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Safety Analysis**

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CONTENTS

1	OBJECTIVES AND SCOPE	7
1.1	Socio-Economic Objectives and Strategic Aspects	7
1.2	Scientific/Technological Objectives	7
2	WORK PROGRAMME AND RESULTS	8
2.1	Establishment of Best Practice Guidelines (WP 1)	9
2.1.1	General Aspects	9
2.1.2	Errors in CFD Simulations	10
2.1.3	Existing CFD Simulations and Experimental Data	11
2.1.4	ECORA Specific Considerations and Templates	11
2.1.5	Application of the BPG to the ECORA Test Cases	11
2.2	Evaluation of CFD Analysis of Primary Loop (WP 2)	13
2.2.1	Flow and Heat Transfer in Nuclear Reactor Cores	13
2.2.2	Pressurized Thermal Shocks	14
2.2.3	Boron Dilution and Non-Symmetric Loop Operation	14
2.3	Definition of Physical Models and Test Cases for PTS-Analysis (WP 3)	15
2.3.1	Selection of PTS-Relevant Test Cases	16
2.3.2	Selection of PTS-Relevant Physical Models	17
2.3.3	Calculation of PTS-Relevant Verification Test Cases	18
2.4	Software Development and Verification (WP 4)	19
2.4.1	VAL01: Impinging Jet with Heat Transfer	19
2.4.2	VAL02: Impinging Water Jet in Air Environment	21
2.4.3	VAL03: Jet Impingement on a Free Surface	22
2.4.4	VAL04: Contact Condensation in Stratified Steam-Water Flow	25
2.5	Software Validation (WP 5)	28
2.5.1	The Upper Plenum Test Facility (UPTF)	28
2.5.2	Single-Phase Calculations	29
2.5.3	Two-Phase Calculations	33
2.5.4	Conclusions	36
2.6	Evaluation of CFD Analysis of Containment (WP 6)	37
2.6.1	Validation of CFD for Containment Phenomena	37
2.6.2	Evaluation of the Available Database	40
2.7	Pre-Test Analysis of Selected SETH PANDA Tests (WP 7)	42
2.7.1	Definition of the Tasks	42
2.7.2	Results	44
2.7.3	Conclusions	48
2.8	Evaluation of Application of CFD Codes to Reactor Safety (WP 8)	49
2.8.1	Use of Single-Phase CFD	49
2.8.2	Use of Two-Phase Flow CFD	51
2.8.3	Recommendations for Code Customisation	53
2.8.4	Recommendations for Single-Phase CFD Development	55
2.8.5	Recommendations for Two-Phase CFD Development	56
3	MANAGEMENT AND COORDINATION ASPECTS	59
3.1	Contractual Matters	59
3.2	Dissemination of Results	61
4	REFERENCES	63

List of Figures

Figure 1: Organizational structure of ECORA.....	9
Figure 2: PTS-relevant flow phenomena.....	16
Figure 3: Impinging jet geometry.....	20
Figure 4: Nusselt number distribution with discretisation of second order accuracy.....	21
Figure 5: Geometry for test case VAL02.....	21
Figure 6: Distribution of the pressure coefficient along the surface.....	22
Figure 7: Experimental setup.....	23
Figure 8: Comparison of the numerical (left) and experimental (right) void fraction profile as a function of the depth below the initial water surface, along the centre line of the nozzle (please note the different scales on the diagrams).....	24
Figure 9: Void fraction map at different successive times.....	25
Figure 10: Radial profiles of void fraction at 1 mm depth, mesh 1 and mesh 2.....	25
Figure 11: Schematic of the stratified flow in a 2-D duct.....	26
Figure 12: Water temperature profiles at the measurement station, NEPTUNE results: top - lower Reynolds number of steam; bottom - higher Reynolds number of steam....	26
Figure 13: Water temperature profiles at the measurement station, CFX-5 results: left – lower Reynolds number of steam; right – higher Reynolds number of steam.....	27
Figure 14: Location of the key temperature measurement positions, and probe numbering.....	29
Figure 15: Vessel and fluid temperatures on the vessel and cold leg walls (left) and a cross-section through the middle of the cold leg with ECC injection (right).....	31
Figure 16: Stalk 3 results of the CFX-5 reference calculation (left) and UPTF experiment (right). For legend see Figure 14.....	32
Figure 17: Level 750 mm results of the CFX-5 reference calculation (left) and UPTF experiment (right). For legend see Figure 14.....	32
Figure 18: Level 4500 mm results of the CFX-5 reference calculation (left) and UPTF experiment (right). For legend see Figure 14.....	32
Figure 19: Vessel and fluid temperatures on the vessel and cold leg walls (left) a cross-section through the middle of the cold leg with ECC injection (right).....	33
Figure 20: Water velocity at Stalk 5 (for position 3 and 5 see Figure 14).....	34
Figure 21: Iso-surface of constant velocity (0.3 m/s), coloured by temperature (left) and Velocity vectors and temperature distribution @ t = 50 s (right).....	35
Figure 22: Configuration for the two PANDA SETH tests selected for the ECORA project.....	43
Figure 23: Test 9 Steam concentration distribution at 250 s along a horizontal line crossing the plume.....	45
Figure 24: Test 17 Gas temperature distribution on a horizontal line crossing the jet	47
Figure 25: Test 17. Steam concentration vertical distribution in Drywell 2 at 1000 s.....	47

List of Tables

Table I: Overview of the performed CFX-5 computations for UPTF Test 1.....	30
Table II: Overview of the performed CFX-5 computations for UPTF TRAM C1	34
Table III: Summary of containment phenomena.....	37
Table IV: Summary of available CFD applications	38
Table V: Main areas of required experimental work	40
Table VI: List of deliverables.....	59

LIST OF ABBREVIATIONS AND SYMBOLS

ABWR	Advanced Boiling Water Reactor
BDBA	Beyond Design Basis Accident
BPG	Best Practice Guidelines
BWR	Boiling Water Reactor
CFD	Computational Fluid Dynamics
CHF	Critical Heat Flux
DNB	Departure from Nuclear Boiling
ECC	Emergency Core Cooling
EPR	European Pressurised water Reactor
ERCOFTAC	European Research Community for Flow, Turbulence and Combustion
FWP	Framework Programme
GCR	Gas Cooled Reactor
IAEA	International Atomic Energy Agency
LES	Large Eddy Simulation
LMFBR	Liquid Metal Fast Breeder Reactor
LOCA	Loss Of Coolant Accident
LWR	Light Water Reactor
NEA	Nuclear Energy Agency
OECD	Organisation for Economic Co-operation and Development
PTS	Pressurized Thermal Shock
PWR	Pressurized Water Reactor
RANS	Reynolds-Averaged Navier Stokes
RPV	Reactor Pressure Vessel
RSM	Reynolds Stress Model
SST	Shear Stress Transport Model
FEFV	Finite-Element-Finite –Volume
UPTF	Upper Plenum Test Facility
URANS	Unsteady Reynolds Averaged Navier Stokes
VVER	Russian type of pressurised water reactor

EXECUTIVE SUMMARY

The objective of the ECORA project is to evaluate the capabilities of Computational Fluid Dynamics (CFD) software packages for simulating flows in the primary system and containment of nuclear reactors. The interest in the application of CFD methods arises from the importance of three-dimensional flow effects in these reactor components, which one-dimensional system codes cannot predict. Therefore, the ECORA project will identify application areas for detailed three-dimensional CFD calculations and make recommendations for software improvements.

The software assessment includes the establishment of Best Practice Guidelines (BPG) and standards regarding the use of CFD software and the evaluation of CFD results for safety analysis. Quality criteria for the application of CFD software are standardised. CFD results are only accepted after these quality criteria are satisfied. Thus, a general basis for assessing merits and weaknesses of particular models and codes is formed on a European basis. CFD simulations having an accepted quality level will increase confidence in the application of CFD-tools.

In addition, a comprehensive and systematic software engineering approach for extending and customising CFD codes for nuclear safety analyses has been formulated and applied. The adaptation of CFD software for nuclear reactor flow simulations is shown by implementing enhanced two-phase flow, turbulence, and energy transfer models relevant for Pressurized Thermal Shock (PTS) applications into the CFX, and Neptune software. An analysis of selected UPTF and PANDA experiments was performed to validate CFD software in relation to PTS phenomena in the primary system and severe accident management in the containment. The following results have been achieved:

- The ECORA BPGs (see Ref. [1]) were applied in the European projects FLOMIX-R, ASTAR and ITEM. In common workshops and project meetings BPG calculations were presented and discussed (see Refs. [2] and [3]).
- Surveys of existing CFD calculations and experimental data for primary loop (see Refs. [4], [5], [6]) and containment flows (see Refs. [7], [8]) have been performed.
- Relevant flow phenomena and models and methods for the simulation of PTS-relevant flows are documented in Refs [9] and [10]. The implemented models were verified by calculating selected test cases following the ECORA BPGs, see Ref. [11].
- Simulations for PTS-relevant single-phase flow and two-phase flow validation and demonstration test cases have been performed according to BPGs. They are documented in Refs. [12] to [14].
- A prototype of the CFD code CFX-5 containing newly implemented and improved models was made available to the ECORA partners.
- Test cases from the SETH PANDA experiments were selected and scoping calculations for a buoyant steam jet were performed (see Ref. [15]) following the ECORA BPGs.
- Pre-test calculations for the SETH PANDA experiments Test 9 and Test 17 were made, a comparison with experiments is documented in Ref. [16].
- A comprehensive analysis on the use of CFD codes in nuclear reactor applications and recommendations for code development and customisation is documented in Refs. [17] and [18]
- In October 2003, the ECORA project was audited and successfully certified for the international ISO 9001:2000 standard.
- During the Final Meeting at NRG, Petten, the partners agreed to proceed with a follow-up action of this project to achieve the sustainability of the ECORA results, see Ref. [19].

1 OBJECTIVES AND SCOPE

1.1 Socio-Economic Objectives and Strategic Aspects

The major objectives of the ECORA project are to consolidate the use of CFD methods in nuclear safety analysis by providing an overview of the state-of-the-art of their capabilities for safety-relevant applications, and to define CFD code improvements that are necessary for nuclear engineering applications. CFD codes were tested in a concerted validation exercise. This assessment produced requirements for improving the CFD codes used in ECORA. The increase in predictive power and better understanding of PTS and containment flows, which were primarily investigated in the project, provide a firmer basis for the development and practical implementation of engineered safety features and accident management measures. This will allow for higher safety, achieved at reduced cost.

The ECORA project was a multi-disciplinary research effort, which brought together highly skilled experts from different engineering fields. The consortium comprised thermal-hydraulic experts, code developers, safety experts and engineers from the nuclear industry, as well as CFD experts. The development of internationally verified and validated methods and practices helps to improve the analysis of potential accident situations and of operating conditions. It will also contribute to a better management of the plant lifetime.

In ECORA, CFD quality criteria were standardized before the application of CFD software, and results were only accepted once the set quality criteria have been met. This standardization was done on a European basis. The ‘certified’ results form a more rational basis for assessing merits and weaknesses of particular models and codes than individual national efforts. Achievement of an accepted quality level also increases confidence in the results, and reduces the amount of overlapping research. This, in turn, leads to cost savings on a European basis, and allows progress the state-of-the-art rather than on double-checking results on a national basis.

Further benefit to EC policies comes from the involvement of non-nuclear users interested in the application of CFD software for thermal-hydraulic two-phase flow problems. For instance, the same procedures and largely similar models can be used for improved simulations of coal and oil combustion in fossil power engineering and of cavitation in hydraulic power plants. The chemical and process industry has a major interest in a deeper understanding of multi-phase flow mixing and reactions. Hence, the interest of several non-nuclear industry branches will further promote an effective application of the acquired knowledge and of the developed software.

1.2 Scientific/Technological Objectives

The objectives of the ECORA project were to assess the capabilities of current CFD software packages for safety analyses of existing installations and evolutionary reactors, to establish guidelines for their correct use, to identify perspective application areas for three-dimensional flow calculations, and to indicate necessary code improvements for simulations of safety-relevant accident scenarios. The assessment included the validation of CFD codes with respect to severe accident management in the containment and to PTS

phenomena in the primary system of PWRs. Moreover, the feasibility of tailoring CFD codes for reactor safety analysis was demonstrated by implementation, verification and validation of selected physical models relevant for PTS analysis. In the verification step the correct programming and implementation of the models was checked. In the validation step, the numerical results were compared to experimental data for reactor-safety relevant phenomena. Furthermore, requirements were formulated for customized versions of CFD packages with features tailored to the needs of the nuclear industry.

The project had several measurable objectives and steps to reach this goal:

- Establishment of Best Practice Guidelines for ensuring high-quality results and for the formalised judgement of CFD calculations and experimental data
- Assessment of the potential, of difficulties, and of limitations of CFD methods for flows in the primary system and in LWR containments, with special emphasis on mixing phenomena such as PTS
- Definition of experimental needs for the verification and validation of CFD software for flows in the primary system and in LWR containments
- Identification of improvements and extensions to the current CFD packages that are necessary for primary loop and containment flow analysis
- Implementation and validation of improved turbulence and two-phase flow models for the simulation of PTS phenomena in PWR primary systems
- Comprehensive evaluation of the application of CFD codes for reactor safety applications
- Identification of research needs for customising CFD software for nuclear application needs

The project helped to improve understanding of merits and limitations of CFD for reactor safety analysis. It also contributes to the definition of realistic expectations regarding these methods. The ECORA results are used within the proposed 6th framework project NURESIM. Model and code improvements are implemented into CFX-5 and NEPTUNE which are publicly available.

2 WORK PROGRAMME AND RESULTS

The ECORA project started with the establishment of BPGs for the use of CFD codes and the assessment of calculated results and experimental data. The rules established in this Work Package 1 (WP 1) helped to ensure a systematic and consistent approach to the survey, interpretation and assessment of CFD results for flows in the primary system and in the containment of nuclear reactors.

After completion of WP 1, the project was divided into two branches, see Figure 1. The first branch was concerned with CFD analysis in the primary loop. A comprehensive survey of CFD simulations and data was conducted in WP2. PTS phenomena and their modelling were considered in particular detail. The insights gained in WP2 helped to support the selection of special PTS models and test cases in WP 3. These models were implemented in WP 4, and the CFD software was customized to facilitate its use for reactor safety applications. The validation of the new models took place in WP 5. The experiences made in these work packages fed into WP 8, and supported a comprehensive approach to the use of CFD codes in nuclear safety analysis.

The second branch of ECORA dealt with CFD analysis in reactor containments. The current capabilities of CFD codes were evaluated in WP 6. In WP 7, pre-test calculations were performed using selected SETH PANDA data. Finally, the obtained results and experiences were summarised in a comprehensive evaluation of CFD applications in reactor safety in WP 8. In addition, development needs and directions for future developments were provided.

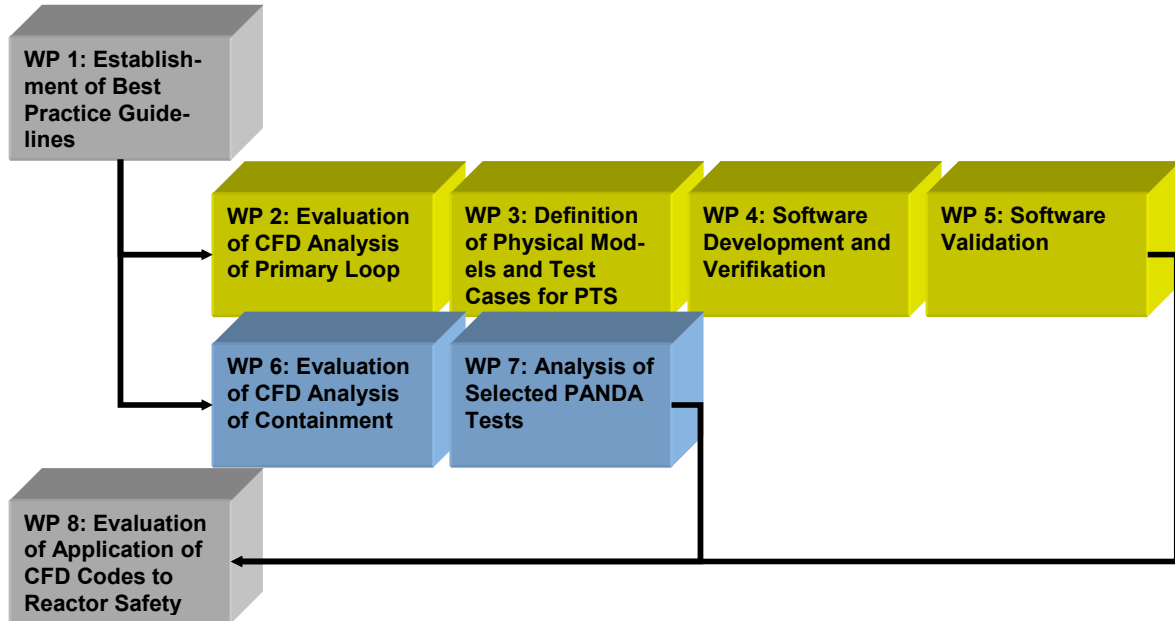


Figure 1: Organizational structure of ECORA

2.1 Establishment of Best Practice Guidelines (WP 1)

2.1.1 General Aspects

One of the central aspects of the ECORA project was the definition and application of Best Practice Guidelines (BPG) for CFD code validation for reactor safety applications. It is to be emphasised that the purpose of this activity, was the combination of “Best Practice” and “Validation”. No attempt was made to provide guidelines for the use of CFD codes for industrial reactor safety applications. The reason for this restriction was that the numerous physical phenomena and the associated physical models have to be tested (validated) against simpler building-block experiments, to demonstrate their proper formulation and modelling accuracy before they can be applied with confidence to more complex applications. Validation of physical model formulations requires a strict discrimination between errors resulting from the model formulation and errors from other sources. A second and equally important outcome of the application of BPG is the resulting information on the computational resources required for an accurate solution. This is of major importance for the estimation of the computing times and hardware requirements for the application of CFD tools to complex industrial applications. It also serves as a basis for the separation of industrial applications, which can be handled by today’s CFD techniques and those which are not within reach due to excessive CPU/Memory requirements.

At the start of the project, BPG have been compiled in a report (D01-best-practice-guidelines.doc) by AEA Technology GmbH (now ANSYS Germany GmbH) and submitted for review to the partners in this work package. Comments of the partners have been included in the document. The BPG were then provided to all partners to serve as a basis for the test case simulations within the project.

It was clear from the start of the present work package that the application of BPG in any rigorous way would be limited to the less complex cases within the project. Nevertheless, it was required from all partners to follow the procedures as far as possible for their validation studies. As detailed below, the BPG have been applied successfully to a number of the ECORA test cases.

2.1.2 Errors in CFD Simulations

A central aspect of the BPG was the identification of all potential errors, which can influence the accuracy of a CFD simulation for the validation cases. The discussion identified the following sources of error:

- Numerical errors
- Model errors
- User errors
- Software errors
- Application uncertainties

Numerical errors result from the differences between the exact equations and the discretised equations solved by the CFD code. For consistent discretisation schemes, these errors can be reduced by an increased spatial grid density and/or by smaller time steps.

Modelling errors result from the necessity to describe flow phenomena like turbulence, combustion, and multi-phase flows by empirical models. For turbulent flows, the necessity for using empirical models derives from the excessive computational effort to solve the exact model equations with a Direct Numerical Simulation (DNS) approach. Turbulence models are therefore required to bridge the gap between the real flow and the statistically averaged equations. Other examples are combustion models and models for interpenetrating continua, e.g. two-fluid models for two-phase flows.

User errors result from inadequate use of CFD software. They are usually a result of insufficient expertise by the CFD user. They can be reduced or avoided by additional training and experience in combination with a high quality project management and by provision and use of Best Practice Guidelines and associated checklists.

Software errors are the result of an inconsistency between the documented equations and the actual implementation in the CFD software. They are usually a result of programming errors.

Application uncertainties are related to insufficient information to define a CFD simulation. A typical example is insufficient information on the boundary conditions, etc..

In addition to the general description of the sources of errors in CFD simulations, strategies for their omission/quantifications are given in the report in the form of guidelines.

2.1.3 Existing CFD Simulations and Experimental Data

In order to be able to utilize also information from other sources, a section on the evaluation of existing CFD simulations was added. The application of these guidelines allows the judgement of the quality of CFD simulation carried out by other groups/projects.

The central aspect in a validation exercise is the availability of high-quality experimental data. It is not sufficient to only investigate sources of errors in the CFD simulations, but to also categorise and quantify the errors in the experiments. A chapter was included in the report, which gives information concerning the selection of experiments for verification, validation and demonstration of CFD codes for reactor safety applications. Examples have been given as to appropriate experiments for the different phases of CFD code/model evaluation.

2.1.4 ECORA Specific Considerations and Templates

Specific considerations for the application of the BPG to the ECORA project have been written. They discuss the different phases of the test case set-up, from geometry generation to grid generation to boundary conditions. Small sections for the selection of physical models have been included (turbulence models and multiphase models). In addition, the chapters in the report relevant for the CFD simulation and the reporting have been listed.

In the appendix, an example for the structure of the test case selection report has been added. It structures the process of test case selection according to:

- The goals of the simulation.
- The description of the test case.
- Quality assessment of the test case.
- Recommendations for CFD simulation.
- Conclusions of the suitability of the test case.

Also in the appendix, a template for the structure of a report for the evaluation of existing CFD results has been included. Finally, the structure proposed for validation reports within the ECORA project has been defined, which was intended as a guideline for the preparation of test case reports within the project. The structure was set-up in a way that all aspects discussed in the BPG were addressed in the report.

2.1.5 Application of the BPG to the ECORA Test Cases

It was clear from the start that the strict application of the BPG would not be feasible for all test cases in the project, due to the large computing resources required. However, it was also agreed that validation studies, without the consideration of the BPG would be of very limited value. The BPG guidelines were therefore applied to all validation studies within the ECORA project, albeit on a different level of detail.

Examples of the comprehensive application of the BPG are summarized in the present report (Chapter 2.3, 2.4):

- VER01: Oscillating Manometer
- VER02: Liquid Sloshing

- VAL01: Impinging single phase jet with heat transfer
- VAL02: Impinging water jet in air environment
- VAL03: Impinging jet on a free surface
- VAL04: Contact condensation in stratified steam-water flow

The main conclusions from the application of the BPG were that some of the cases could be carried out in full consistency with the define procedures (VER01, VAL01 VAL02). Particularly for VAL01 and VAL02, consistent grid refinement procedures could be employed, resulting in a reliable comparison with the experimental data. For both cases, the agreement with the data was very high.

For other cases, the best practice procedures revealed convergence or modelling problems. In case VER02, good quantitative agreement between measurements and simulation could be obtained. However, grid and time step refinement resulted in an increasing resolution of flow details (inclusion of air bubbles in water), which prevented a convergence to a well defined solution. This is a typical situation for flows with free surfaces, where grid refinement eventually results in additional flow details, which might not be desired within the simulation.

For VAL03, the jet impingement resulted in substantially too high air-entrainment into the water with different codes (see chapter 2.4.3). This is a result of the deficiency of the physical models in the impingement region. The results indicate a need for refined two-phase modelling in this region. In addition, it was observed that the numerical accuracy deteriorated under grid refinement. This is most likely also a result of the unphysical behaviour of the models in the impingement region.

The simulation of the flow with contact condensation resulted in a qualitatively good comparison with the data, when all physical aspects were included in the simulation. The current formulation of the condensation models would however require an even finer resolution of the free surface than possible in the simulations.

For the complex applications, involving parts of actual reactors (or models thereof) the BPG could only be applied in a limited fashion. This was expected from the start, as the computing requirements, particularly for transient simulations are already very large. However, even for these cases, important information on the uncertainties in the simulation and the comparison with the data could be obtained. For the UPTF test case, it was shown in a sensitivity study that the use of a porous media approach to simulate the piping in the lower plenum, resulted in oscillations in the simulation, which were not present in the experiments. The detailed geometric modelling of the lower plenum resulted in a stabilization of the simulations. Tests with different spatial and temporal discretisation schemes proved some sensitivity of the simulations to the details of the numerical formulation. This is an indication that additional grid resolution would be required, which was currently not feasible due to limited computer resources. A time step corresponding to $CFL \approx 1$ was needed in the downcomer. Improvements in the prediction have been observed with inclusion of buoyancy modifications in the turbulence model.

Comments on the feasibility of the BPG were provided by PSI. They address the use of BPG in complex geometries with multiple physical phenomena. Particularly for transient flows, the estimates show that the strict application of the procedures is currently not feasible. Other issues, like geometry reduction and boundary layer resolution are also discussed.

It is important to note that the cases where the application of the BPG proved not straightforward should not be used as an argument against the procedures. The information on model-, convergence- or principle deficiencies of today's CFD formulations is an essential basis for future improvements, particularly in multi-phase flow simulations. One could also argue that areas, where no sensitivity studies to numerical or other uncertainties can be performed, are outside the realm of reliable CFD simulations today. However, with the increase of computing power and advanced (statistical) strategies for uncertainty analysis, more and more of these cases will be tractable.

2.2 Evaluation of CFD Analysis of Primary Loop (WP 2)

Within the WP2, a survey of available CFD applications and of experimental data for primary loop applications was conducted and documented in Refs [4] and [5]. The survey included PTS, boron dilution scenarios, steam line break, and flow distribution at the entrance to the core. Particularly, CFD calculations and comparison of the results with experimental data on slug mixing and flow distribution obtained within the 5th FWP project FLOMIX-R, and International Standard Problems (ISP-43) were integrated into this survey. Basic fluid dynamic problems related to turbulent and transient mixing of velocity and temperature fields were considered.

The results of the EUROFASTNET project in relation to limitations and proposed improvements for physical modelling of two-phase flows were considered. Merits of the various turbulence models and numerical schemes were evaluated, and the need to implement more accurate and efficient models and numerical methods was established. Sensitivity studies of the impact of grid nodalisation, numerical schemes and turbulence models on the numerical results were reviewed. Requirements for additional experiments were also identified.

The calculation times for full-scale calculations were estimated and compared with the capabilities of current computers expected to become available within the next decade. This gave a realistic picture of the future possibilities of CFD analyses, and of restrictions posed by simulation time and memory requirements. The current perspective on the application of CFD methods to more complex situations including two-phase flows were evaluated in Ref. [6]. Research needs were defined for developing customized versions of the codes. As an example of established development needs, PTS phenomena and related modelling were considered in more detail.

2.2.1 Flow and Heat Transfer in Nuclear Reactor Cores

In the field of single-phase flow and heat transfer in nuclear reactor cores, two main problem areas can be identified: coolant mixing in the rod-to-rod and rod-to-wall gaps, and effects of spacers (mainly mixing vanes) on coolant mixing. Both these problems are important also to application of sub-channel codes, which are the main tools used in thermal-hydraulic analyses of nuclear reactor cores. Coolant mixing is introduced into these codes by means of semi-empirical correlations for "mixing coefficients" and these correlations are dependent on geometry and other parameters of corresponding experiments. Application of CFD-type codes could decrease the number of needed experiments or provide data, which is difficult or even impossible to measure. In the case of two-phase flow, determination of critical heat flux is the most important. The role of CFD codes here is more difficult, since modelling of two-phase flows suitable for these codes is not

mature enough to be used with confidence. Nevertheless, there are several papers treating rod-to-rod or rod-to-wall gap mixing. The effects of spacers are even more difficult to simulate and very few experimental results are available as most vane designs are proprietary.

2.2.2 Pressurized Thermal Shocks

Pressurized thermal shock is a complex phenomenon involving among others mixing of both forced and buoyant jets/plumes, jet impingement on curved surfaces, plunging jets, and interaction of parallel jets/plumes. In WP 3, some experiments focused on these separate phenomena were used for verification/validation of CFD computer codes. In WP 2, attention was paid to European experimental facilities where “integral” tests were performed. These include German UPTF and HDR facilities, and Finnish FORTUM (former IVO) facility simulating the VVER-440 Loviisa reactor vessel. As for the former two facilities, it is possible to download the data from some tests, but most tests are confidential. Data from several tests on the FORTUM facility was made available within the FLOMIX-R project and a number of CFD analyses were performed in an attempt to find the most suitable approach to this problem. The ECORA and FLOMIX-R results indicate that the behaviour of the cold water plume in the reactor downcomer is affected by the modelling of the structures in the lower plenum.

2.2.3 Boron Dilution and Non-Symmetric Loop Operation

During boron-dilution events, a volume (slug) of boron-deficient water enters the reactor core after start of the main circulation pump, or after recovery of natural circulation. In contrast to the PTS cases with thermal stratification (“cold plumes”), the slug fills the cold leg cross section completely, and flow rates are usually higher. Experiments are therefore focused on mixing in the reactor downcomer and in the lower plenum in front of the reactor core inlets. Main experimental facilities, which are still in operation, are ROCOM (FZR, Germany) modelling the Konvoi reactor, OKB Gidropress (Russia) modelling the VVER-1000 reactor, and Vattenfall (Sweden) modelling the Westinghouse three-loop reactor. Very detailed results of measurements are available also from experiments on the University of Maryland four-leg loop, performed within the OECD/NEA ISP-43.

In the 1:5-scaled ROCOM test facility four different groups of mixing scenarios have been performed:

- Flow distribution measurement at constant flow rates with mass flow rate, the number of operating loops, the status of non-operating loop and the friction losses varied.
- Slug mixing experiments with a change of the flow rate in one or several loops.
- Density driven experiments leading to determination of the critical Froude number for the transition from momentum driven to density driven flow.
- Mixing experiments for determination of the boron dilution distribution at the reactor outlet.

Concentrations at the reactor core inlet and velocity field in the reactor downcomer were measured.

Selected tests were simulated with different commercial CFD codes within the FLOMIX-R project. Again, importance of modelling the lower plenum structures is even more than in the PTS case. Final conclusions are under preparation, but they will be made public soon.

Three tests were performed on the OKB Gidropress experimental facility (Figure 4) with different final flow rate. Temperatures at the reactor core inlet were measured. Selected tests were simulated within the FLOMIX-R project with CFX and FLUENT computer codes. Some problems with uncertainty of the measured quantities (loop flow rates) and with probable, but unknown wall heat transfer caused differences of measured and computed results.

At the University of Maryland 2x4 Loop facility measurement from two tests are available:

- “Front mixing” test when an infinite slug of cold water enters the model of RPV.
- “Slug mixing” test when finite-volume slug of cold water enters the model of RPV.

In these tests, two distinct flow patterns appeared: Buoyancy controlled flow when cold water flows vertically downward in the reactor downcomer driven by density differences, and momentum controlled flow when typical “butterfly-type” pattern is visible in the downcomer. The two types of flow were found even during repeated “identical” runs. One possible explanation could be based on slightly different temperature of the cold water in different runs in situation when the tests are performed in critical region of Froude number. Within the ISP-43, CFD simulations of the “blind” type were performed, and in the simulations, the two types of flow were encountered. It would be useful to perform detailed follow-up simulations of the tests in order to identify possible case(s) of the observed discrepancies.

The Vattenfall experiments are similar to the OKB Gidropress tests; in both cases, a slug of finite volume enters the reactor core. Measurements of concentrations at the “core” inlet and velocities in downcomer were planned for four transient cases: VATT-01 (big slug), VATT-02 (medium-size slug), VATT-03 (small slug) and VATT-04 (slow transient) were planned within the FLOMIX-R project. Both steady state (only velocity field was calculated) and transient of the case VATT-02 was simulated within the project by several groups with FLUENT and CFX codes.

Practically in all CFD analyses of the boron dilution cases, averaged quantities were captured quite well, but distributions of boron concentration at reactor inlet showed discrepancies. Measured positions of minima and maxima were only approximately reproduced by simulations. There were problems with grid-independency of solutions due to limited computer resources. Modelling of internals influenced the results and it was recommended to model them in detail.

2.3 Definition of Physical Models and Test Cases for PTS-Analysis (WP 3)

The flow conditions in the primary system of a pressurised water reactor (PWR) during emergency cooling (ECC) is one of the two reactor safety applications chosen for the validation of CFD codes within the ECORA project. The ECC system of a PWR delivers

cold water to the primary system during a so-called ‘loss-of-coolant accident’ (LOCA). Since the operational temperature and pressure are high, typically 350°C and 150 bar, a rapid temperature drop can lead to an excessive structural load on the reactor pressure vessel. This is called a pressurised thermal shock (PTS).

2.3.1 Selection of PTS-Relevant Test Cases

Figure 2 shows a typical situation encountered in a PTS scenario. Cold water from the ECC system is injected into the cold leg of a PWR to control the effects of a LOCA. The impinging cold water can lead to thermal shocks on the reactor vessel due to combined stresses from rapid temperature and/or pressure changes. This in turn can lead to potential mechanical failure of the walls. The dominant fluid and heat transfer phenomena involved in this scenario are:

- Impingement of single-phase flow jets
- Impingement of two-phase flow jets
- Impinging jet heat transfer
- Turbulent mixing of momentum and energy in and downstream of the impingement zone
- Stratified two-phase flow (or free surface flow) within ducts
- Phase change at the steam-water interface (condensation, evaporation)

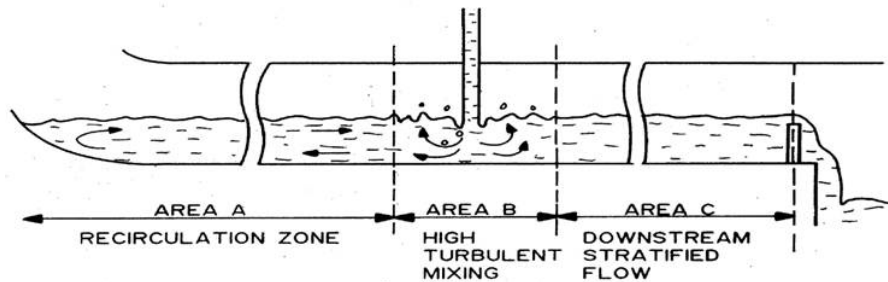


Figure 2: PTS-relevant flow phenomena

After identification of the most important flow phenomena, test cases which relate to these phenomena have been identified and documented in the report D05a (see, Ref. [9]). The test cases are subdivided into single-effect studies, which are used for initial verification and validation of the CFD software, and combined-effect studies, which approximate industrially relevant geometries and operating conditions. The overall strategy was to start software development considering single-effect phenomena, and then proceed to combined effects.

The verification test cases have been proposed by CEA and are discussed in Ref. [11]. They relate to unsteady-state free surface (or stratified) flows, and are:

- VER01: Gravitational oscillations of water in a U-shaped tube
- VER02: Centralized liquid sloshing in a cylindrical pool

The validation test cases are focused on a separate examination of the single physical effects:

- VAL01: Axisymmetric single-phase air jet in air environment, impinging on a heated flat plate
- VAL02: Water jet in air environment impinging on an inclined flat plate
- VAL03: Jet impingement on free surface
- VAL04: Contact condensation on stratified steam/water flow

Test cases VAL01 and VAL02 have been proposed by AEA. VAL01 is a fully turbulent single-phase air jet impinging on a heated flat plate. It relates to the heat transfer and turbulent mixing aspect of a PTS scenario. Mean flow, turbulence and heat transfer data are available. VAL02 is a two-phase water jet, hitting a horizontal or inclined flat plate. The test case represents injection of water into a steam-filled cold leg. Velocity, pressure and jet thickness data are available. VAL03 and VAL04 have been proposed by NRG. VAL03 is an axisymmetric, turbulent water jet impinging orthogonally on a free surface. During this process air is entrained and air bubbles are carried under and dispersed. In VAL04 the direct contact condensation of steam is investigated at a stratified free water surface in a horizontal pipe. In addition, the effect of non-condensable gas on the condensation rate was studied. Finally, the following studies for complex, multi-phase phenomena were proposed as industrial test cases by GRS:

- DEM01: UPTF Test 1
- DEM02: UPTF TRAM C1

The purpose of the demonstration test case DEM01 was to check the ability of the applied CFD codes to simulate correctly the single-phase, thermal mixing and stratification phenomena in horizontal pipes. DEM02 was intended as first PTS test of the two-phase flow models in the CFD codes. The simulation of the demonstration test cases was performed within WP 5 demonstrating code customisation and improvements for PTS-relevant applications.

2.3.2 Selection of PTS-Relevant Physical Models

A selection of PTS-relevant mathematical models is documented in Ref. [10]. It deals with the CFD modelling and simulation of condensation in dispersed and stratified two-phase flows. The main focus is on modelling of transport processes at the vapour-liquid interface, damping of turbulence at free surfaces in stratified flows, and the calculation of the interfacial area density in flows of complex morphology.

CFD software, which is used to predict PTS relevant flow phenomena, must satisfy the following criteria:

- The software must reproduce the test case data within a given error band.
- The software must produce these results in a consistent and convergent manner, i.e. it must be shown empirically that numerical solution errors of the method are bounded and become smaller as the spatial and temporal grids get refined.
- Conservation of the global mass, momentum and energy balances must be guaranteed within the iteration and/or discretisation accuracy.
- The software must be robust. However, a mathematical convergence proof for three-dimensional CFD methods, which could be used as an absolute benchmark

for robustness, does not exist. Therefore, robustness of the CFD methods can only be defined in a statistical sense. For instance, a code is said to be ‚robust’ if it runs and converges for more than 80 % of the test cases it is subject to.

The ‘optimum’ CFD software needs to satisfy the above requirements, at the same minimizing computing time and computer memory demands.

2.3.3 Calculation of PTS-Relevant Verification Test Cases

The two verification test cases have been calculated with CFX-5 and Neptune. The results are documented in Ref. [11]. The purpose of these test cases was to check robustness and accuracy of the numerical methods. Different factors influencing accuracy of the results were identified and analysed separately.

2.3.3.1 VER01: Oscillating Manometer

The first verification test case VER01 is the oscillating manometer documented in Ref. [20]. It consists in calculating the motion of one liquid phase in a U-shaped tube. The tube is closed at both ends. Initially, it contains water in its upper part and air in its lower part. The liquid level is the same in the two parts of the pipe. The initial velocity of the liquid is non zero with a uniform value. In this case the two phases are mechanically uncoupled. Gravity forces are present. The motion of a volume fraction front has to be represented without diffusion. Therefore, stratified flows must be correctly calculated. The problem deals not only with the numerical features, but also with physical modelling. The test case is useful to investigate the accuracy of mass balance and the ability of the code to conserve total pressure along a stream line.

Though the manometer problem is a good test of front-capturing capabilities, as they exist in hyperbolic numerical schemes, parabolic/elliptic solvers cope adequately with the problem, provided second-order differencing schemes are utilised, and there is sufficient mesh resolution. Additionally, there are positive benefits from employing an explicit interface-tracking technique. Satisfactory results are obtained with the Neptune and CFX 4 and CFX-5 codes.

2.3.3.2 VER02: Liquid Sloshing

The test deals with an experiment in which the main phenomenon is free surface oscillations. The flow is transient; the fluid is water in an air environment. A cylindrical pool is divided into two concentric parts. Initially, the water column in the inner cylinder is higher than the water level in the external cylinder. Initially, the water column is released and a sloshing motion of the liquid between the symmetry axis and the outer wall of the cylindrical pool is initiated. The main goal of the simulation is to compute the free surface flow and to predict the motion of the free surface correctly. The original test case is documented in Ref. [21] A cylindrical water column with a diameter of 11 cm and an initial height of 20 cm, is centred in a cylindrical pool with an outer diameter of 44 cm. The initial water level in the pool is 5 cm (D1X-3 experiment). The water sloshing is initiated by lifting quickly the sheet around the inner cylinder. The test case is useful to investigate the following numerical features:

- A large interface between air and water crosses the mesh in this case. It is therefore of interest to check the robustness of the algorithms with regard to residual phases treatment and variations of volume fraction between 0 and 1
- The case is useful to check numerical diffusion and, possibly, dispersion, laying an emphasis on the damping of main oscillations. The case is also useful to distinguish the role of physical modelling and the role of numerical features, when the interfaces get smeared or the waves get damped.
- Accuracy of mass balances
- CPU time required for calculations

Another goal of the simulation of the verification tests is to apply the BPG defined in WP 1 to the current test case. The purpose of the procedures defined in the BPG is to quantify or minimize all numerical errors. Satisfactory results are obtained regarding robustness and accuracy of numerical methods, and the conservation of mass and momentum with the Neptune and CFX code.

2.4 Software Development and Verification (WP 4)

The objective of WP 4 was the implementation and validation of PTS-relevant models. These comprise turbulence, heat transfer and two-phase flow models, including models for phase interaction, evaporation, condensation and boiling. The models are implemented into CFX-5 and NEPTUNE. CEA and EDF use the NEPTUNE code for two phase flow applications. A significant part of the effort is related to the optimisation of the numerical method and the enhancement of the coupling algorithms to achieve fast convergence and robustness of the codes for the complex flows considered. The results are documented in Ref. [12]. In addition, the CFX-5 software has been made available to the ECORA partners in the frame of deliverable D08.

2.4.1 VAL01: Impinging Jet with Heat Transfer

The validation test case VAL01 deals with a single-phase jet impinging on a heated surface. The main goal of the simulation was to compute the heat transfer from the surface to the flow and the velocity profiles near the impingement region. An important aspect of the simulation was the evaluation of the near wall treatment of the CFD methods, which has a significant influence on the accuracy of heat transfer predictions. Jet impingement with heat transfer occurs in PTS scenarios, when cold water is injected into the cold leg of PWRs to control the effects of a LOCA.

The original test cases are documented in Refs. [22], [23], [24]. The experimental data are publicly available from the Classic ERCOFTAC Database, Case 25 of the Classic ERCOFTAC Database at <http://cf.me.umist.ac.uk/ercoftac> (ERCOFTAC is the European Research Community for Flow, Turbulence and Combustion, see www.ercoftac.org).

An axisymmetric, turbulent jet impinges orthogonally on a large plane surface, as shown in Figure 3. The plate is heated by the uniformly distributed heat flux. The flow is statistically steady-state; the fluid is air in air environment. Two Reynolds numbers have been considered, 23,000 and 70,000. They are based on the diameter of the inflow pipe, the bulk velocity and the molecular viscosity of air at standard conditions. The height of the jet discharge above the plate ranges from 2-10 diameters, with particular attention focused on $H/D=2$ and $H/D=6$. Typical temperature differences between the heated flat

plate at a radial position of eight pipe diameters and the incoming air jet are of the order of 10 K. Before discharge, the air passes through a smooth pipe sufficiently long to ensure fully developed flow at the exit plane of the pipe.

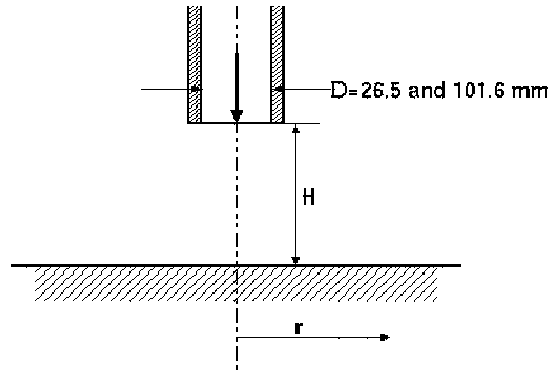


Figure 3: Impinging jet geometry

2.4.1.1 Summary of the Results, Calculated by the ANSYS Group Using CFX-5

The SST model of turbulence with the automatic wall treatment for velocity and temperature was setup for the CFX-5 calculations. The wall treatment procedure switches between the logarithmic wall function and the resolved viscous sublayer depending on the local grid resolution. A series of refined grids was used for the quality assurance.

A validation study for the predictions of the heat transfer between a heated surface and a normally impinging jet has been performed here in accordance with the ECORA BPGs. One set of experimental data ($Re=23000$, $H/D=2$) has been used for the extensive validation of the CFD code and the turbulence model. A quantitative analysis has been performed for the maximum Nusselt number and its radial distribution over the plate as the target variables. An uncertainty analysis has been performed to check the influence of the far field boundary location.

The results, computed for the Reynolds number of 23,000, reveal good agreement with the experimental data both for the Nusselt number and for the velocity profiles near the wall surface at different radial locations. Figure 4 shows the convergence of the Nusselt number distribution on the five grids for the second order accurate discretisation. For the higher Reynolds number of 70,000 the agreement is not as good. Deviation from the experiment becomes more pronounced with the increase of the distance between the pipe outlet and the heated plate surface. This fact can be explained by the general limitation of the eddy viscosity models, which are more suitable for the flows along the solid surfaces. Flows of the more complex pattern, like the impinging jet flow, typically require either special customising of the eddy viscosity model (streamline curvature correction, correction of the turbulence production in the impingement stagnation zone), or the application of the Reynolds stress transport models (RSM). Therefore for the future calculations of test cases with the higher Reynolds numbers and/or larger H/D ratios application of RSM is recommended.

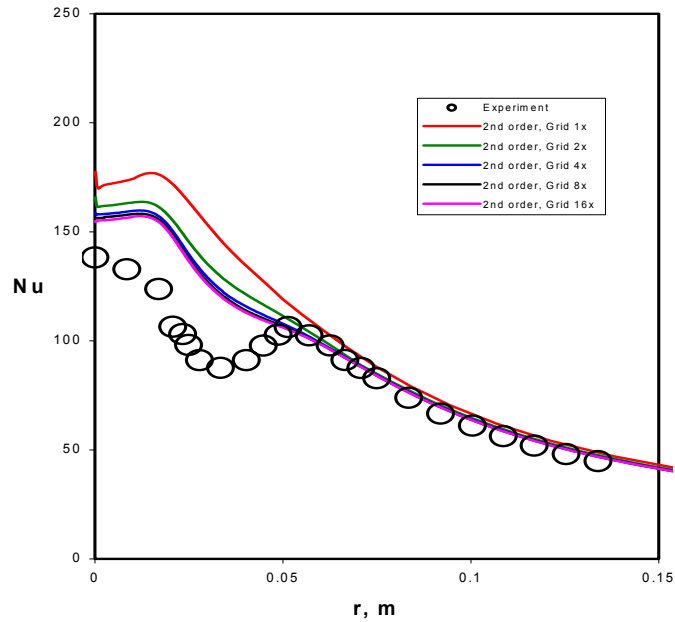


Figure 4: Nusselt number distribution with discretisation of second order accuracy

2.4.2 VAL02: Impinging Water Jet in Air Environment

This three-dimensional validation test case VAL02 relates to a water jet in air environment impinging on an inclined flat plate. It is representative of cold water injection in the steam-filled cold leg. In the experiments, an axisymmetric turbulent water jet generated by an injector hits an inclined flat plate. The geometry is shown in Figure 5. The flow is statistically steady-state. The fluid is water in air environment. Two different inclinations of the plate have been investigated, namely $\gamma = 0^\circ$ and 30° . The mean jet inlet velocity is 19.8 m/s. The jet inlet diameter is 0.03 m, resulting in inlet Reynolds number of 5.94×10^5 , which is in the turbulent flow regime. In the experiment, the pressure distribution on the flat plate was measured. The original test cases are documented in Refs. [25] and [26]

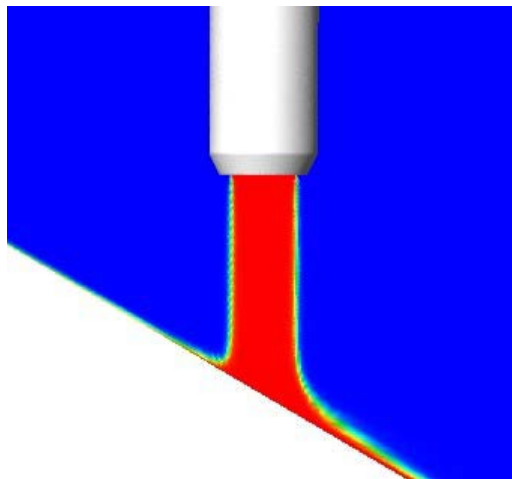


Figure 5: Geometry for test case VAL02

2.4.2.1 Summary of the Results, Calculated by the GRS Group Using CFX-5

The homogeneous multi-phase flow model combined with the SST-turbulence model of CFX-5 has been applied to the test case VAL02. The applied free surface flow model and the turbulence model are suitable to calculate this flow type with good accuracy. The test case has been calculated on three successively refined hybrid grids for the plate inclinations of 0° and 30° . Numerical iteration and solution errors have been quantified following the ECORA BPGs. The discretisation error has been quantified by refining numerical grids and by using discretisation schemes with different truncation error order. In addition, calculations have been performed using the automatic grid refinement option of CFX-5. Comparison with data shows very good agreement on the finest grids for the test case with 30° inclination angle, see Figure 6.

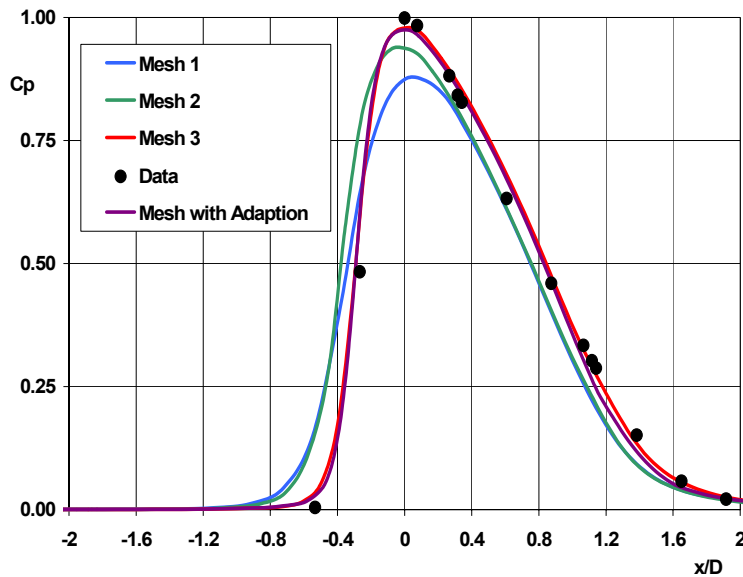


Figure 6: Distribution of the pressure coefficient along the surface

2.4.3 VAL03: Jet Impingement on a Free Surface

Jet impingement on a free surface can occur in PTS scenario, when the ECC water is injected into a partially steam-filled cold leg of the PWR. The processes, taking place in this scenario, i.e. steam carry under, subsequent dispersion and condensation of steam bubbles in the bulk liquid, are very complicated. In order to reduce the complexity of the problem a validation experiment is chosen, which neglects the thermal and the phase change effects. In the experimental study of Bonetto and Lahey, see Ref. [27], jet impingement is studied in air environment. The experimental setup is shown in Figure 7. Water is injected through a 5.1 mm diameter nozzle which impinges normally on a water pool.

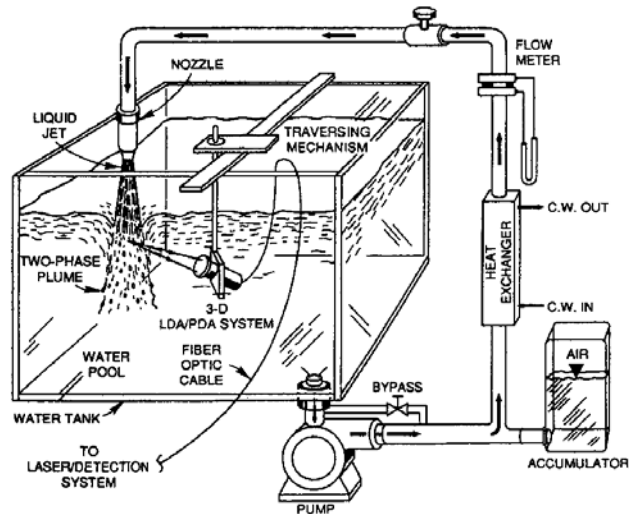


Figure 7: Experimental setup

The experimental system is tested by studying the expected axial symmetry of the volume fraction profile. It was observed to be symmetric within the 1% error in the volume fraction. So, in the computational study, a two-dimensional axisymmetric geometry is used.

In the experimental programme the turbulence intensity of the liquid jet (u_L'/u_L^{mean}) is varied to create a smooth jet (intensity of 0.8 %) and a rough jet (intensity of 3.0 %). For the rough jet, which is used for the validation study, the mean bubble size was measured to be 2.0 mm. Besides this variation in turbulence intensity, also the height of the nozzle above the water surface is varied in the experiment. For the validation study, a nozzle height of 30 mm is chosen. In the experiment, the radial distribution of the volume fraction was measured at three different levels beneath the pool surface. In the centre of the nozzle, the volume fraction was measured as a function of depth. These four volume fraction profiles are compared with the computational results.

2.4.3.1 Summary of the Results, Calculated by the NRG Group Using CFX-5

A conventional two-fluid model was used for this simulation, with the interfacial area density and the drag force modelled using correlations for the dispersed bubbles in the continuous liquid. The turbulent dispersion force was taken into account using a correlation by Lopez de Bertodano, available with CFX-5. A steady-state flow was calculated by solving the Reynolds-averaged Navier-Stokes equations. The assumption of the statistically steady-state flow is based on the experimentally observed flow behaviour.

The analysis started by estimating the numerical errors, according to the ECORA BPG. It turned out that strict application of the BPG was impossible because the convergence degree was not sufficient for the successively refined meshes. Good convergence was achieved only with relatively coarse grids. With grids finer than 6 grid cells per jet radius no properly converged results could be obtained. Nevertheless, the results obtained using the three different coarser grids enabled the authors to estimate the discretisation error. Namely, the error in the height of the radial volume fraction profile was about 10%, and the error in the width of the profile was between 10-15%.

Subsequently, comparison of the numerical and experimental results revealed that the air carry under by the water jet is over predicted by a factor of 4, which is much larger than the numerical error. A typical result is shown in Figure 8 in form of the vertical distribution of void fraction. It is demonstrated that this significant over prediction is caused by application of the interfacial transport models for the dispersed two-phase flow regime, whereas models for the separated two-phase flow regime and special atomisation models are required to accurately model the water jet. This over prediction of carry under would, in real PTS applications, lead to an underestimation of the severity of the PTS, since the steam condensing in the bulk liquid heats up the cold ECC water.

It is therefore concluded that the standard two-fluid model is not suited for simulation of the plunging jet phenomena. A three- or four-fluid approach with the separate phases allocated for the continuous gas and the dispersed bubbles is necessary here, with special treatment of the impingement zone. Since a real PTS scenario is more complicated than this test case due to the thermal effects, it must also be concluded that it will require even more model development before these problems can be tackled.

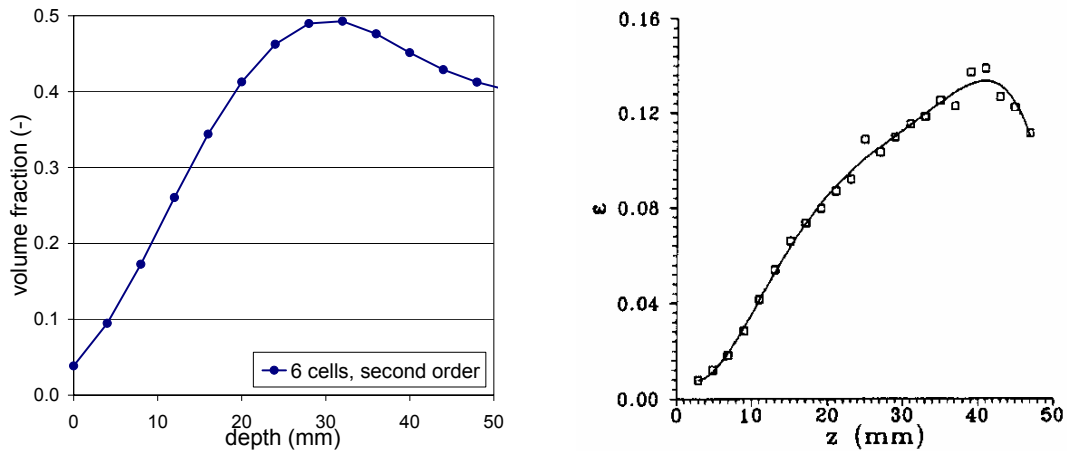


Figure 8: Comparison of the numerical (left) and experimental (right) void fraction profile as a function of the depth below the initial water surface, along the centre line of the nozzle (please note the different scales on the diagrams)

2.4.3.2 Summary of the Results, Calculated by the CEA Group Using NEPTUNE

The modelling approach used for the simulation with NEPTUNE was also based on the two-fluid description. Different from the setup by NRG, both phases were treated as the continuous fluids, and the correspondent correlations typical for the free surface flows were used to model the interfacial area density and the drag force. Besides, the flow regime was setup not as the statistically steady-state one, as done by the NRG group, but as the transient flow (an Unsteady RANS, or URANS approach). The transient flow behaviour is illustrated by Figure 9. Calculations were carried out on three different grids, with different spatial resolution and different height of the computational domain.

Similar to the CFX-5 results, the NEPTUNE simulations revealed the strong overestimation of the air entrainment by a plunging jet. Figure 10 demonstrate this issue by comparing the calculated and the measured radial void fraction distributions.

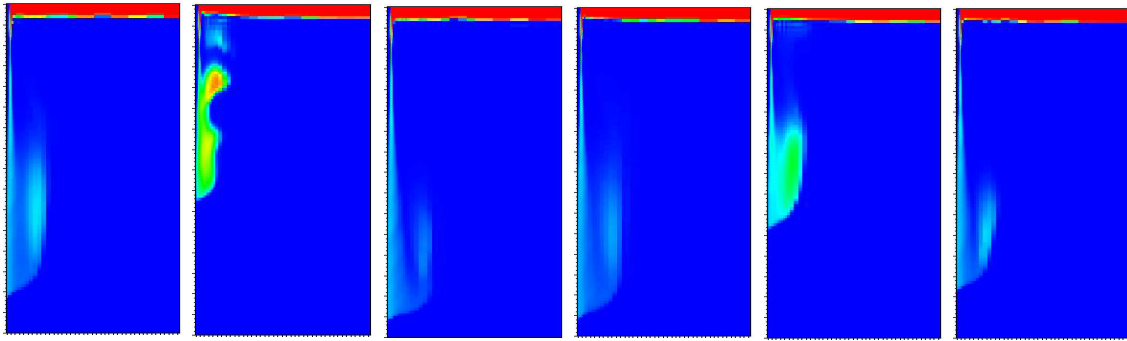


Figure 9: Void fraction map at different successive times

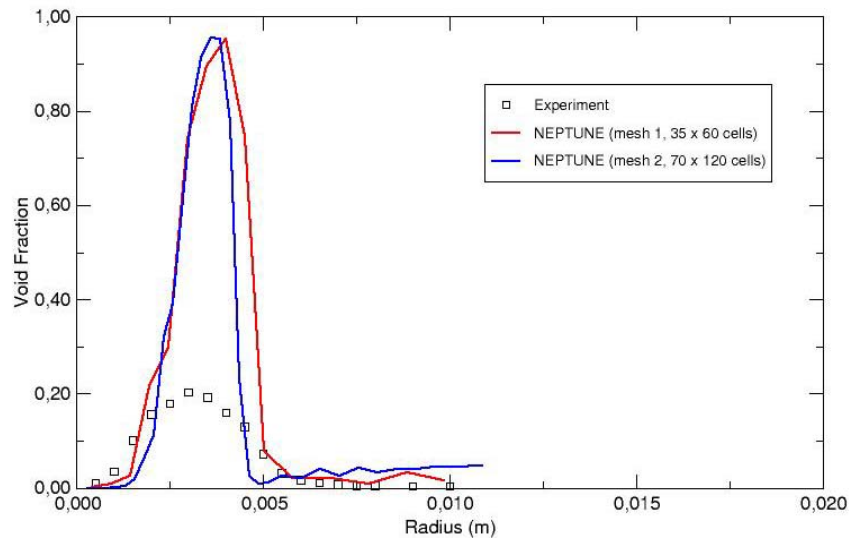


Figure 10: Radial profiles of void fraction at 1 mm depth, mesh 1 and mesh 2.

2.4.4 VAL04: Contact Condensation in Stratified Steam-Water Flow

The VAL04 test case deals with the contact condensation in the two-phase stratified steam-water flow. The main goal of the simulation is to compute heat and mass transport from saturated vapour to liquid over a free surface and the temperature profiles across the liquid flow in a duct. An important aspect of the simulation is the evaluation of how the CFD methods treat turbulent transport near the free surface, which primarily determines the inter-phase heat and mass transfer predictions. Contact condensation on the free surfaces occurs in PTS scenario, when the injected cold water flows together with steam through the cold leg and the other primary loop parts of PWRs.

A schematic of this test case, depicted in Figure 11, represents a 2-D horizontal stratified co-current flow of sub-cooled water and saturated dry steam along a straight channel with adiabatic walls. It has been documented in detail in Ref. [12]. The original test cases are documented in Refs. [28] to [30]. Experimental data have been performed at the Technical University of Munich using the LAOKOON test facility. They include the water and steam flow rates at the feed cross section, the inlet water temperature, and the temperature distribution across the water layer at one given location, where a vertical ar-

ray of thermocouples is installed. The pressure level inside the channel and the water layer height are also known.

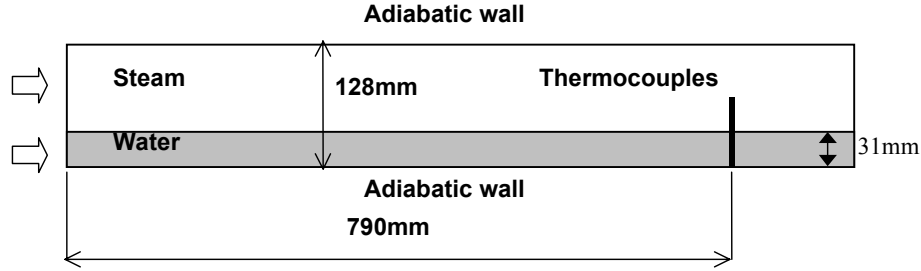


Figure 11: Schematic of the stratified flow in a 2-D duct

According to the experimental evidence this flow is stationary and two-dimensional. The Reynolds number of water was in the range between 20,000 and 30,000. Two co-current flow regimes were selected, which differ in the steam Reynolds number value, namely $5.1 \cdot 10^5$ and $3.4 \cdot 10^5$ at the inlet. The pressure level was close to 7 bar in the higher Reynolds number case, and 4 bar in the lower Reynolds number case. Due to the carefully designed inlet and outlet of water the free surface is plane and horizontal everywhere. No waves were visually observed in the experiment. During the condensation the latent heat of phase transition is released and fully consumed for heating up the initially sub-cooled water. The correspondent temperature gradient, normal to the free surface, develops in water. Therefore the condensation rate is limited by the transport rate of heat from the free surface to the bulk water flow.

2.4.4.1 Summary of the Results, Calculated by the EDF Group Using NEPTUNE

A model of condensation, used by the EDF group, was based on a modified interface renewal concept by Hughes and Duffey in Ref. [31]. A small parametric study was done for the high Reynolds number configuration in order to better understand the behaviour of the condensation model.

Figure 12 shows the water temperature profiles at the measurement section. The computation curve of the water temperature is in a good agreement with the experimental data. Near the channel bottom, the water temperature obtained with the Neptune CFD code is colder than expected, which might be caused by the weakness of the $k-\varepsilon$ turbulence model near a wall and by the too small turbulent diffusion.

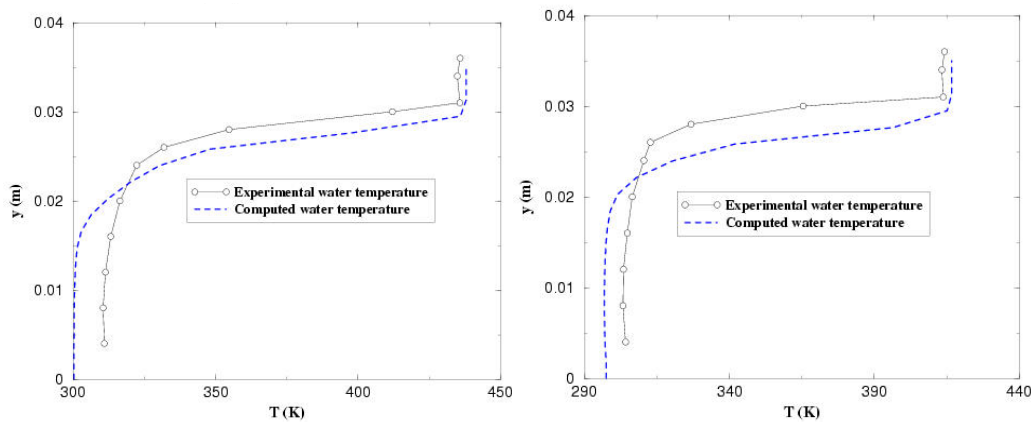


Figure 12: Water temperature profiles at the measurement station, NEPTUNE results: top - lower Reynolds number of steam; bottom - higher Reynolds number of steam.

2.4.4.2 Summary of the Results, Calculated by the ANSYS Group Using CFX-5

A model of condensation, used with CFX-5, follows an approach of resolving the viscous sub-layer in both phases near the interface. It implies the necessary damping of turbulence and asymptotically high heat transfer and drag coefficients at the interface. The resulting temperature profiles at the measurement probe location, calculated with and without the mass sources due to the phase change, are shown in Figure 13. The result obtained for the higher Reynolds number case shows very good agreement with the experiment. In particular, the effect of the latent heat release is clearly visible there. It results in elevation of the bulk water temperature up to the experimentally observed level. No converged solution was obtained for the lower Reynolds number of steam with condensation. However comparison of Figure 13 shows that it is feasible, once the convergence issue is resolved, to calculate correct temperature profiles for the lower Reynolds number case.

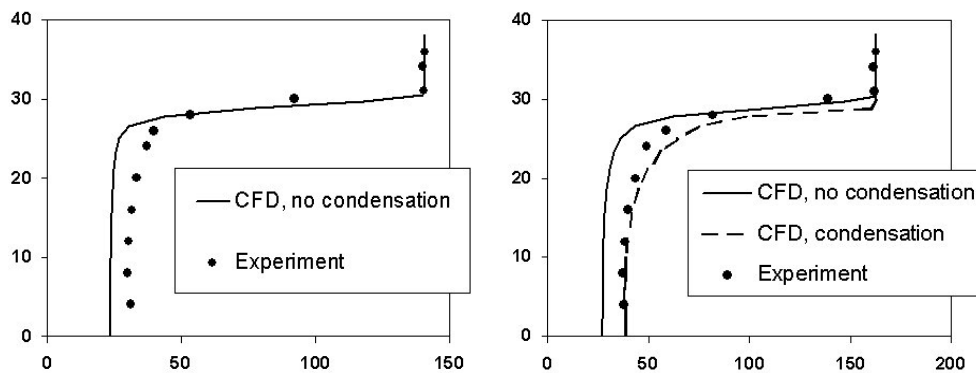


Figure 13: Water temperature profiles at the measurement station, CFX-5 results: left – lower Reynolds number of steam; right – higher Reynolds number of steam.

2.4.4.3 Conclusion

The PTS-relevant physical models and the correspondent numerical algorithms, implemented in the two CFD solvers CFX-5 and Neptune, have been validated by comparison with the experimental data. The four test cases, selected for the validation, cover all major effects of PTS flow inside a cold leg, except for the fast transient pressure waves. The first two cases, dealing with the single phase and the two phase jet impinging on a solid wall, have been calculated with CFX-5. They have demonstrated good accuracy of the SST turbulence model for the complex flows with strong normal stresses near a stagnation point. This, in turn, provided for the accurate prediction of the wall temperature distribution in the first case VAL01 “Single phase jet impingement on a heated wall” and the wall pressure distribution in the second case VAL02 “Impinging water jet in air environment”. The second test case has also proved accuracy and efficiency of the homogeneous free surface model of CFX-5. Due to the stability and efficiency of the solver the whole analysis could be performed according to the ECORA BPGs as follows:

- Accuracy of the results has been quantitatively estimated using the representative target values
- The necessary convergence criteria have been found.
- A grid refinement study has been performed on a series of grids.

- Potential uncertainty sources in formulating of boundary conditions have been analysed.

The validation test cases VAL03 and VAL04, dealing with the momentum, heat and mass transfer between the two phases, required application of the full-scale multi-fluid model. They have been calculated using NEPTUNE and CFX-5. The test case VAL03 “Impinging water jet on a free surface” turned out especially challenging because of the free surface disruption and entrainment of air bubbles by a plunging jet. Here the physical model adequacy and the numerical robustness have been found insufficient by both groups. A recommended improvement of the physical model is based on allocating a third phase for the dispersed bubbles and using an empirical model for bubble formation. Another modelling issue highlighted by this test case, concerned the proper modelling of turbulence in a very complex impingement zone. The last test case VAL04 “Condensation in stratified steam-water flow” has also demonstrated serious modelling and convergence issues in both codes tested. Nevertheless, the calculated temperature profiles agreed reasonably well with measurements. As a result of the mentioned issues, only limited attempts to apply the “Best Practice Guidelines” have been made for the VAL03 and VAL04 test cases. The necessary model improvements include the following points:

- Adequate and efficient modelling of turbulence damping near a free surface.
- Grid-independent modelling of interfacial drag and heat transfer on a free surface.
- Accurate discretisation of the buoyancy force by the Volume-of-Fluid methods
- Improvement of numerical stability and convergence

2.5 Software Validation (WP 5)

After the successful implementation and validation of PTS-relevant models for turbulence, heat transfer and two-phase flow modelling in WP 4, these models have been applied to a full-scale industrial problem in WP 5. The objective of this work package was to assess the performance of the CFX-5 and Neptune CFD code for an integral PTS experiment. For this purpose, experiments performed in the Upper Plenum Test Facility (UPTF) were chosen in WP 3. From the extensive experimental program of this facility two tests were selected:

- UPTF Test 1: Single-phase experiment
- UPTF TRAM C1: Two-phase experiment

In WP 5, the single-phase experiment was analysed by NRG. Besides this work, also a reference calculation as performed by EDF to validate the Neptune code is considered. The two-phase experiment was analysed by GRS. A detailed report of the assessment for these two cases can be found in Refs. [13] and [14].

2.5.1 The Upper Plenum Test Facility (UPTF)

The UPTF was a full-scale simulation of the primary system of the four loop 1300 MWe Siemens/KWU Pressurized Water Reactor (PWR) at Grafenrheinfeld in Germany. The test vessel upper plenum internals, the downcomer, and the primary coolant piping were replicas of the reference plant. However, other important components of the PWR such as the core, the coolant pumps, the steam generator, and the containment were replaced by simulators which simulated the thermal-hydraulic behaviour in these components dur-

ing end-of-blow down, refill, and reflood phases of a large break Loss-Of-Coolant Accident (LOCA). Both hot leg and cold leg breaks of various sizes have been simulated in the UPTF. The Emergency Core Cooling (ECC) injection systems of the UPTF were designed to simulate the various ECC systems of PWRs in Germany, Japan, and the US.

Temperature measurements have been performed at various locations in the UPTF geometry. The results of the simulations were compared at those positions, which were most relevant for PTS phenomena. The temperature measurements in the intact cold leg, where the ECC injections occur, and the measurements in the downcomer directly under this cold leg were selected. In Figure 14 these measurement positions are indicated.

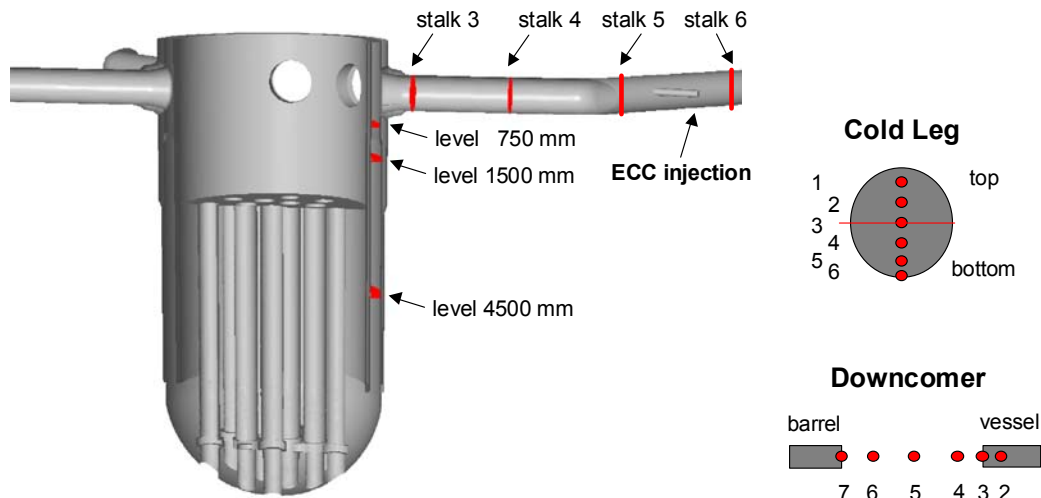


Figure 14: Location of the key temperature measurement positions, and probe numbering.

2.5.2 Single-Phase Calculations

2.5.2.1 UPTF Test 1 Conditions

The UPTF Test 1 was performed in order to investigate fluid-fluid mixing in the cold leg and downcomer as taking place during a small break LOCA. This fluid-fluid mixing results from the high pressure injection of the cold ECC water into the cold leg at a time when the reactor coolant system is at an elevated temperature. This mixing relates to the reactor safety issue of PTS.

For PTS, a key concern is how the injected cold water mixes with the hot primary water. In general, if the mixing is good, a slow cool down occurs which provides sufficient time to prevent the development of significant temperature gradients in the wall of the Reactor Pressure Vessel (RPV). Good mixing takes place when there is flow in the loops, even when the flow results from natural circulation only. However, in certain SBLOCA scenarios, it is possible that stagnant flow conditions occur in one or more loops. For this situation, the flow in the cold leg is thermally stratified. Namely, the ECC injection results in a cold stream, which flows along the bottom of the cold leg from the injection nozzle to the downcomer, whereas a hot stream flows along the top of the cold leg counter current to the cold stream. This situation is investigated in UPTF Test 1.

For UPTF Test 1, the primary system was initially filled with stagnant hot water at 463 K (190 °C). The cold ECC water was injected into a single cold leg. The ECC water injection mass flow rate was equal to 40 kg/s and the temperature of this ECC water was equal to 300 K (27 °C).

2.5.2.2 Summary of Results Calculated by NRG Using CFX-5

The different turbulence models and meshes used in the NRG computations are summarised in Table I. Cases A and B have been executed in order to determine whether detailed modelling of the UPTF internals is required. Simulations showed spurious circumferential flow oscillations in the downcomer for an empty lower plenum in combination with the commonly applied porous medium approach for representation of the UPTF core. Furthermore, it has been shown that the pump volume has to be taken into account, since a large amount of the ECC water flows towards the pump and accumulates there. In a real accident scenario, it is therefore important to correctly predict the amount of ECC water flowing towards the pump, since this water will never reach the core.

Table I: Overview of the performed CFX-5 computations for UPTF Test 1.

Case	Turbulence model	Turbulence modification	Core model	Pump volume	Time step	Discretisation space, time	Mesh size
A	SST-k- ω	none	porous	no	0.5 s	1 st , 1 st	1.155.153
B	SST-k- ω	buoyancy	internals	yes	0.5 s	1 st , 1 st	2.052.315
C	k- ϵ	buoyancy	internals	yes	0.5 s	1 st , 1 st	2.052.315
D	SST-k- ω	buoyancy	internals	yes	0.5 s	2 nd , 1 st	2.052.315
E	SST-k- ω	buoyancy	internals	yes	0.05 s	2 nd , 2 nd	2.052.315
F	SST-k- ω	buoyancy	internals	yes	0.05 s	2 nd , 2 nd	2.871.450
G	RSM	buoyancy	internals	yes	0.05 s	2 nd , 2 nd	2.871.450

Turbulence modelling has been investigated by comparing results of a simulation of the SST-k- ω without (case A) and with (case B) inclusion of the turbulence production/destruction term due to buoyancy. From a comparison of these two cases, it has been concluded that this modification to the standard turbulence model is required in order to achieve a good representation of the stratification occurring in the cold leg. Once this term is included, the results of the SST-k- ω (case B) and standard k- ϵ turbulence model (case C) are practically identical. Finally, an ω -based Reynolds stress turbulence model has been used (case G). The results from this calculation show a better agreement with experimental observations for the amplitude of the oscillations in the downcomer. These oscillations are over predicted by the two-equation turbulence model (case F). It is important to notice that correct prediction of these oscillations is required in order to analyse phenomena like PTS and thermal fatigue. Since these oscillations turn out to an effect on the wall temperature, and thus on the correct prediction of the severity of the PTS, an attempt was made to quantify the oscillations in the experiments. However, the Fast Fourier Transformation of the experimentally observed oscillations did not show any dominant frequencies present in the signals.

Besides determining the effect of the geometrical assumptions and turbulence modelling, as described before, the other calculations in Table I are related to the ECORA Best Practice Guidelines. Since modelling the UPTF geometry is computationally very demanding, it is impossible to strictly follow the BPG, which, e.g., state that a 2×2×2 re-

finement should be performed. Instead, a 1st order solution (case B) will be compared with a 2nd order solution (case D). This comparison demonstrated that it is plausible to assume that the mesh in the cold leg is sufficiently fine; however, the results in the downcomer are still mesh dependent. Therefore, a mesh which is locally refined in the downcomer was generated. In this new mesh, it is ensured that correct y^+ values are obtained (case F). The temporal discretisation is checked by performing a simulation with a reduced time step size and 2nd order temporal discretisation (case E). This reduced time step size is needed in order to reliably capture the oscillations in the downcomer which determine the vessel wall temperature.

Case F in Table I is the reference case, since here the best mesh and time step size was used. In Figure 15 the temperature distribution on the vessel cold leg walls can be seen. Strong mixing of the cold ECC water with the hot liquid, initially present in the system, is observed in the region of the upward directed ECC injection tube. Further downstream, strong stratification is observed in the cold leg. The cold water flows towards the reactor vessel and in the direction of the pump simulator, where the cold water accumulates until it has reached the level of the top of the cold leg (after about 160 s). The stratification in the part of the cold leg leading to the reactor vessel remains at a constant level throughout the transient. The cold water plume flows downwards past the vessel wall. Some slow oscillations can be observed in the circumferential direction. In the same figure, a detailed view of the flow in the downcomer is presented. At the connection of the reactor vessel with the cold leg, the flow remains attached to the vessel wall, but starts to detach and re-attach at a lower level in the downcomer. These oscillations, which are much faster than the circumferential oscillations, cause hot and cold regions to emerge. In the bottom of the reactor vessel the hot and cold regions are fully mixed by the turbulent flow between the lower plenum internals.

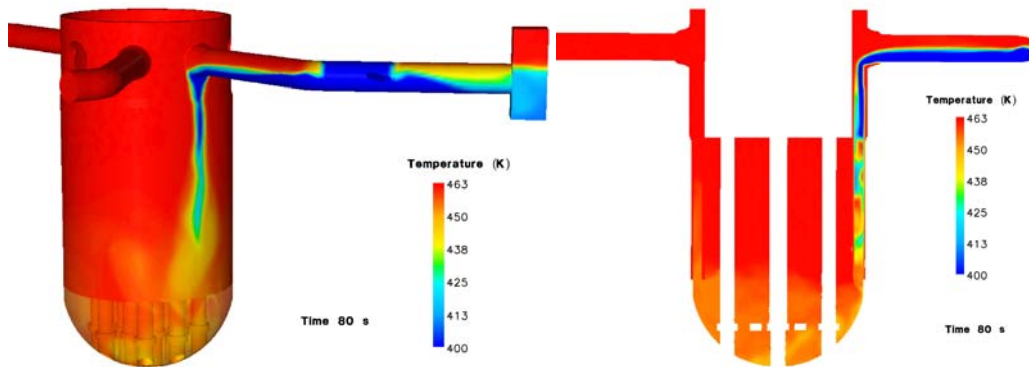


Figure 15: Vessel and fluid temperatures on the vessel and cold leg walls (left) and a cross-section through the middle of the cold leg with ECC injection (right).

The computed temperature profiles in the cold leg are compared with the experimental results from the UPTF Test 1 in Figure 16. From this comparison, it can be concluded that the stratification in the cold leg is accurately predicted by the CFD code. The calculated lowest temperature in the cold leg, which is the most important factor for determining the severity of the thermal shock, is within 3 % of the experimental value.

A second comparison is made for the results in the downcomer in Figure 17 and Figure 18. In the experimental results in the downcomer large oscillations are observed at every height. In the CFD results, these oscillations are not found at the highest measurement

positions. This is caused by the previously mentioned attachment of the cold plume to the vessel wall, which results in an overestimation of the cooling of the vessel wall. The predicted temperature drop $\Delta T = T - T_{\text{initial}}$ is typically overestimated by 50 to 100 %. At the lower level (see Figure 18) oscillations are observed, but the temperature drop still remains overestimated by 60 to 90 %.

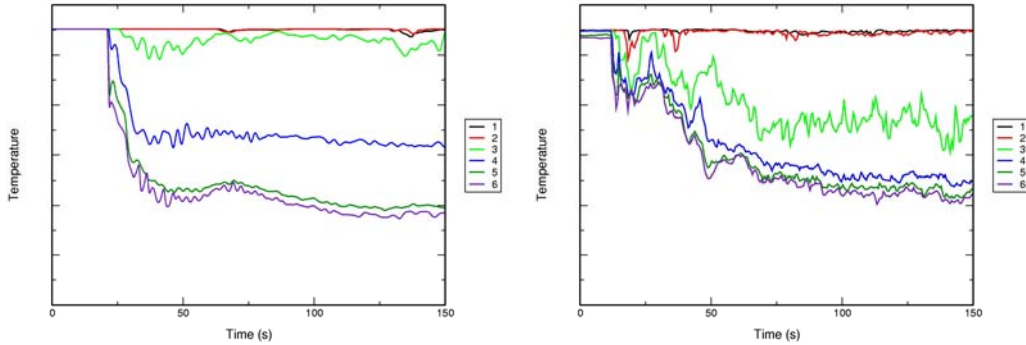


Figure 16: Stalk 3 results of the CFX-5 reference calculation (left) and UPTF experiment (right). For legend see Figure 14.

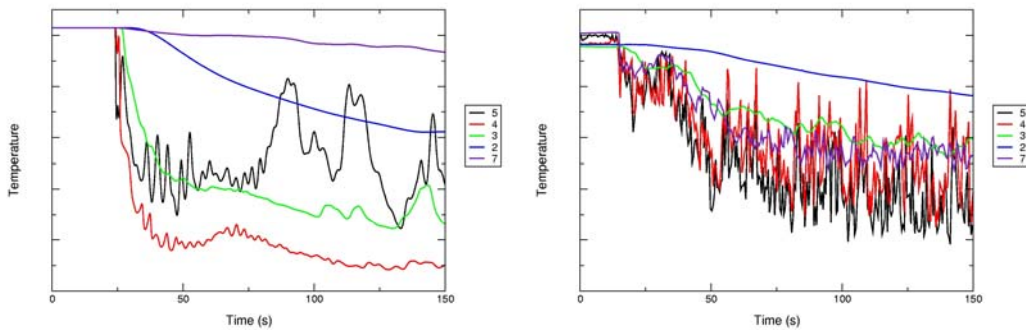


Figure 17: Level 750 mm results of the CFX-5 reference calculation (left) and UPTF experiment (right). For legend see Figure 14.

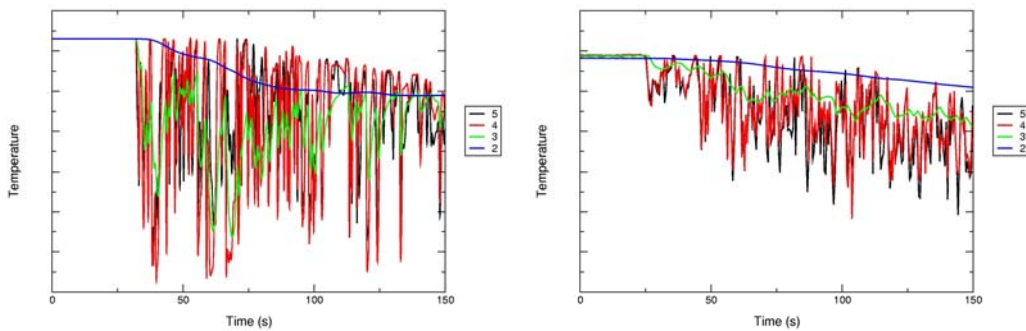


Figure 18: Level 4500 mm results of the CFX-5 reference calculation (left) and UPTF experiment (right). For legend see Figure 14.

2.5.2.3 Results from EDF

Reference calculations performed by EDF with the finite-element code N3S, now Code_Saturne, are available for the same UPTF test, see Ref. [32]. Using the standard k-

ϵ model turbulence model, important physical flow phenomena, like fluctuations of the cold-water plume when entering the downcomer, see Figure 19. There was good agreement between numerical results and data.

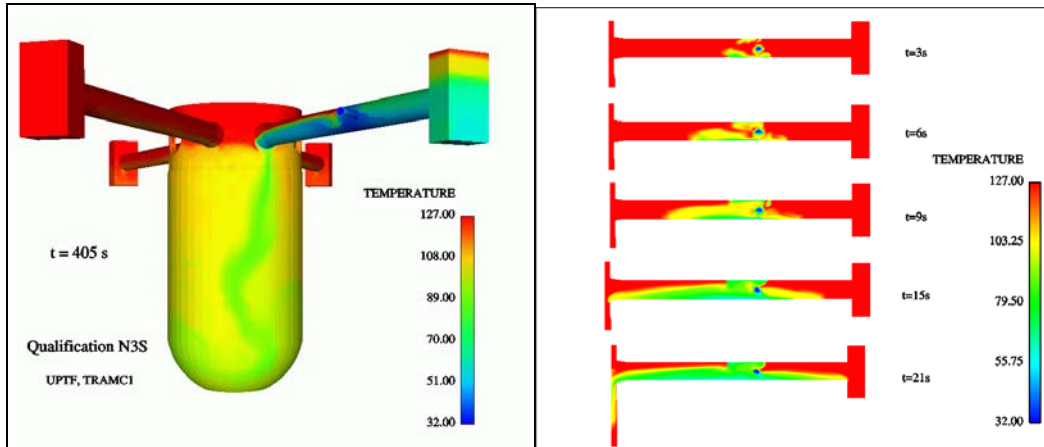


Figure 19: Vessel and fluid temperatures on the vessel and cold leg walls (left) a cross-section through the middle of the cold leg with ECC injection (right)

2.5.3 Two-Phase Calculations

2.5.3.1 UPTF TRAM C1 Test Conditions

The UPTF TRAM C1 was performed to steam-water flow in the intact cold legs and in the downcomer of a pressurized water reactor (PWR) during the end of blow-down of a cold leg loss-of-coolant-accident (LOCA). The coolant water of the primary system flows rapidly through the break, and a significant fraction of the water flashes to steam. The pressure in the primary system decreases as the blow-down progresses. When the pressure has reached a threshold value, the accumulators begin to inject emergency core coolant water (ECC) into the cold legs. This is the point in time where the test cases start.

In the experiments, nitrogen was injected into the system to prevent condensation effects. In the test case UPTF TRAM C1 Run21a2 the water level in the cold leg was just above the cold leg centreline. The initial water and nitrogen temperature was 461 K. The cold ECC water was injected into a single cold leg. The ECC water injection average mass flow rate was equal to 20 kg/s and the average temperature was 304 K.

2.5.3.2 Summary of Results Calculated by GRS Using CFX-5

In this two-phase flow simulation, the same CFX-5 free surface model was used, which has been successfully validated using the test cases VER01, VER02, and VAL02. In order to verify the basic operation of the models and to perform a first quality check of the results within reasonable computing times, only one quarter of the full UPTF geometry, as used by NRG, was modelled. For this geometry a hexahedral mesh with 444,583 elements was generated. The sequence of calculations in this simplified geometry conducted by GRS is summarised in Table II.

Table II: Overview of the performed CFX-5 computations for UPTF TRAM C1

Case	Turbulence model	Thermal model	Physical properties	Time span	Average Time step	Discretisation space , time
A	SST-k- ω	Isothermal	constant	50 s	0.04 s	1 st , 1 st
B	SST-k- ω	Isothermal	constant	50 s	0.004 s	2 nd , 2 nd
C	SST-k- ω	Thermal	func.(T)	100 s	0.065 s	2 nd , 2 nd

Even for this complex two-phase calculation in a large geometry an attempt was made to apply the ECORA BPG. Although strict application is not feasible due to the computational demand of, e.g., mesh refinement. A comparison was made of the calculations with first (case A) and second (case B) order discretisation schemes on the same grid. The target variable for the isothermal calculations is the superficial velocity of water. Figure 20 shows the velocity distribution at the centre and the bottom of the cold leg at Stalk 5. At this position, which is close to the ECC injection nozzle, the water velocity at the bottom of the cold leg is much higher than at the free surface. The first order scheme shows damping of the velocity fluctuations.

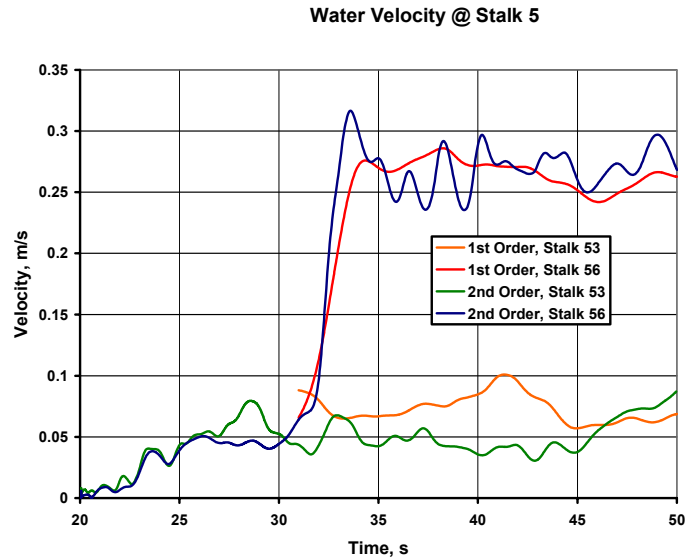


Figure 20: Water velocity at Stalk 5 (for position 3 and 5 see Figure 14)

The differences between the first and second-order solutions are, however, not large and the dominant frequencies are resolved quite well in both calculations. The numerical error for the target quantities in the isothermal simulations is approximately of the same order of magnitude as the difference between the first and second-order results, which amounts to approximately 10%.

After the quantification of the numerical error, a thermal calculation was performed (case C). Figure 21 show the development of the 0.3 m/s iso-surface of water at $t = 50$ s. The

iso-surfaces are coloured by temperature. The cross section plots at the measurement stalks indicate a stationary position of the free surface. At the ECC nozzle, the cold-water jet bends downwards, mixes with the surrounding fluid and flows toward the downcomer and the pump simulator.

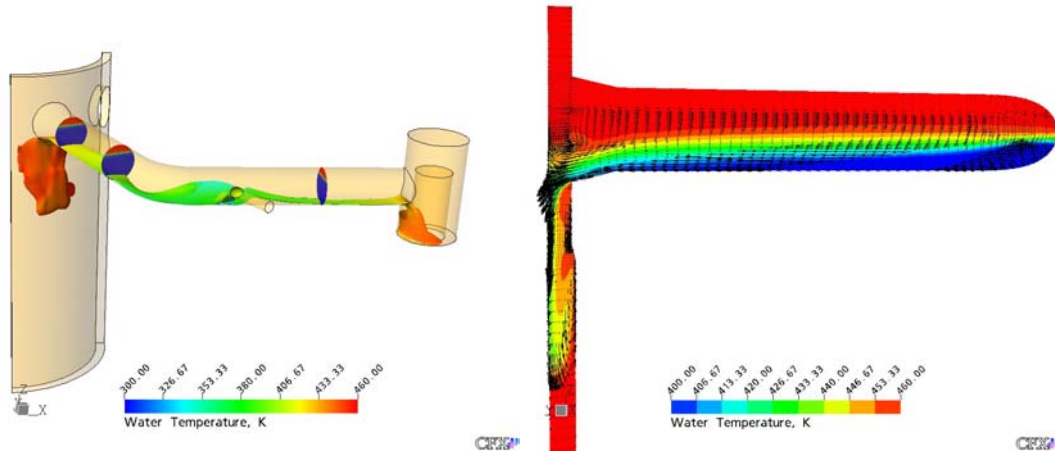


Figure 21: Iso-surface of constant velocity (0.3 m/s), coloured by temperature (left) and Velocity vectors and temperature distribution @ $t = 50$ s (right)

The ECC water mixes rapidly. This can be deduced from the temperature of the iso-surface after 50 s, which amounts already to 380 K. For reference, the inlet temperature at the ECC injection nozzle is 304 K. Between the ECC nozzle and the downcomer, the iso-surface becomes thinner because of mixing with the surroundings. After 50 s, the water iso-surface is in the downcomer, where it is heated by a larger water volume. The water also flows back into the pump simulator.

Figure 21 also shows a planar view of the velocity and temperature distribution at $t = 50$ s at the centre plane of the cold leg. Counter-current flow is observed in the cold leg. The cold water flows at the bottom towards the downcomer. The warmer water, which is close to the free surface flows with similar velocities towards the injection nozzle. The large velocity gradients in the transition layer generate turbulence and enhance mixing.

Finally, the results of the thermal two-phase flow calculation were assessed by comparison of experimental data with the computed temperature distribution in the cold leg. At Stalk 3, which is close to the downcomer, temperature stratification is observed after 40 s simulation time. At this time, the temperature in the water layer decreases, whereas it remains unchanged above the water layer. The temperature increase of the ECC water from its inlet value of 304 K to more than 400 K is well simulated. The vertical temperature distribution and the free surface position are also in good agreement with data.

The results for Stalk 4, which is shortly after the cold leg bend are similar. The earlier onset of cooling, the stratification and the lower absolute temperatures are all in satisfactory agreement with data. However, at this position the data show high-frequency oscillations, which are not visible in the calculations. Assuming that the data are correct, these discrepancies could have the following reasons:

- Grid and time steps are too coarse producing too much numerical damping

- Use of a statistical turbulence model, which is known to predict too large eddy viscosities and length scales for transient situations

The exact reason could not be identified within the current calculations.

2.5.4 Conclusions

In this work package, the performance of CFX-5 and the Neptune CFD codes have been assessed for prediction of the PTS phenomena occurring in an integral PTS experiment. For this purpose, the experimental data from the full-scale Upper Plenum Test Facility has been compared with results from the CFD codes. The following conclusions have been drawn:

- The single-phase flow calculation with CFX-5 and Code_Saturne showed good agreement for the prediction of the thermal mixing and stratification phenomena occurring in the cold leg. A detailed study with CFX-5 showed that the CFD model does not accurately capture the flow behaviour in the downcomer.
- The two-phase flow calculation with CFX-5 showed satisfactory results for the prediction of the two-phase flow and thermal stratification in the cold leg.
- For a large demonstration case as this UPTF geometry, it is impossible to strictly follow the ECORA BPG. However, comparison of first and second order discretisation scheme solutions (as performed in the both the single and two-phase CFX-5 calculation) can be used to estimate the numerical error.

The largest discrepancy in both the single and two-phase calculations is observed for quickly fluctuating flow phenomena. Although no definite conclusions can be drawn at this stage, it is highly probably that the use of statistical turbulence models is the cause for this discrepancy. The state-of-the-art in turbulence modelling now includes more refined approaches like Large Eddy Simulations (LES), hybrid RANS – LES approaches called Detached Eddy Simulation (DES), or even Scale-Adaptive Simulation (SAS). These models have hardly been investigated for NRS application, but show great potential for this important class of problems.

Since the BPG could not be strictly applied for the UPTF cases, the risk exists that the outcome of ECORA will be that the BPG are only applicable to small scale problems of no interest to realistic large scale NRS problems. It is our opinion that the establishment of ‘quality and trust’ in CFD in general, and NRS CFD in particular, starts with an accepted and applied quality document; the BPG. Therefore, it is of the highest importance to establish practical BPG for these large scale cases.

These final and most complex demonstration cases in the ECORA project are not only a challenge for the available models, but also for the available computer power. Notice that both the single and two-phase CFX-5 cases required several weeks computation time on parallel computers. Therefore, in order to use CFD calculations for reactor safety applications of the type investigated in the work package, an important task is a reduction of calculation times by, e.g., using adaptive algorithms in space and time. Another important issue that has to be addressed is the application of BPG for these large scale calculations.

2.6 Evaluation of CFD Analysis of Containment (WP 6)

The main objective of WP 6 is the evaluation of the current CFD codes with respect to their potential for analysing containment flows. A second step, the available experimental database is assessed and recommendations for future experiments are given.

2.6.1 Validation of CFD for Containment Phenomena

This task is addressed in Ref. [7]. This report evaluates the application of CFD codes to processes and phenomena which can be observed under accidental conditions in a nuclear containment. The focus is on the assessment of the state-of-the-art and the derivation of future requirements in order to provide requirements for the definition of future experiments and to formulate needs for code development. The first step in this report is the analysis of the complexity of processes involved and the determination of the phenomena suitable for CFD simulation. Examples of the validation of CFD codes against experiments are presented. Seventeen validation cases are discussed. Attention is paid to the description of the work carried out, the methods used as well as to the quality assurance of the results obtained. Mixing plays a dominant role and is somehow involved in all cases. According to the main target of eventually providing CFD simulations for real containments, six examples are presented. Experimental data are not available for these studies, therefore a careful validation before the step to full scale can be performed, is mandatory. For some of the containment studies a direct link to the validation chapter is obvious. A considerable progress on both the hardware and software side has been achieved during the last years, thus enabling step by step the up-scaling from the experimental level to full containment size.

2.6.1.1 Relevant Containment Phenomena

The phenomena known to occur under accidental conditions inside and outside of a containment are summarised in the following Table III. This table tries to classify the known phenomena according to their relevance in terms containment failure and source terms to the environment.

Table III: Summary of containment phenomena

Phenomenon		Ranking in terms of containment integrity	Ranking in terms of source terms to environment	CFD Modelling
Gas Dispersion		Low	Low	Many activities
Reacting Flows				
	Hydrogen combustion	High	High	Many activities
	Pool and cable fires	Medium	Medium	Some work
	Catalytic reactions	No	No	Some work

Phenomenon	Ranking in terms of containment integrity	Ranking in terms of source terms to environment	CFD Modelling	
Multi-phase				
	Condensation	No	Low	Few work
	Aerosol transport	No	High	Few work
	Melt particles	Medium	No	Unknown
	Evaporation	No	No	
External dynamic loads				
	Fire	Medium	High	Some work
	Missiles	High	No	Started

Table III identifies the physical phenomena, which create in several combinations with each other complex and very challenging tasks for CFD codes. To date there is no code to predict the full spectrum of issues. A further complication is the size together with the complexity of a nuclear containment. Almost all processes can evolve freely in space and have consequently to be considered in full three dimensions. Even combinations of selected issues provide often difficulties. From the high ranked issues hydrogen behaviour got a lot of attention through the last years. This is reflected in the number of validation cases and containment applications in this report. Mixing in general is involved in almost each of the phenomena listed above. However, it is necessary to address this basic item also separately for better understanding. Some of validation cases are devoted to pure mixing studies.

2.6.1.2 CFD Code Validation

A summary of CFD validation work is given in Table IV. More details are discussed in D10, see Ref. [7].

Table IV: Summary of available CFD applications

Investigated Phenomena	Simulation of Experiments	Application to Containment Issues
Mixing of Gases		
Multi-Component Mixture, Heat Transfer	HYJET	
Multi-Component Mixture, Turbulence, Buoyancy	LSGMF	Hydrogen accumulation in the reactor building
Multi-Component Mixture, Turbulence, condensation, evaporation	Panda	Hydrogen distribution

Investigated Phenomena	Simulation of Experiments	Application to Containment Issues
Jet mixing	CEASAR	
Jet flow, Supersonic regime		Pipe rupture
Hydrogen Combustion		
Combustion, Turbulence	FLAME , NUPEC	Full containment, Steam generator
Catalytic Recombination of Hydrogen		
Surface reactions, radiation	Gx at BMC	
Compartment Fires		
Combustion, radiation, turbulence	VTT	
Condensation		
Wall condensation, temperature stratification, mixing	Phebus FPT1, Panda	

All validation projects are presented in a unified format, thus giving the reader the ability to easily compare differences in the approach, the model set-up and the results obtained. The individual paragraphs are grouped as follows:

- General description
- Description of measurements
- Key words
- CFD Simulation:
 - Geometry
 - Mesh
 - Selected and applied models
 - Boundary conditions
 - Initial conditions
 - Fluid properties
 - Results
 - Conclusions

Additionally, to each project included in report D10, an independent questionnaire was filled and can be used to readily access the simulation work in a very concise manner. The questionnaires will form the core for a database on CFD validation cases.

2.6.1.3 Conclusions

The simulations of experiments reveal the high standard of CFD simulation which has been reached. In many cases either time restrictions or limitations in the hardware resources prohibited an extensive quality assurance investigation of the results obtained. This is a general shortcoming.

There are a number of conclusions that can be drawn. Some are more general and apply to most CFD applications; others are specific to certain phenomena.

- Code application:
 - Quality assurance of the simulations by investigation of grid sensitivity of the solution obtained.
 - Parametric investigation of model parameters which appear to be insecure.
 - Follow Best Practice Guidelines developed in WP1.
 - Derive uncertainty bands when possible.
- Future Needs:
 - Hardware needs:
 - More powerful computers (clusters or shared memory multiprocessors) for larger meshes to better resolve turbulent flows and to run over longer problem times. A full severe accident scenario may require several hours of problem time to be covered.
 - Software needs:
 - More robust parallel solvers.
 - Dynamic grid adaptation for premixed combustion of hydrogen.
 - Coupling with heat conduction, radiation, neutronics, structural mechanics.
 - Physical models:
 - More developed combustion models.
 - Combination of phenomena: combustion – structural response, condensation, radiation – fires or standing flames.
 - Advanced turbulence modelling.
 - Multi-phase model improvements
 - Experimental needs:
 - Special CFD related instrumentation including flow field, species concentrations.
 - Denser grids of data recording for more comprehensive code comparisons.
 - Precise control of boundary conditions.

2.6.2 Evaluation of the Available Database

The available database is analysed in D11 see Ref. [8]. Major recent test facilities like PANDA, MISTRA, ThAI and Battelle Model Containment are discussed. A detailed description is given of the test facilities and instrumentation, the types of experiments performed on the respective facility and the use of the experimental results with respect to code validation.

In Table V areas of necessary future containment related experiments are summarised. This table was extracted from the discussion of major experimental programmes in report D11. Together with the introduced relevance for nuclear safety, investigations for combustion, fires, condensation and special mixing problems should have priority.

Table V: Main areas of required experimental work

Phenomena to be investigated	Experimental Target	Safety Relevance	Comment
Mixing	Inclined jets	Medium	Hydrogen multi-component mixtures
	Buoyant plumes	Medium	Influence of fans
Mixing in a multi-compartment containment	Energy source	High	Influence of recombiners
	Energy sink	High	Influence of condenser
Condensation	Film condensation	Low	Influence of flow fields
	Direct condensation (spray)	High	Spray effectiveness and its influence on mixing
Combustion	High temperatures, large scale, non-uniform mixtures	High	
Recombination	Initiation of deflagrations	Medium	Surface Reactions
Particle Flow	Large particles carried by a critical flow	Medium	
Aerosol behaviour	Particle flows	High	Influence of flow fields
Fires	Cable Fires	High	

Future experiments should take into account:

- The purpose of the tests can be either to study single effects, coupled effect tests or to carry out integral tests. A good practice would be to start with separate effect tests and to develop these progressively into integral experiments (Mistra, BMC). The use of different geometric scales would provide a valuable extra source of information.
- If possible innovative non-intrusive measuring techniques should be employed. As examples gas concentration through sampling and mass spectrometer analysis and more innovative techniques based on optical non-intrusive techniques can be quoted. Velocity (LDV) measurements offer additional possibilities for CFD code validation.
- With the high costs of experiments and to provide test results in reasonable time, international cooperation can help to overcome these problems. Experiments should be designed, that different scales are investigated by different partners (Tosqan, Mistra and ThAI). Such discussions are already taking place in the framework of the 6th FP project SARNET and the OECD/NEA Group of Experts on Containment Code Validation Matrix (CCVM).

2.7 Pre-Test Analysis of Selected SETH PANDA Tests (WP 7)

2.7.1 Definition of the Tasks

The analyses in WP7 are aimed at investigating the capabilities of CFD codes to reproduce flows of interest for the containment response to a hypothetical accident and to provide an evaluation of the applicability of the BPG to these large-scale, transient problems. As the assessment is using data from the large-scale facility PANDA, the exercise can be classified as a demonstration test. Tests that have been designed to provide the adequate database for this basic assessment are carried out in the framework of the OECD SETH project, see Ref. [33]. For all tests, the two upper vessels (drywells) and the large interconnecting pipes are used. Fluid is injected in one vessel (Drywell 1), the gas distribution in this vessel, the distribution of gases and the propagation of the stratification in the adjacent vessel is measured.

The OECD-SETH experimental programme includes tests for horizontal jets, near-wall plumes, and free plumes. Depending on the test series, steam or a mixture of steam and helium are injected in vessels filled with air or a mixture of air and steam. Most tests are performed with a constant pressure at the outlet (vent), and under conditions for which no condensation is expected. In fact, a moderately superheated gas is injected into an ambient where both gas and walls are at a temperature slightly above the saturation temperature at the prescribed pressure. Measurements include pressure, injection and vent flow rates, fluid and wall temperatures, gas concentrations, and velocities at selected locations. PIV measurements are planned for specific regions.

The typical test duration for all tests is a few thousands seconds, which is a computational challenge for simulations with CFD codes using high-quality meshes. Additional information on the experimental programme, its rationale and the available instrumentation is included in Ref. [15]. Two tests (identified by numbers 9 and 17, respectively) belonging to the near-wall plumes series have been selected for ECORA. They relate to a very low-momentum injection (Test 9) and to an injection with higher (but still low) momentum (Test 17). Both tests feature horizontal injection of steam close to the wall of one of the two initially air-filled vessels. This experimental set-up (see Figure 22) produces a flow condition where the buoyancy force acts perpendicular to the inertia of the injected flow. This arrangement is specially challenging for CFD simulations.

In order to establish standards for the evaluation of the capabilities of the codes, the ECORA BPG should be applied for the simulations. However, due to the large computational overhead that they impose, the application of BPG to the analysis of the PANDA SETH tests needed to be evaluated, and realistic goals had to be set. To this aim, a benchmark exercise was conducted (with simplified geometry and boundary conditions) to define the scope of the analyses, and the results were used to define the time span of the tests to simulate and a set of recommendations that the participants in the exercise were expected to apply.

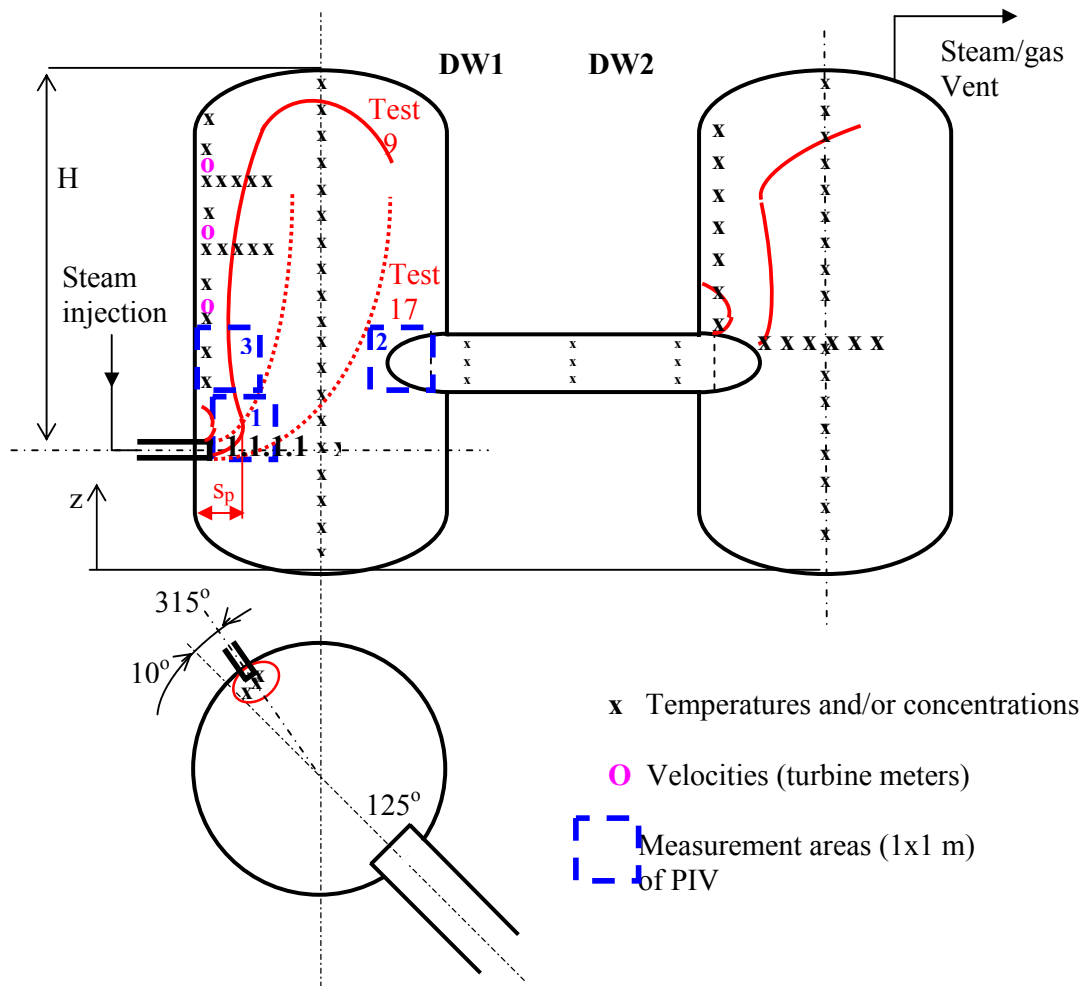


Figure 22: Configuration for the two PANDA SETH tests selected for the ECORA project

The results of the benchmark exercise showed that large computation times were required for the simulation with fine meshes, and small time steps were necessary for achieving a sufficiently accurate solution, which indicated that the currently available computer resources were not sufficient for a complete BPG-conformal analysis of the entire transient of Tests 17 and 9. Indeed, simulations of up to thousands seconds using increasingly fine meshes to obtain converged solutions appeared to be not possible. Simulations with only one, “practical mesh”, was the only realistic option, the application of the BPG being recommended for a portion of the transient only. Therefore, the validation exercise could be conveniently divided in two steps:

- Step 1: A short transient should be analyzed using, to any practical extent, the BPG.
- Step 2: provided that the solution using a ‘practical mesh’ is sufficiently close to that obtained with the finest mesh used in Step 1, the entire transient had to be calculated with that mesh.

The criterion used for deciding whether Step 2 had to be carried out was the convergence of one of the target variables (see below) within certain acceptance limits. Therefore,

simulations for the entire transient in Step 2 had to be carried out only if the results of the calculations for Step 1 (early period of the transient) showed that the simulations performed with a ‘practical mesh’ were sufficiently close to those obtained using the finest mesh.

Specifications for the pre-test analyses were given for: Geometry, simulation times, initial and boundary conditions, sensitivity studies, as well as for the variables to submit. All these specifications are included in D12 Ref. [15], and only the essential parameters for both tests are reported here: Pressure: 130 kPa; initial fluid and wall temperature: 108 °C; temperature of the injected steam: 140 °C. The injection velocity for Tests 9 and 17 are 1 m/s and 5 m/s, respectively.

As the strict application of the BPG would result in a computational effort that was hardly affordable with the current computer power, the guidelines were somewhat relaxed. It was required to perform sensitivity studies with respect to: 1) Mesh, using three meshes (coarse, intermediate, fine); 2) time step (or tolerance on residuals), but only for one mesh (intermediate grid), using at least three time steps. Moreover, as the only model that was expected to have an effect on the calculated results was the turbulence model and the associated wall treatment, the exercise included simulations with at least two turbulence models. As the high-Reynolds number $k-\epsilon$ model is currently the industrial standard for large-scale calculations, all participants were asked to provide simulations with this model.

Target variables were only defined for Step 1, as sensitivity studies were only requested for the early time period. These were the steam molar fractions on a horizontal line in DW1 and a vertical line near the middle section of the interconnecting pipe. The target variables were mainly used for defining the convergence of the simulation, by calculating the RMS of the differences of the distributions obtained with increasingly fine meshes and did not all correspond to measured variables.

2.7.2 Results

The pre-test calculations revealed that the application of the BPG to the analyses of the transient problem in the large-scale geometry of the PANDA facility resulted in a severe computational challenge. Most of the organisations could not perform all the sensitivity studies prescribed, and none of the delivered results can be considered fully converged in the sense of the BPG. For both test cases, the computational overhead was significant: Even for the short period simulations (70 s for Test 17 and 250 s for Test 9), the running time was in the range between several days and a few weeks per run, using state-of-the-art, single-processor computers or, for codes that can be run in parallel mode, small clusters. These large computation times strongly limited the scope of the analyses for most organisations, and prevented a systematic application of the BPG. A comprehensive summary of the analyses carried-out is presented in D13 Ref. [16]. The code-to-code comparison for selected results includes only for Test 17 the comparison with experimental data. The data for Test 9 will be only available later in 2005, and could not be used for the assessment of the codes within the ECORA project.

It would not be practical to include the large number of sensitivity studies that have been made with respect to mesh, time step, etc. in the comparison of the calculations with data. Therefore, for each turbulence model, only the results of the most accurate calcula-

tion were included in the comparison¹. Simulations for Step 1 have been provided in accordance to the assignments. For Step 2, however, fewer contributions were submitted due to the very large computation times and/or to the failure to obtain converged results (within 5 % for the target variables) for Step 1.

Test 9 features a low momentum injection, the inlet velocity being close to 1 m/s. As no data are available and only one calculation was continued to the end of the transient, the comparison of the results is limited to Step 1. The low-momentum injection is calculated to produce a near-wall, which persists through the 4,000 s transient simulation. Figure 23 shows the steam concentration distribution along a horizontal line at an elevation half way between the interconnecting pipe and the hemispherical dome at 250 s (end of Step 1). Three out of four calculations predicted the axis of the plume to be at about 0.5 m from the wall. The VTT simulation, which shows a maximum of the steam concentration close to the wall, is probably affected by a large numerical error, as the coarse mesh used is probably inadequate to resolve the details of the flow. The results showed that meshes with less than 100,000 cells (one Drywell only) are not sufficiently fine to capture the flow structure for the low momentum injection of Test 9.

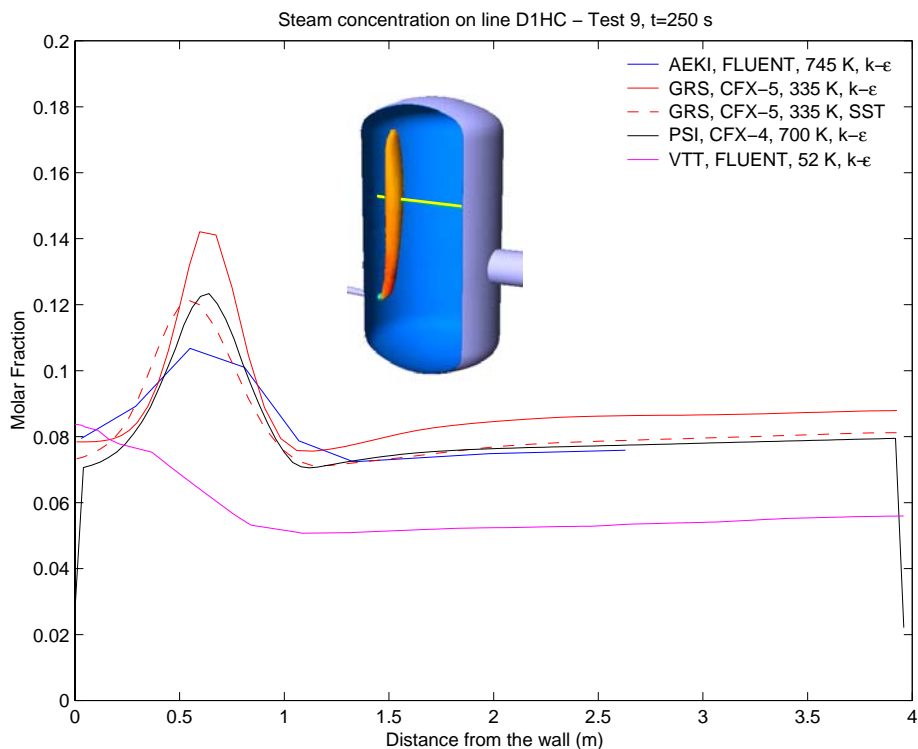


Figure 23: Test 9 Steam concentration distribution at 250 s along a horizontal line crossing the plume

On the other hand, the choice of the turbulence model, various treatments of the heat transfer, physical representation of the fluid properties, as well as assumptions on inlet

¹ The labels in the comparison plots include the name of the organisation, the code used, the number of cells (in thousands) in the mesh, and the turbulence model used (where MixL, Mixing Length; k-ε, k-ε model; RNG, SST, Realizable, other variants of the k-ε model).

turbulence and wall treatment (which resulted in largely different profiles of velocity and other variables inside the injection pipe), did play a less important role than the mesh.

Test 17 featured a higher momentum injection, the inlet velocity being close to 5 m/s. As experimental data are available in Ref. [34], the merits of the models used can be assessed to some extent, although separating the effects of the mesh from those of the model is only possible for one calculation (NRI).

Step 1. The flow structure in Drywell1 can be characterised using the experimental information. The data obtained from a large number of thermocouples show initially a bent jet, which is detached from the wall closer to the injection point and attaches to the opposite wall at an elevation above the interconnecting pipe. The maximum temperature along a horizontal line in the same plane as the injection pipe and close to the top of the interconnecting pipe is further from the injection than the axis of the vessel (i.e. to the right of the axis). Although the position of the maximum is fluctuating, it initially remains at a distance between 2 and 2.5 m from the wall of the injection. Later in the transient, the jet loses buoyancy and the axis of the jet becomes increasingly horizontal. At the end of the transient it nearly enters the interconnecting pipe. The slow variation of the inclination of the initially buoyant jet was confirmed by PIV observations. The relatively large horizontal penetration of the jet results in an anti-clockwise circulation for the whole transient. Figure 24 shows that the calculated results are in a broad band, the predictions indicating a temperature peak between 1.3 and 2.5 m from the wall. All calculations using two-equation models ($k-\varepsilon$ model and its variants) qualitatively predict the large penetration depth of the jet, and correctly predict anti-clockwise circulation, although the results span over more than half a metre. The best agreement was obtained by NRI with the FLUENT code and a rather fine mesh. The observation of the spreading of results is worrying, but shows the importance of arriving at mesh-insensitive results before trying to define the accuracy of the various models. In particular, only the results obtained by NRI can be used for judging the merits of the three turbulence models investigated. For all other organisations, the differences between predictions are likely to be affected by both mesh and model effects. The only calculation with the mixing-length turbulence model produces a much less inclined flow, resulting in clockwise circulation.

Step 2. Figure 25 shows, as an example, the steam concentrations in DW2 measured at various elevations in the time span between 750 and 920 s, as well as interpolated values at 1000 s. It can be observed that the codes using two-equation models are in excellent agreement with the data, the sharp stratification front below the interconnecting pipe being reproduced very well. It is specially to remark that rather large differences in the flow structure predictions in the fluid-receiving vessel (see above) resulted in a minor difference in the steam distribution in the adjacent vessel. On the contrary, TONUS overpredicts the thickness of the interface between the steam-rich upper part of the vessel and the steam-lean bottom, as a consequence of the large diffusivity calculated with the Mixing Length model.

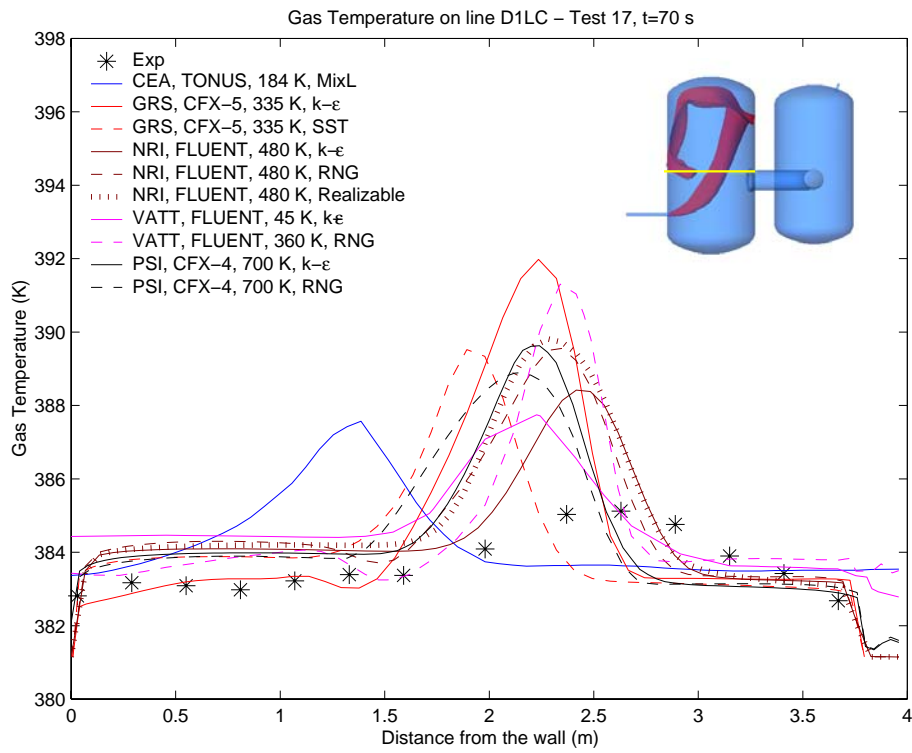


Figure 24: Test 17 Gas temperature distribution on a horizontal line crossing the jet

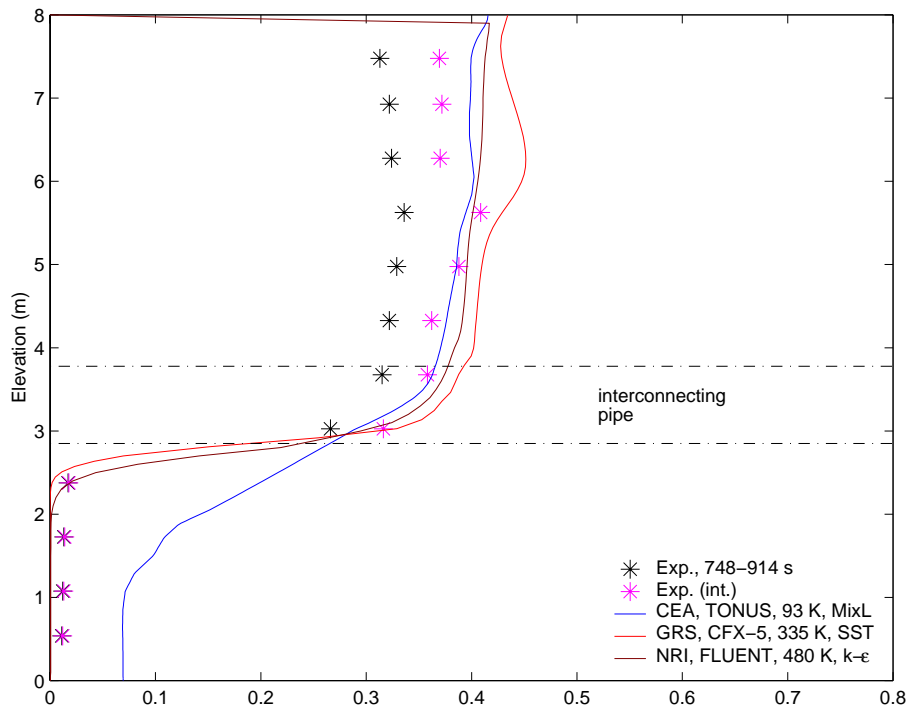


Figure 25: Test 17. Steam concentration vertical distribution in Drywell 2 at 1000 s

2.7.3 Conclusions

In WP7 of the ECORA project the need for a basic assessment of CFD codes for flows relevant for containment analysis has been addressed, using first results of an experimental programme (OECD SETH) specially conceived for this purpose. Some of the conclusions are preliminary, and need to be verified for the conditions specified for the other tests in the OECD programme. Various results of the exercise, however, can be used for evaluating the perspective use of CFD for the analysis of containment of an NPP. The main outcomes of the work performed are:

- The accurate analysis of the flows produced by the injection of buoyant fluid in large-size, interconnected vessels is a computationally challenging task, which requires very large computer resources. For the relatively milder conditions of the low-momentum injection prescribed for Test 9 (for which experimental data are not available yet), the mesh required for obtaining sufficiently accurate results are larger than hundred thousands cells. For the more severe conditions of Test 17, sensitivity studies could only be made for a short transient. These lead to the conclusions that mesh-insensitive results can be achieved with a few hundred thousands cells. The need for such a large mesh and the long times of the transients investigated result in very large computation times.
- Due to the large computational overhead of the analysis, the BPG had to be reduced in scope. Notwithstanding the reduced scope, the BPG could not fully be applied by any organisation. In a strict sense, simulations using a mesh with about 10^6 cells were not proved to have achieved mesh-insensitivity.
- The simulation of the flow in the fluid-receiving vessel is very sensitive to mesh and model choice. As only one simulation was based on the use of a ‘certified’ mesh, it is not possible to speculate on whether the differences between codes would be drastically reduced if ‘mesh-independent’ results were provided by all organisations. The success of the simulation (against experimental data) performed with an ‘certified’ mesh confirms that the application of a systematic sensitivity study (along the lines of the BPG) has a high pay-off.
- On the other hand, the steam transport between vessels and the long-term stratification seems to be less sensitive to the mesh quality. In fact, the adequate predictions obtained with a mesh of similar size as the ‘certified’ one, but not supported by sensitivity studies and evaluation of the accuracy, could lead to the wrong conclusions that the use of a ‘good’ mesh according to engineering judgement and careful choice of numerical methods and time step could be sufficient to produce a trustworthy result. The occasional success of the ‘traditional approach’ should not distract the attention from the need to establish rigorous guidelines.
- The $k-\epsilon$ turbulence model produced good results, and was the only model (in association with a ‘certified’ mesh) to reproduce all aspects of the test for which experimental results are available. Variants of the two-equation models also produced very good results in relation to stratification and gas transport. On the other hand, the simple mixing length model produced results of much less accuracy in relation to all aspects of the transient, the flow structure in the fluid-receiving vessel being totally missed.

In relation to the objective of WP7 in the more general framework of the ECORA project, namely the evaluation of CFD methods for reactor safety analysis, the following conclusions can be drawn:

- The flows analysed in the framework of the ECORA project do not include all the physics (e.g. condensation is not included) of prototypical applications. However, the success obtained in the simulation of the separate-effect tests using appropriate meshes and models can greatly improve the confidence in the methods for containment analysis. Assessment of the codes using other tests of the OECD-SETH programme is an important step in building this confidence.
- The application of the BPG to full containment analysis is out of reach with the currently available computer power, although the use of large computer clusters could permit full-scope analyses of reference scenarios in the future.
- In general, CFD codes seem to be capable to give reliable answers on issues relevant for containment integrity evaluation (such as inter-compartment mass transport mainly investigated here). Moreover, as advanced (and more computationally intensive) turbulence models may not be needed, the use of the BPG for ‘certified’ simulations could become feasible within a relatively short time.

2.8 Evaluation of Application of CFD Codes to Reactor Safety (WP 8)

2.8.1 Use of Single-Phase CFD

Reactor safety analysis related to both PWRs (western type and VVER type) or BWRs mainly relied on system codes where the primary (and secondary) flows are modelled with a rather coarse nodalisation including about 1,000 mesh points or “control volumes”. However some safety issues were clearly identified where a much finer resolution of the simulation tools was required. These issues are often related to situations where the 3D aspects of the flow and the geometrical effects have a significant influence on the safety criterion. Turbulent mixing is a common feature of these flows and the degree of mixing controls the result which directly affects the safety. Single phase CFD tools are then required which may model small scale mixing phenomena with a fine space resolution including 10^5 to 10^7 mesh points. The experimental investigation may also give the answer to the safety problem if the industrial geometry is strictly respected. Reliable simulation tools, after having been validated for each basic flow process and for some prototypic geometry, may allow a fast answer to a new problem and/or a new geometry. Such single phase CFD tools exist and are commonly used in many industrial sectors and are now applied for NRS or for design purposes.

The principal interest of industrial CFD consists in the capability to obtain at a lower cost, valuable information on some physical phenomena. Numerical simulations of industrial processes make it possible to test virtually any configuration, from both qualitative and quantitative points of view, and thus to evaluate and/or discriminate different designs according to pre-determined criteria. These criteria may be linked to economical or technological constraints, and/or to safety and environmental issues. Concerning safety issues in the nuclear industry, CFD has now been recognized as an important tool, as discussed in the IAEA/NEA workshop of November 2002.

In order to produce trustworthy studies on various problems, both “in house” and “commercial” software for thermal hydraulics and industrial fluid mechanics were developed and validated. Commercial codes such as CFX and FLUENT are widely and increasingly used in nuclear reactor safety applications. In the nuclear reactor community, for exam-

ple, the SATURNE code is developed at EDF and the TRIO-U code and CAST3M code are developed at CEA for single phase flow whereas the NEPTUNE platform developed by CEA and EDF includes a two phase flow CFD tool. Two-phase models are also available in commercial codes. A multi-year validation study of the multi-phase capability in CFX-5 for reactor safety applications is currently carried out in a German research project coordinated by GRS (CFD Kompetenzverbund Reaktorsicherheit - German CFD Network in Nuclear Technology). In the 6th Framework Programme, the NURESIM proposal will be an integrated project aiming at developing a common nuclear reactor simulation platform, which will also include two-phase CFD modules. All these codes are engaged in a qualification process in the field of nuclear thermal hydraulics in order to ensure that the software is effectively able to produce relevant results in a clearly defined application field.

Developing and testing the tools has required intensive work on complex physical modelling and numerics, both domains being closely linked in the CFD field. In parallel, experimental data bases are created, including separate effect tests and real-size industry-like experiments; they are used to validate the physical modelling implemented in the codes. A comprehensive measurement data base on turbulent mixing inside the reactor pressure vessel has been created within the EC project FLOMIX-R on fluid mixing and flow distribution in the primary circuit of PWR. This data base gained from experiments at various test facilities representing different types of European reactors (German KONVOI, Westinghouse and Framatome –ANP PWRs, VVER) is made available for CFD code validation purposes.

Although the design of the first PWRs was mainly based on an experimental approach, in particular for evaluating the loads applied on the structures, present numerical tools are now able to model the structures even with complex geometry using a 3D numerical model and to solve the complex physical aspects of the flows. Different flow features take place in normal operating conditions, like jet impact, flow reversal, piping swirl effect, and in accidental conditions, buoyancy effects or dilution problems are encountered, either in the primary system or in the reactor containment in the event of a Loss of Coolant Accident (LOCA). For the new reactors such as the EPR, the experimental approach is coupled to the numerical approach to provide elements required by the design.

Although not addressed in the framework of the ECORA project, other thermal-hydraulic phenomena require the use of CFD for safety assessment: for example, hydrogen combustion issues (addressed in the 4th FP projects HDC (see, Ref. [35] and HYCOM (see Ref. [36]) or the 5th FP EXPRO (<http://batchelor.uc3m.es/expro/expro.html>), as well as phenomena representative of Generation IV reactors such as Gas-Cooled Reactors (decay heat removal phenomena, depressurisations, thermal fatigue, etc) – see for example Refs. [37] and [38] or also the proceedings of the HTR-2002 conference for examples of application of CFD to such problems. The development of Best Practice Guidelines for those particular applications is also needed, and would prove beneficial to the overall quality of the simulations.

2.8.1.1 Nuclear Reactor Safety Problems where Single Phase CFD is Recommended

A good maturity of both the tool and the user is reached or can be reached in a reasonable term and single phase CFD can be a very powerful tool for better understanding

physical behaviour and one may recommend using it for a number of flow configurations encountered in safety analyses such as:

- Boron dilution
- Mixing of cold and hot water in steam line break event
- Hot-leg temperature heterogeneity
- Pressurised thermal shock (PTS)
- Counter-current flow of hot steam in hot leg for severe accident investigations of a possible “induced break”
- Thermal fatigue (e.g. in T-junctions)
- Hydrogen distribution and combustion in containment

In addition to these problems, which are related to the present generation of water reactors, there are also a number of issues for advanced (including gas-cooled) reactors. A few examples are:

- Natural circulation in LMFBRs
- Coolability & flow induced vibration of APWR radial reflector
- Flow in lower plenum of ABWR
- Depressurisation of a GCR
- Decay heat removal in a GCR
- Thermal loading on structures, etc.
- Containment integrity (peak pressure) during the long-term cooling of innovative reactors with passive safety systems, particularly in a BDBA scenarios, see Ref. [39]

2.8.2 Use of Two-Phase Flow CFD

The EC project EUROFASTNET, which was a pre-runner to ECORA, has identified industrial needs for three-dimensional simulation of nuclear reactor thermo-hydraulics. These include safety, performance, design, availability and increase of life span of nuclear reactors (see Ref. [40]). The requirements with the highest industrial priority are fuel performance, fluid-structure interaction, thermal shocks due to safety injection and stratification in circuits. As a consequence, the ‘Extension of CFD Codes to Two-Phase Safety Problems’ has become the subject of *Writing Groups on CFD Issues*, which has been established by the OECD/NEA. The report produced by this Writing Group (see, Ref. [41]) covers a wide range of NRS problems in pressurized water reactors (PWR), boiling water reactors (BWR), steam generators, heat exchangers, containment flows and components with three-dimensional structures like spacer grids. High priority is given to critical heat flux conditions in the core, to two-phase pressurized thermal shocks (PTS), and to thermal fatigue and stratification in the primary system of PWRs.

The reports in Refs. [40] and [41] embrace all aspects of two-phase flow CFD in NRS. In the ASTAR project, some test cases of interest for two-phase flow modelling were investigated, and BPGs were also applied to produce better quality solutions (see, Ref. [42]) and (see, Ref. [43]). In the ECORA project, only a subset of the cases described in Ref. [41] was investigated, namely the CFD simulation of flows in the primary system and containment of PWRs. Two-phase flow phenomena were studied for PTS-relevant flow conditions during the injection of emergency core cooling water into the cold leg of PWRs. The following discussion will be focussed on these topics.

2.8.2.1 Nuclear Reactor Safety Problems where Two-Phase CFD is Recommended

Two-phase CFD tools are far less mature than single phase tools. However, it is recommended to further develop such tools for a number of nuclear safety issues. Due to the lower maturity, the activity should include:

- Identification of the relevant basic phenomena which need to be modelled for a given application
- Assessment of the model including verification, validation and demonstration tests
- Definition of new R&D work for a more detailed validation, for a better numerical efficiency, and a better accuracy and reliability of predictions

Such a process has been applied within ECORA to the two-phase PTS scenario. The dominant fluid and heat transfer phenomena involved in this two-phase flow scenarios are:

- Impingement of two-phase flow jets
- Impinging jet heat transfer
- Turbulent mixing of momentum and energy in and downstream of the impingement zone
- Stratified two-phase flow (or free surface flow) within ducts
- Phase change, like condensation at the steam-water interface

These phenomena were investigated in ECORA. The respective test cases which were calculated in ECORA are documented in Ref. [9]. The ECORA test cases were subdivided into verification, validation and demonstration tests. A detailed description of the results is given in Ref. [12]. The calculations in ECORA have shown a satisfactory performance of the employed CFD codes for single-phase flow problems, and for two-phase flow problems with single dominant interface morphology. This includes free surface flows, or bubbly flows. However, for cases with more than one morphology, for instance for a jet impinging on free surface flow with bubble entrainment or for the transition of bubble to churn flow, the available two-phase models show poor results and need to be improved. The same is true for multi-phase flows with heat transfer and mass transfer at the interface. For the latter, the numerical schemes and the physical models need enhancements. A prerequisite for these model improvements is, however, the provision of adequate experimental data to develop, calibrate and validate these models.

The test calculations in ECORA have also shown that the calculation times for typical PWR assemblies (cold legs, downcomer, lower plenum, core, and hot legs, see Ref. [13]) are still very large (order of weeks on current parallel machines). Improvements in the numerical methods, and advancements like error-based grid and time-step adaptation, are therefore necessary to make CFD a tool for comparing and assessing different scenarios in NRS.

The ECORA project has made a contribution to the assessment of the state-of-the-art of two-phase flow CFD in NRS. Also, a number of useful model improvements have been made in ECORA. It is, however, still difficult to 'recommend NRS problems' for CFD. If a problem is suitable or not depends on the accuracy expectations and on the computational investments one is willing to make. As said above, many two-phase flow problems with single morphologies (free surfaces, bubble flows, droplet flows, water jets, ...) can

be predicted quite well. However, there are still large uncertainties for flows with more than one morphology, and for flows with mass transfer at the interface (condensation, boiling, and cavitation). Also, calculation times for these kinds of flows may become prohibitive. Therefore, while many of the flows described in Table I of Ref. [41] can now be tackled from a research and development perspective, the available CFD codes are not yet sufficiently mature for a day-to-day industrial application.

Independent of the test case and the problem at hand, ECORA has shown that the application of the BPGs developed as part of the project, can substantially reduce uncertainties, lead to more valid conclusions about model performance vs. performance of the numerical method, and can therefore help to accelerate development and progress of three-dimensional CFD in NRS. A similar approach should be followed for other important issues with two-phase flow such as:

- DNB, dry-out and CHF investigations
- Direct contact condensation : ECC injection or steam discharge in a pool
- Condensation induced water hammer
- Pool heat exchangers: Thermal stratification and mixing problems
- Corrosion, erosion and deposition
- Two-phase flow in valves, safety valves
- Flow oscillations in BWRs
- Steam generator tube vibration
- Pipe flow with cavitation

2.8.3 Recommendations for Code Customisation

The fluid flow problems considered in ECORA, as well as information gathered at meetings with other European projects like ASTAR and FLOMIX-R, have shown that CFD applications in nuclear reactor safety are focussed on internal flows. Examples are the single and multi-phase flows in hot and cold legs, downcomers, pressure vessels and containments. In ECORA, BPGs have been developed for these flow categories. Customisations of CFD software are also recommended, which encompass these BPGs. The recommended customisation of the CFD codes can facilitate the set-up of CFD calculations and the interpretation of the CFD results, as well as optimise the solution process. The net result will be higher result quality, an increased trust in the results, and reduced user influence.

2.8.3.1 Geometry Model

The first step in performing a CFD calculation is the generation of a geometry model. This geometry model must include all the details influencing the flow. For instance, calculations in ECORA and FLOMIX-R have shown that only a detailed modelling of the structures in the lower plenum and at the core entrance will lead to realistic flow predictions. Since many reactor components are geometrically similar for European pressure reactors, parameterized geometry models could be provided for such components. These parameterised models could then be quickly adjusted to different applications by changing the appropriate dimensions. Pre-made models for cold and hot legs, ECC-nozzles, downcomers, and core structures could then be combined in a modular fashion using a solid (or volume) modeller.

2.8.3.2 Mesh Generation

After the geometry of the flow domain is available, it needs to be meshed. As stated above, NRS applications involve mainly internal flows. These require special care in order to obtain proper resolution of the walls. The generated grids should also be scalable, which means that their quality should not change when the mesh size is changed. Generation of such high-quality grids can be aided by the following customisations:

- Guidance about which element types (tetrahedral, hexahedral, prisms, ...) are recommended for which reactor component and application
- Provision of pre-designed, scalable hexahedral block structures for typical NRS components, like downcomers, hot and cold legs, etc.
- Estimators for the required near-wall resolution based on typical flow parameters like Reynolds or Peclet numbers
- Development of grid-quality metrics, including recommendations and information on grid density, skewness, aspect ratios, expansion factors
- Construction of vertical applications for generating meshes in typical reactor components using the BPGs developed in ECORA

2.8.3.3 Physical Models and Boundary Conditions

One of the major results of ECORA BPGs was the selection of state-of-the-art physical models for predicting turbulent flows, turbulent heat transfer, and multi-phase flows in NRS applications. A logical customisation of the applied CFD software is therefore to encapsulate the best models for specific applications in 'Application Libraries'. Typical applications could be pressurized thermal shocks, Boron mixing, buoyant flows in containments, etc.

The same principle could then be extended to boundary condition setting and to numerical control parameters. Customisations for boundary conditions could include recommended values for positioning of inlet and outlet boundaries, turbulence quantities at inlet cross sections, preferred outlet boundary condition settings, guidance on the general near-wall treatment for given geometries, and the use of rough or smooth wall boundary conditions. Customisation of the numerical control parameters could provide guidance about time-step sizes for given applications, choice of convergence criteria, and recommendations on appropriate spatial and temporal discretisation schemes.

These customisations would narrow the physical model, boundary condition and numerical control parameter choices for novice users on the basis of the expertise of experienced users. The result would be higher and more consistent result quality.

Another recommendation is the customisation of material data (fluid and solid properties). These could be shared for typical fluids like steam/water, nitrogen, hydrogen, and typical solids used for reactor walls and claddings.

2.8.3.4 Solver Run and Quality Control

Extensions and customisations for the CFD flow solver and for quality control are recommended in the following areas:

- Most calculations in NRS are for transient, three-dimensional flows. A major issue for these flows are the long calculation times. A much-needed extension of

current CFD codes is, therefore, to provide algorithms for adaptive time stepping. These algorithms should adjust the time steps to either preserve a given numerical accuracy (solution error-based adaptation) or maintain a given iterative convergence level per time step. By using small time steps only when they are needed, and by increasing the time-steps otherwise, calculation times can be minimized for a given result quality.

- A logical extension of the above would be to also adapt the spatial grid during transient runs. In this way, a given amount of grid points could be used in the most efficient manner, or a given accuracy could be maintained by adding and withdrawing grid points from critical zones. It is, however, recognized that spatial, transient adaptation is a rather complex development project.
- A very helpful feature for monitoring transient CFD runs would be to post-process results during the calculation. In other words, the flow solver should continuously feed information to the post-processor. Anomalies and problems with transient flow calculations, or discrepancies to data could then be recognized immediately and countermeasures could be taken. This would be more efficient than the currently used sequential processing of solver and post-processor.

Customisations for efficient post-processing and analysis of NRS calculations, which extend the currently available functionality, are:

- Easy creation of post-processing surfaces at a given distance from boundaries (lofted surfaces), for instance in the centre of downcomers or in the interior of hot and cold legs
- Easy definition of surface normals and cutting planes based on these surface normals; examples are cutting planes normal to the path of hot and cold legs
- Provision of macros for calculating values which are relevant for NRS, like the position as a function of time of maximum and minimum temperatures or concentrations or of maximum and minimum temperature, pressure or concentration gradients (relevant for fatigue and structural analysis)
- Possibility to transfer mechanical (forces, moments) and thermal loads (temperatures, heat fluxes) to structural mechanics and fatigue software
- Allowance for two-way fluid structure interaction in order to follow transient development of cracks and other structural failures
- Provision of project data management software to keep track of the large amount of data and runs typically involved in NRS applications

2.8.4 Recommendations for Single-Phase CFD Development

Single phase CFD tools are already mature for being applied to many NRS issues. The need for further developments was identified.

2.8.4.1 Extension of the Scope of Single Phase CFD Applications

Extension to porous media: Many reactor applications require a modelling of some reactor components with CFD in open medium (e.g. downcomer, lower plenum, upper plenum in a Pressure vessel) and a modelling of some other components (reactor core) with a porous body approach. Since turbulent mixing is often a main concern (in steam line break, boron mixing,...) the physical coupling between turbulence description in the open medium and in the porous body requires further modelling effort and validation.

Coupling with other disciplines: Many reactor applications require coupling of CFD with simulations tools for neutron kinetics, fuel thermo-mechanics and structure mechanics. Such coupling should be made easier by a standardisation of the code architecture and of module interfaces. This is a major objective of the NURESIM Integrated Project.

2.8.4.2 Improvements of the Physical Modelling

Using either RANS or LES turbulence models requires the use of wall functions in order to avoid too fine meshes in all wall boundary layers. Such wall functions for momentum and energy equations exist and are well established for ideal cases but might be improved in more complex situations such as a natural circulation (or mixed forced-natural convection) boundary layer, in presence of an impinging jet or of a flow detachment and for heated boundary layer with strong variations of physical properties.

LES now often replaces RANS models to benefit from the capacity to predict large scale fluctuations or for transients where time scales related to mean value variations and to large eddies are similar. Being more recently developed, LES still require improvements concerning wall functions, low Reynolds number zones, and the control of the numerical viscosity. High-Reynolds number flows could be better treated by developing a coupling between RANS and LES or using a hybrid method which combines the advantages of RANS and LES.

2.8.4.3 Improvements of the Numerical Efficiency of the Solvers

The main limitation of present CFD tools is still the large CPU time which is required for industrial applications. Any further progress in the efficiency of the numerical schemes would be welcomed by all users.

Adaptive mesh refinement methods should be generalised since they provide a better accuracy with a minimum increase of CPU time. In particular, similar methods should be developed for LES. However LES+Parallel+Adaptation does not seem efficient, as adaptation would be required for every time step. Grid nodes would cluster around each single resolved eddy. Turbulent structures are best resolved on a ‘uniform’ grid. An alternative would be an adaptation based on the averaged quantities.

First generation finite-volume or finite-difference solvers used structured meshing and staggered variable arrangement. These methods were very stable, robust, could preserve mass and energy and solve the momentum balance with a reasonable accuracy. The present generation of solvers prefers finite-volume methods with body fitted meshing and co-located variable arrangement. These methods offer new capabilities to be adapted to complex geometry, can also preserve mass and energy but may lose a little accuracy. Attempts to combine advantages of both and more generally to improve accuracy and robustness are in progress, such as the finite-element/finite-volume (FEFV) method. It is recommended to continue the development of robust numerical schemes with higher resolution and sharper interface prediction capabilities on given grids

2.8.5 Recommendations for Two-Phase CFD Development

Two-phase CFD tools are not yet very mature and require long term developments in many aspects. Physical modelling will require a long term effort and numerical scheme capabilities can still be better evaluated with respect to the requirements. Many applica-

tions of two-phase CFD also require a coupling with other thermal hydraulic modules and with other disciplines. Recommendations for further R&D on two phase CFD are given below.

2.8.5.1 Improving the Predictive Capability by Improved Physical Modelling

Present two-phase CFD tools have already proven reasonable predictive capabilities for some specific applications where the flow regime is a priori well known. Modelling in two phase CFD tool includes several aspects:

- Selection of the system of equations and of the averaging procedure
- Identification of local flow structure, which can be dispersed liquid, dispersed gas, separate-phase, or a mixture of them
- Modelling wall transfers through wall functions
- Modelling turbulent transfers
- Modelling interfacial heat and mass transfers
- Modelling source terms of additional equations such as interfacial area, bubble number density,...

For all these aspects further R&D is required. Further, basic research items are:

- No clear definition of what is the space and time filtering of the basic equations has been formulated so far. The Bonetto-Lahey test case demonstrated that the choice of the space resolution of the model is of prime importance. More theoretical work is necessary to specify what can be simulated and what should be modelled.
- An identification of the local flow configuration has to be based on calculated local variables. Still no universal approach exists and this prevents CFD from being a simulation tool capable of covering the whole range of flow regimes.

The modelling of bubbly flows requires the following work:

- Turbulence modelling seems to be presently limited to extrapolations of the single phase two-equation models (e.g. k - ϵ -model) by adding interfacial production terms. The limits of such approaches have already been reached and multi-scale approaches are necessary to take account of the different nature of the turbulence produced in wall shear layers and the turbulence produced in bubble wakes.
- Identification of the interface structure is currently using a transport equation for a bubble number density or an interfacial area concentration. However coalescence and break-up phenomena have to be modelled and further modelling effort is required for improving the available models. Moreover several additional equations would be necessary in poly-dispersed bubbly flows to characterize the bubble size spectrum. Further work is still required for having reliable closure relations for such additional equations.
- If expression for drag and virtual mass forces tend to converge, lift and turbulent diffusion forces are still tuned from one experiment to another. This indicates that more generic models need still to be developed.
- Wall functions for momentum and energy equations are often taken from single-phase flow whereas flow processes near the wall are significantly different in two-phase flow.

The modelling of droplet flows requires the following developments:

- Identification of the interface structure is currently using a transport equation for a droplet number density or an interfacial area concentration. However several additional equations would be necessary in poly-dispersed droplet flows to characterize the droplet size spectrum. Further work is required for having reliable closure relations for such additional equations. The identification of all possible mechanisms for droplet break up or coalescence still requires further investigations.
- Turbulent diffusion forces require more generic models and the modelling of droplet deposition upon vertical films or on free surfaces requires further investigations.
- Wall functions for momentum and energy equations are often taken from single phase flow whereas flow processes near the wall are significantly different in two-phase flow.

Modelling of free surface requires work in the following areas:

- The interface structure of stratified flows with a free surface may be influenced by friction forces, surface tension, wave propagation, condensation or vaporization, turbulence of both the gas flow and the liquid flow. The most difficult part is the prediction of the local wave structure since it is the result of local perturbations but also of propagation from everywhere in the flow domain.
- Turbulent diffusion controls heat and mass transfer at the free surface. Present models for the interfacial turbulence are not as well established as for wall shear layers. Complex interactions between turbulence and waves exist, which are not yet well understood.
- Droplet entrainment from the wave crests are presently not modelled with adequate accuracy for local scale modelling.
- Breaking of waves with entrainment of bubbles below the free surface plays a role in the interfacial transfer and requires specific efforts.

Considering the two-phase PTS issue which was investigated in ECORA, progress has been obtained for modelling some physical processes like

- Interfacial transfer of momentum, heat and mass at a free surface
- Effects of turbulent diffusion upon condensation
- Turbulence production below the jet
- Turbulence production in wall shear layers and in interfacial shear layer

Further effort should be directed to the modelling of the following physical processes:

- Entrainment of steam bubbles below the water level
- Condensation on the jet before mixing
- Interactions between interfacial waves, interfacial turbulence production and condensation
- Effects of temperature stratification upon turbulent diffusion
- Interface configuration in the top section of the downcomer
- Flow separation in downcomer at cold leg nozzle
- Heat transfer with cold leg and RPV walls

2.8.5.2 Concluding Remarks

Two-phase modelling with CFD is a complex problem and the present CFD codes are far from mature. There are numerous areas where the models are deficient and it is important to prioritise these, to enable the most important safety issues to be addressed as soon as possible. The safety community should therefore:

- Prioritise the safety issues
- Identify the dominant phenomena for which reliable two-phase CFD models are needed
- Advise the code developers accordingly
- Plan future validation tests accordingly

3 MANAGEMENT AND COORDINATION ASPECTS

3.1 Contractual Matters

A Unified Consortium Agreement (UCA) with a special confidentiality agreement for the use of selected UPTF experiments and PANDA data has been signed by all ECORA partners. In addition, the ECORA project was audited and successfully certified for the international ISO 9001:2000 standard [40]. Finally, the ECORA Technology Implementation Plan (TIP) has been submitted. It contains a single part 2, as all partners are implementing the same dissemination and usage scheme.

The project reports and financial coordination is running in line with the scheduled resources. A delay in the deliverable D13 of WP 8 and, as a consequence, the final reports D16 and D17, see section 3.1, was anticipated and approved by the responsible EC officer.

Table VI: List of deliverables

Deliverable No ²	Deliverable title	Delivery date ³	Nature ⁴	Dissemination level ⁵
D01	Best Practice Guidelines for judgement of CFD results, use of CFD software, and judgement of experimental data.	5	Re	PU

² Deliverable numbers in order of delivery dates: D1 – Dn

³ Month in which the deliverables will be available. Month 0 marking the start of the project, and all delivery dates being relative to this start date.

⁴ Please indicate the nature of the deliverable using one of the following codes:

Re = Report **Da** = Data set **Eq** = Equipment
Pr = Prototype **Si** = Simulation **Th** = Theory
De = Demonstrator **Me** = Methodology **O** = other (describe in annex)

⁵ Please indicate the dissemination level using one of the following codes:

PU = Public
RE = Restricted to a group specified by the consortium (including the Commission Services).
CO = Confidential, only for members of the consortium (including the Commission Services).

Deliverable No²	Deliverable title	Delivery date³	Nature⁴	Dissemination level⁵
D02	Review report of CFD applications to primary loop and recommendations	15	Re	PU
D03	Review report of experimental data base on mixing in primary loop and future needs	15	Re	PU
D04	Review report of two-phase flow modelling capabilities and recommendations	27	Re	PU
D05a	Report describing selected PTS-relevant test cases	12	Re	RE
D05b	Report describing selected physical models	16	Re	RE
D06	Documentation of verification test cases	18	Re	RE
D07	Documentation of CFD code performance for PTS analysis	24	Re	RE
D08	Results and performance of the software with improved models	26	Pr	CO
D9.1	Demonstration Test Case: ECORA DEM01: UPTF Test1, Run21	38	Re	RE
D9.2	Demonstration Test Case: ECORA DEM02: UPTF TRAM C1, Run21a2	38	Re	CO
D10	Review report on CFD applications to large-scale experiments and full-scale containment analysis and recommendations for CFD code use	15	Re	PU
D11	Review report on experimental data base on containment related safety issues and future needs	39	Re	PU
D12	Summary of selected tests and criteria applied to choice of models, mesh and numerical methods	36	Re	RE
D13	Results of the pre-test calculations	40	Re	RE
D14	Recommendations on use of CFD codes in nuclear safety analysis	36	Re	PU
D15	Recommendations for code development and customisation	36	Re	PU
M01	Minutes of UPTF-meeting	1	Re	PU
M02	Minutes of kick-off meeting	1	Re	PU
M03	Minutes of second project meeting	3	Re	PU
M04	Minutes of third project meeting	7	Re	PU
M05	Minutes of PANDA-meetings	10	Re	PU
M06	Minutes of mid-term meeting	18	Re	PU
M07	Minutes of fifth project meeting	24	Re	PU

Deliverable No ²	Deliverable title	Delivery date ³	Nature ⁴	Dissemination level ⁵
M08	Minutes of sixth project meeting	32	Re	PU
M09	Minutes of final meeting	36	Re	PU
D16	Final summary report	40	Re	PU
D17	Condensed final summary report	40	Re	PU

3.2 Dissemination of Results

Representatives of the projects ERCOFTAC/QNET-CFD, FLOMIX-R, ASTAR and ITEM expressed strong interest to cooperate with ECORA. The technical coordinators of these projects have obtained copies of the ECORA BPGs with the stipulation to return general comments on the BPGs, and to report about any experience gained in applying the BPGs. Many ECORA partners have contributed to the ASTAR conference which took place on 17 – 18 September 2003 at GRS. ASTAR has a new deliverable, the ASTAR BPGs, which will feed into the ECORA BPGs. FLOMIX-R and ITEM also used templates from the ECORA BPGs for the description of numerical and experimental test cases. A common ECORA/FLOMIX-R workshop took place on 15 – 16 March 2004 organised by CFX Germany. Several FLOMIX-R simulations of Boron dilution mixing were presented where the ECORA BPGs had been successfully applied. In addition, the ECORA BPGs have been presented at the OECD/NEA writing groups on CFD issues in NRS which want to issue similar guidelines for the use of CFD in NRS.

A POST-FISA workshop on ‘advanced multi-physics computations in nuclear reactor safety’ was organised by the ECORA coordinators. The objectives of this workshop were the discussion of nuclear reactor safety simulation challenges from the industrial, regulatory and utility point of view. Representatives of European and US nuclear reactor safety organisations presented the state-of-the-art of nuclear reactor simulation tools, and described current development challenges and on-going research programmes. The presentations related to the fields of computational fluid dynamics (CFD), computational neutronics, system codes, multi-scale methods, and to the coupling of these methods for multi-physics applications. Collaboration opportunities were identified for multi-physics simulation platforms, and for the assessment of mathematical models in nuclear reactor safety. Finally, the importance of quality assurance guidelines for simulations was discussed using the example of the ERCOFTAC and ECORA CFD Best Practise Guidelines

Documentation is made available via the Internet to achieve a high degree of topicality and to be in a position to maintain and extend the BPGs and related documents during and beyond the project term. The ECORA website at <http://domino.grs.de/ecora/ecora.nsf> contains the project documents and the results from the validation test cases including the experimental data. The main findings and conclusions of the project are presented in publications and conferences, e.g. FISA conference, ASTAR and ANSYS-FZR workshop on multi-phase flows. The ECORA paper presented at the FISA 2003 conference is published in the Journal for Nuclear Engineering and Design.

The models developed within the project are implemented in industrial and commercial CFD software packages and will therefore be easily accessible by industry and research institutions. Implementation in industrial software packages will guarantee that the models will be maintained and refined after the project.

The work performed in ECORA improves understanding of merits and limitations of CFD, and contributes to define realistic goals of these methods in safety analysis. Additionally, the project aims at reinforcing the network among the European Centres of Competence on CFD, to achieve consensus and common understanding on key technical/scientific issues related to the use of CFD methods for reactor safety analysis.

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