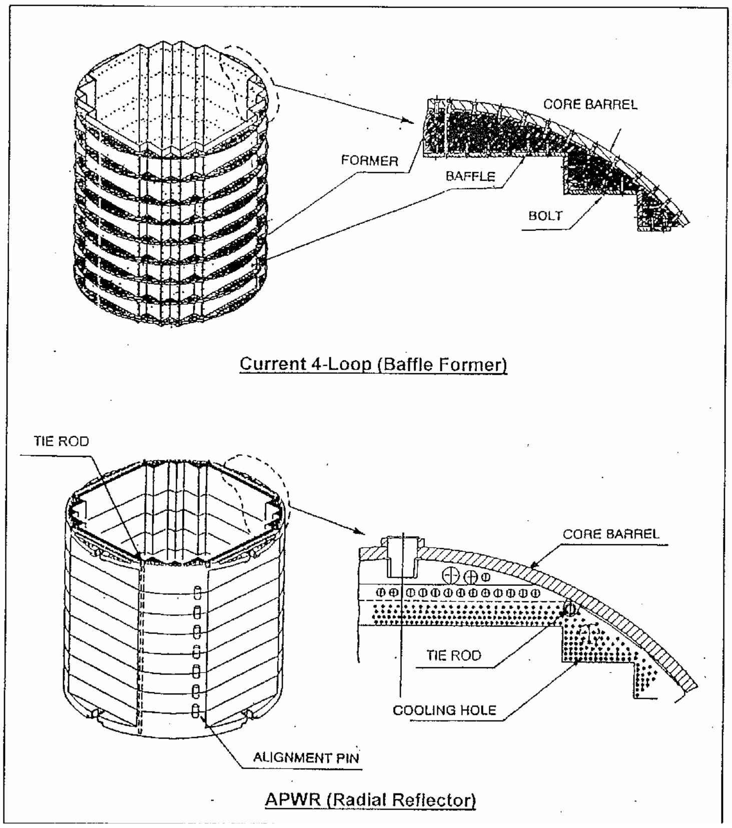


Figure 4. **APWR Radial Reflector and Baffle Former**

4.2 VVER

The VVER-440 geometry differs considerably from that of a western PWR. The height of the reactor core is smaller than in most western PWR designs while the volume of the lower plenum is larger, because of the extra space required by the fuel followers of the control rods. The fuel rods are in a triangular arrangement. Each fuel assembly is hexagonal with a shroud. The VVER-440 design has six primary circuits (VVER-1000 has four primary circuits) with horizontal steam generators. VVER reactors have hot leg nozzles above the cold leg nozzles. Another unique feature of the VVER-440 (not of the VVER-1000) geometry is the hot loop seals. Horizontal steam generators are less effective in both driving and stopping natural circulation in the loops than western U-tube or vertical once-through designs. Even in the case of Steam Generator (SG) heat transfer reversal (*i.e.* due to primary cool-down by break and ECCS), there is still a possibility that ECCS injection of cold water into the reactor downcomer produces sufficient driving force for natural circulation in the loop (“non-standard natural circulation”). This phenomenon was found in NRI calculations with the system code RELAP5 (see Král [0]), but there is no experimental confirmation known to us.

Mixing of primary coolant in a reactor is a very important phenomenon affecting reactor safety. In Table 1 partially taken over from Tuomisto (1987) [0], several parameters affecting primary coolant mixing are compared for selected nuclear power plants. The number of primary loops determines the tendency of downcomer flow to keep a vertical direction, which in the case of the Dukovany NPP is strengthened by guiding vertical baffles in the region of the accumulator (and LPIS) nozzles. Such flow exhibits lower mixing than the case of swirling and re-circulation flow in the downcomer, see Höhne et al. (1999) [0]. The situation of cold and hot leg nozzles at different levels makes the upper downcomer free of obstacles and enhances mixing. The same can be said for larger downcomer width, but here the ratio of loop volume to the sum of volumes of the downcomer and lower plenum also plays a role. This ratio is 1:3 for VVER-440, and 1:1 for a typical western NPP (PWR), see Gango (1997) [0]. A lower ratio is more favourable for mixing. However, the thermal shield in the downcomer can cause “dead zones” with low mixing.

Existence of loop gate valves brings new possible boron dilution scenarios in comparison with western NPPs. The value of the superficial Froude number ($Fr_{CL,HPI}$) affects backflow to the loop seal, mixing and stratification at the High Pressure Injection (HPI) nozzle and in the cold leg, and counter flow in the cold leg between the HPI and reactor vessel. The position of the HPI nozzle also affects mixing in this region. In the Dukovany NPP, there are orifices at the HPI nozzles, which enhance mixing of injected coolant before its entry to cold leg. The steam generator design affects the form of a slug of boron deficient coolant flowing from the hot leg loop seal to the cold leg. Existence of a perforated core barrel bottom and perforated plates in the lower plenum enhances mixing of coolant entering reactor core. Designs of the reactor coolant pump and the pump suction leg determine if backflow of coolant to the loop seal is possible.

In summary, areas of a VVER where CFD would be applied have substantial differences in geometry and flow patterns from the corresponding regions in a standard western PWR. Detailed guidelines for application of CFD to a VVER should be expected to be modified accordingly, and, in particular, be more extensive for the downcomer and lower plenum.

Table 1**: Parameters of the VVER reactor designs important from the point of view of primary coolant mixing and comparison with western PWR.**

Parameter	***Dukovany NPP (VVER-440/213)***	***Temelín NPP (VVER-1000)***	***Loviisa NPP (VVER-440/213)***	***Western PWR***
Number of primary loops	6	4	6	3 - 4
Cold and hot leg nozzles	at different levels	at different levels	at different levels	at the same level
Downcomer gap, mm	150 - 269	185 - 263	150 – 269	250 - 300
Thermal shield in the downcomer	no	no	No	yes
Loop gate valves	yes	no	Yes	no
Reactor coolant pump intake	bottom	bottom	Side	bottom
$Fr_{CL,HPI}$	high	high	High	low
HPI-nozzle in the cold leg	top, orifice	top, angle 45 deg	Bottom	top
Steam generator	horizontal	horizontal	Horizontal	vertical
Perforated flow distributor plate in the lower plenum	yes	yes	Yes	no
Backflow to loop seal	possible	possible	Impossible	possible
Ice condenser	none	none	Yes	no

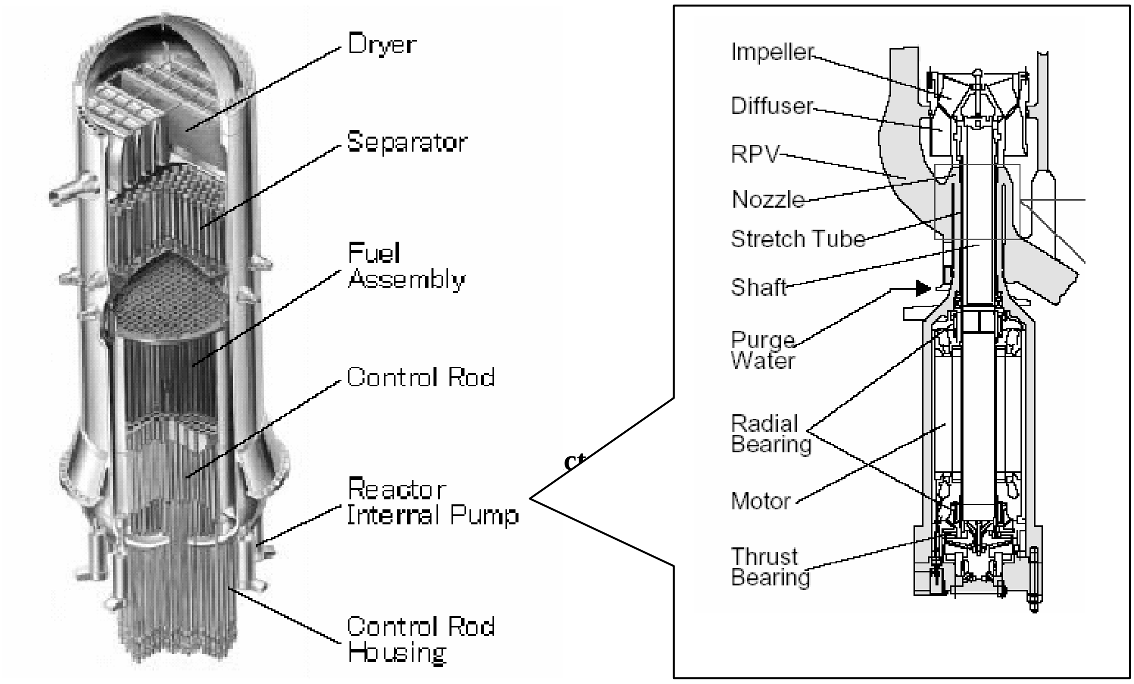
4.3 BWR and ABWR

By their nature Boiling Water Reactors have more limited regions where single phase CFD can be applied. This is true of both standard, and advanced BWR's. Major differences (improvements) between ABWR and current BWR include:

- The improved core design of the ABWR is rated at 1,350 MWe, where the reactor core consists of 872 fuel assemblies of the improved 8x8 type.
- Safety and reliability enhancement
  - Reduction of possibility of occurrence of ECCS. Elimination of accident of re-circulation pipe break can be realized by reactor internal pumps. (Figure 5)
  - Reduction of possibility of occurrence of a control rod drop accident through the newly designed control rod drive

CFD has been useful in understanding mixing of core return flow and feedwater flow in the downcomer, which affects the core inlet temperature distribution. This temperature distribution is also affected by the closely packed internal structures in the lower plenum. As with cross-flow in a PWR core, special considerations are needed to correctly evaluate the flow rate which passes in the very small flow paths between these structures. Flow induced vibration is also an issue for these structures. When evaluating the fluid pressure fluctuations in the lower plenum, special guidelines are needed for application of the LES model to this complex geometry.

As with PWRs, CFD is important for analysis of the containment under severe accident conditions. More specific discussion can be found in the report by the writing group on Assessment of CFD Codes for NRS Problems.



4.4 HTGR

High Temperature Gas Cooled Reactors are an obvious target for single phase CFD analysis, but not emphasized here because of their relative rarity. During normal operation, CFD is required to understand threats of thermal fatigue and development of hot spots associated with fluid mixing and heat transfer. However, significant safety analysis will generally require coupling of CFD capabilities with 3-D conduction, radiation transport modelling, and neutron kinetics. LOCA analysis requires multicomponent single phase flow to follow ingress of air, and chemical reaction models for air/graphite interaction.

BPGs are needed because of complex and unique geometries, and the wide range of flows with transitions from laminar to turbulent and back.

5. Recommended BPG document structure

Structure of BPG documents can be deduced from the examples provided in the previous section and more detailed examples in the report by the Writing Group on Assessment of CFD Codes for NRS Problems. At the highest level we see a large contrast in geometries and flows to be analyzed. Guidelines can be expected to differ substantially between analysis of flow in a containment building and analysis of flow through the guide tubes in a BWR's lower plenum. This is analogous to the problem faced by a company such as General Motors when building guidelines to cover body design calculations of flow around the vehicle and design of a heat exchanger to transfer heat from the engine coolant to the passenger compartment. As General Motors concluded, we believe that it is appropriate to generate separate BPG documents for important reactor subsystems.

The examples given are specific to CFD, but imply a need for written guidelines indicating when traditional porous-media systems codes (e.g. CATHARE, RELAP5) are no longer appropriate, and describing the level of CFD turbulence modelling (RANS, LES, DNS) needed. Precise choice of a CFD tool might be also governed by the best mesh technology for the problem. Large open regions such as a downcomer or water tank might best lend themselves to a standard structured mesh. On the other hand, the lower plenum of a BWR might be better modelled with an unstructured mesh. A heat exchanger in a large water tank might work best with an overset grid technology.

The range of physical conditions in the examples, reflect the standard range of choices of physical models between and within CFD codes. Is an incompressible code an acceptable approximation? If so, what is an appropriate buoyancy model? Application of wall functions is going to vary between tightly spaced internal structures and walls of open regions. The range of geometries and flows discussed can't be covered by a single turbulence model. In a containment analysis you might reasonably expect better results with some zoned modelling of turbulence, using different models near the jet from a pipe break and in areas with buoyancy driven convection.

Generic advice can be provided for verification of models employed, and for validation of results. However, specific guidelines are also necessary for adequate validation of specific subsystems and transients.

A general document would begin with an executive summary, giving both practitioners and managers a clear idea of the extent of the effort required to produce defensible results and training necessary for a competent CFD practitioner. The body of the document would consist of a section on selection of the appropriate CFD software, a section of general guidance on establishing the initial model, a section on quantification of numerical and physical model errors, and a section on validation of results against experimental data. Extensive references should be provided to take advantage of the wealth of existing guidance and examples in the literature.

As already indicated, a general BPG document should be supplemented with BPGs for each specific subsystem that needs CFD analysis. Sufficient experience exists now to generate such a document for pressurized thermal shock, boron dilution (*e.g.* ISP-43), hydrogen mixing in a containment or thermal mixing in a steam generator plenum during a severe accident scenario. One or more of these would serve as template BPGs for other subsystem simulations.

5.1 General guidelines document

A suggested outline is provided below for the general BPG.

1. Executive Summary
2. Introduction
3. Terminology
4. Problem Definition
    PIRT
    Special Phenomena
5. Selecting an Appropriate Simulation Tool
    5.1 Classic Thermal-Hydraulic System Code
    5.2 Component Code (porous)
    5.3 CFD Code
6. User Selection of Physical Models
    6.1 Selection of Turbulence Models
        6.1.1 RANS
            6.1.1.1 Boundary Conditions
            6.1.1.2 Near Wall Models
        6.1.2 LES
        6.1.3 DES
    6.2 Buoyancy Model
    6.3 Heat Transfer
7. User Control of the Numerical Model
    7.1 Transient or Steady Model
    7.2 Grid Requirements
        7.2.1 Resolution of Boundaries
        7.2.2 Grid Quality

- 7.3 Discretization Schemes
  - 7.3.1 Space
  - 7.3.2 Time
- 7.4 Convergence Control
- 7.5 Code Specific Considerations

8. Verification of Calculation, Numerical Model
   - 8.1 Target Variables
   - 8.2 Iteration Error
   - 8.3 Discretization Error
9. Validation of Results
   - 9.1 Validation Methodology
   - 9.2 Target Variables and Metrics
   - 9.3 Sensitivity to Parameter Variations
   - 9.4 Treatment of Experimental Uncertainties
10. Documentation
11. Summary of Specific NRS Cases
12. Summary

To a large degree sections of this outline can be regarded as separable tasks. Annex 1 provides a summary of individuals responsible for each of these tasks, the estimated level of effort, and the completion date.

5.2 Documents with specific guidelines

A document created for a specific application (*e.g.* hydrogen mixing in a containment) would follow the general outline above. However, the sections on “Special Phenomena”, and “Specification of the Input Model and Associated Code Options” would be much more specific and detailed. In the latter section particular attention would be given to the initial specification of a grid. Verification and Validation would primarily provide application specific examples and appropriate references.

Known cases requiring specific guidelines include:

- Hydrogen mixing in the containment;
- Western PWR, Cold Leg connection to the Downcomer
  - PTS
  - Boron Dilution Transient
  - Standard Operating conditions
- Western PWR Lower Plenum

- Western PWR Upper Plenum
- VVER Downcomer
- VVER Lower Plenum
- BWR-ABWR Lower Plenum
- Western PWR Hot Leg and Steam Generator Inlet Plenum (induced break)
- In containment water storage tanks
- APWR Accumulator

Creation of these specific guidelines is a different exercise from creation of a general Guidelines document. Each document needs to be tightly coupled to a project in which a well designed CFD analysis is being performed. One very good venue for creation of such documents would be the process of creation and execution of appropriate international standard test problems and similar benchmark activities. The OECD/NEA should provide guidance for creation of these documents and an organized repository for the final products.

Chapter 11 of the general BPGs should be updated periodically to reflect all existing specific guidelines. Ideally, the general BPGs would exist as a Web based HTML document maintained by the OECD/NEA, with cross links to all application specific documents. The application specific documents could in turn cross-link back to the general document as appropriate.

6. Conclusions and recommendations

Our writing group sees a strong need for an OECD/NEA sponsored set of guidelines for use of Computational Fluid Dynamics in Nuclear Reactor Safety analyses. We have reviewed the ECORA guidelines [0] and consider them to be an excellent starting point, but see enough necessary extensions beyond ECORA to justify another document. In addition we feel that Best Practice Guidelines documents should be issued by OECD/NEA to provide maximum international participation in writing and circulation of the documents. We have considered options of documents that are internally complete versus those that rely heavily on references to other works such as ECORA. To maximize the benefit to analysts, we recommend creation of an internally complete document. This approach was used successfully by MARNET [0], building on the ERCOFTAC guidelines [0].

As indicated in the previous section, we also recommend creation of more than one document. A general best practices guide at the level of the ECORA or ERCOFTAC would follow the outline provided in the Section 0. With this as a template, organizations with direct experience in a specific analysis would contribute information to the OECD/NEA for inclusion in an application specific document. The process of creating and exercising international standard problems would be a particularly good venue for creation of these specific BPGs.

A writing group should be formed within the auspices of OECD/NEA to create the general Best Practices Guidelines document. The group would also be responsible for assembling the application specific guidelines documents, based on input provided by organizations directly involved in the specific CFD analysis. In addition the group would have responsibility for setting up a Web-based format for this document and related application specific guidelines, and a continuing responsibility for updating the Web based document as new specific guidelines are produced. However, we do not envision the BPG writing group continuing as an independent entity beyond June 2006. Given overlapping membership and responsibilities, any work related to application specific guidelines should be picked up as part of follow-on efforts by the groups on assessment and two-phase needs as they deal with benchmark activities.

The recommended schedule for the writing group and estimated resources are reflected in Annex 1. If approval is given by GAMA and CSNI before the end of this year, initial writing will begin in January 2005. A first meeting in March 2005 will discuss introductory sections and general organization of the remaining tasks. A second meeting in September 2005 will review contributions to Chapters 5 through 7 of the document and discuss remaining contributions. In March 2006 contributions to the remaining Chapters (8 through 12) will be reviewed and tasks assigned to complete a final draft. A meeting will be held in June 2006 to review the final draft and agree on any last minute changes before submittal to GAMA.

REFERENCES

1. AIAA, "*AIAA Guide for the Verification and Validation of Computational Fluid Dynamics Simulations*," AIAA Report G-077-1988, 1998.

2. Casey, M., and Wintergerste, T., (ed.), "*Special Interest Group on 'Quality and Trust in Industrial CFD' Best Practice Guidelines, Version 1*," ERCOFTAC Report, 2000.

3. Casey, M., and Wintergerste, T., *"The best practice guidelines for CFD - A European initiative on quality and trust,"* American Society of Mechanical Engineers, Pressure Vessels and Piping Division (Publication) *PVP*, v 448, n 1, p 1-10, 2002.

4. Menter, F., *"CFD Best Practice Guidelines for CFD Code Validation for Reactor-Safety Applications,"* European Commission, 5th EURATOM Framework Programme, Draft Report, EVOL-ECORA-D1, February 2002.

5. Roache, P.J., *"Verification and Validation in Computational Science and Engineering,"* Hermosa Publishers, pp. 403-412, 1998.

6. Mahaffy, J. H., Micaelli, J.-C., Royen, J. (ed.), *"Proceedings of an exploratory meeting of experts to define an action plan on the application of computational fluid dynamics (CFD) to nuclear reactor safety problems"*, Aix en Provence - 15-16 May 2002, Nuclear Energy Agency, Committee on the Safety of Nuclear Installations, Report NEA/CSNI/R(2002)16 .

7. Paillere, H., Kumbaro, A., Farcia-Cascales, J., Bestion, D, Mimouni, S., Laporta, A., Staedke, H., Franchello, G., Graf U.,. Romstedt P,. Toro, E.F.,. Romenski, E., Deconinck, H., Valero, E. Ricchiuto, M, de Cachard, F., Smith, B., *"Advanced Three-Dimensional Two-Phase Flow simulation Tool for Application to Reactor Safety (ASTAR)"*, Proceedings of the FISA 2003 Conference EU Research in Reactor Safety, European Commission, Luxembourg, pp 502 – 509, 10-13 Nov. 2003,.

8. Weiss, F.-P. , Rohde, U., Karlsson, R., Hemström, B., Lillington, J., Scheuerer, M., Tuomisto, H., Toppila, T., Dury, T. , Cvan, M., Muhlbauer, P, Toth, I., Elter, J., Bezrokov, Y., *"Fluid Mixing and Flow Distribution in the Reactor Circuit (FLOMIX-R)"*, Proceedings of the FISA 2003 Conference EU Research in Reactor Safety, European Commission, Luxembourg, , pp 198 - 204,10-13 Nov. 2003.

9. WS Atkins Consultants, "*Best Practices Guidelines for Marine Applications of CFD"*, MARNET-CFD Report, 2002.

10. Oberkampf, W. L. and Trucano, T. G., *"Verification and Validation in Computational Fluid Dynamics"*, Sandia National Laboratories Report SAND2002-059, 2002.

11. Oberkampf, W. L. and Aeschliman, D. P., *"Joint Computational/Experimental Aerodynamics Research on a Hypersonic Vehicle: Part 1, Experimental Results"*, AIAA Journal, Vol. 30, No. 8, pp. 2000,2009, 1992.

12. Walker, M. A., and Oberkampf, W. L., *"Joint Computational/Experimental Aerodynamics Research on a Hypersonic Vehicle: Part 2, Computational Results"*, AIAA Journal, Vol. 30, No. 8, pp. 2010,2016, 1992.

13. Aeschliman, D. P., and Oberkampf, W. L., *"Experimental Methodology for Computational Fluid Dynamics Code Validation"*, Sandia National Laboratories Report SAND95-1189, 1997.

14. Oberkampf, W. L., Aeschliman, D. P., Henfling, J. F., and Larson, D. E., *"Surface Pressure Measurements for CFD Code Validation in Hypersonic Flow"*, AIAA Paper No. 95-2273, 26th Fluid Dynamics Conference, San Diego CA, 1995.

15. Roy, C. J., McWherter-Payne, M. A., and Oberkampf, W. L., *"Verification and Validation for Laminar Hypersonic Flowfields"*, AIAA2000-2550, Fluids 2000 Conference, Denver, CO, 2000.

16. Oberkampf, W. L., Trucano, T. G., Hirsch, C., *"Verification, Validation and Predictive Capability in Computational Engineering and Physics"*, Foundations for Verification and Validation in the 21st Century Workshop," Johns Hopkins Applied Physics Laboratory, October 2002, SANDIA National Laboratories Report SAND2003-3769, 2003.

17. Hatton, L. *"The T Experiments: Errors in Scientific Software"*, IEEE Computational Science & Engineering, Vol.4, No.2, pp. 27-38, 1997.

18. Oberkampf, W. L., Blottner, F. G., and Aeshliman, D. P., *"Methodology for Computational Fluid Dynamics Code Verification/Validation"*, AIAA Paper 95-2226, 26th AIAA Fluid Dynamics Conference, San Diego, California, 19-22 June 1995.

19. Salari, K., Knupp, P., Roache, P. J., and Steinberg, S. *"TVD Applied to Radionuclide Transport in Fractured Porous Media"*, Numerical Method in Water Resources, Denver, Colorado 1992.

20. Salari, K., Blaine, R. L., Economy, K., and Roache, P. J., *"Grid Resolution Studies of Radionuclide Transport in Fractured Porous Media"*, Quantification of Uncertainty in Computational Fluids Dynamics – 1995 (Johnson, R. W. and Hughes E. D. eds..), Joint JSME-ASME Fluid Mechanics Meeting, ASME FED Vol. 213, Hilton Head, South Carolina, August 14-18, , pp. 25-30, 1995.

21. Lester, D. H., Jansen, G., and Burkholder, H. C. *"Migration of Radionuclide Chains Through an Absorbing Medium"*, AIChE Symposium Series, vol. 71, no. 152, 1981.

22. The International HYDROCOIN Project, *"Groundwater Hydrology Modelling Strategies for Performance Assessment of Nuclear Waste Disposal. Level 1: Code Verification"*, NEA/OECD, Paris 1988.

23. Macian-Juan, R., Ivanov, K., Mahaffy, J.H., *"Numerical diffusion and the tracking of solute fields in system codes: Part III. Application to a boron dilution transient analysis in the AP600"*, NED, Vol. 179, pp. 345-356, 1998.

24. Král, P., *"Non-Standard Natural Circulation in Primary Circuit of VVER-440. Behavior of Horizontal Steam Generator in this Regime"*, Fifth International Seminar on Horizontal Steam Generators. Lappeenranta, March 2001. Also Report ÚJV 11616 T.

25. Tuomisto, H., *"Thermal-hydraulics of the Loviisa Reactor Pressure Vessel Overcooling Transients"*, Report IVO-A-01/87, Helsinki 1987.

26. Höhne, T., Rohde, U., Weiss, F.-P., *“Experimental and Numerical Investigation of the Coolant Mixing During Fast Deboration Transients”*, 9th AER Symposium on VVER Reactor Physics and Reactor Safety, Demänovska Dolina, Slovakia, October 4-8 1999.

27. Gango, P., *“Numerical Boron Mixing Studies for Loviisa Nuclear Power Plant”*, Nucl. Eng. Design 177(1997) 239-254.

GLOSSARY

AIAA	American Institute of Aeronautics and Astronautics
ASME	American Society of Mechanical Engineers
BPGs	Best Practice Guidelines
CFD	Computational Fluid Dynamics
DNS	Direct Numerical Simulation
ECCS	Emergency Core Cooling System
ECORA	Evaluation of Computational Fluid Dynamic Methods for Reactor Safety Analysis
ERCOFTAC	European Research Community on Flow, Turbulence and Combustion
$Fr_{CL,\ HPI}$	"Superficial" Froude Number; $Fr_{CL,\ HPI}=(Q_{HPI}/A_{CL})/(g\ D_{CL}\ \Delta\rho/\rho)^{1/2}$
HPI	High Pressure Injection
LES	Large Eddy Simulation
LPIS	Low Pressure Injection System
NRS	Nuclear Reactor Safety
NPP	Nuclear Power Plant
PIRT	Phenomena Identification Ranking Table
PTS	Pressurized Thermal Shock
RANS	Reynolds-Averaged Navier-Stokes
SG	Steam Generator
V&V	Verification and Validation

ANNEX I
TASK ASSIGNMENTS, RESOURCES, AND END PRODUCTS

The table below is an estimate of organizational responsibility, level of effort, and schedule for creation of the general BPG document. It is based on structure of this writing group, and subject to changes resulting from consultation with potential participants, and changes in membership for the document's writing group.

TASK	Lead	Support	Person-days	Report to Writing Group
1. *Executive Summary*	U.S. NRC		1 day	April 2006
2. *Introduction*	U.S. NRC		2 days	Jan. 2005
3. *Terminology*	U.S. NRC		0.5 days	Jan. 2005
4. *Problem Definition*	PSI	JNES	10 days	Jan. 2005
4.1 PIRT	U.S. NRC		5 days	Jan. 2005
4.2 Special Phenomena	Vattenfall	All	10 days	Jan. 2005
5. *Selection of Appropriate Simulation Tool*	CEA		2 days	Jan. 2005
5.1 Classic Thermo-Hydraulic System Code	U.S. NRC	CEA	3 days	Jan. 2005
5.2 Component Code (Porous CFD)	CEA		3 days	Jan. 2005
5.3 CFD Code	PSI		3 days	Jan. 2005
6. *User Selection of Physical Model*	IRSN		2 days	July. 2005
6.1 Selection of Turbulence Models	CEA		2 days	July. 2005
6.1.1 RANS	CEA		8 days	July. 2005
6.1.2 LES	CEA	ANSYS	8 days	July. 2005
6.1.3 DES	CEA	ANSYS	8 days	July. 2005
6.2 Buoyancy Model	CEA		5 days	July. 2005
6.3 Heat Transfer	JAERI	GRS	5 days	July. 2005
7. *User Control of the Numerical Model*	U.S. NRC		5 days	July. 2005
7.1 Transient or Steady Model	U.S. NRC		2 days	July. 2005
7.2 Grid Requirements	GRS		10 days	July 2005
7.3 Discretization Schemes	U.S. NRC		10 days	July. 2005
7.4 Convergence Control	PSI		2 days	July. 2005
7.5 Code Specific Considerations	U.S. NRC		10 days	July. 2005
8. *Verification of Calculation/Numerical Model*	GRS		5 days	Jan. 2006
8.1 Target Variables	GRS		5 days	Jan. 2006
8.2 Iteration Error	GRS		5 days	Jan. 2006
8.3 Discretization Error	GRS		5 days	Jan. 2006

TASK	**Lead**	**Support**	**Person-days**	**Report to Writing Group**
9. *Validation of Results*	GRS		5 days	Jan. 2006
9.1 Validation Methodology	NRI		5 days	Jan. 2006
9.2 Target Variables and Metrics	Halden		10 days	Jan. 2006
9.3 Sensitivity to Parameter Variations	U.S. NRC	GRS	10 days	Jan. 2006
9.4 Treatment of Experimental Uncertainties	Halden	FZR	10 days	Jan. 2006
10. *Documentation*	NRI		3 days	Jan. 2006
11. Summary of Specific NRS Cases	IRSN		2 days	Jan. 2006
12. Summary	U.S. NRC		2 days	Jan. 2006
				Final Report: May 2006