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Use of computational fluid dynamics codes for safety analysis of nuclear reactor systems

Summary report of a technical meeting jointly organized by the International Atomic Energy Agency and the Nuclear Energy Agency of the Organisation for Economic Co-operation and Development held in Pisa, Italy, 11–14 November 2002

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FOREWORD

Safety analysis is an important tool for justifying the safety of nuclear power plants. Typically, this type of analysis is performed by means of system computer codes with one dimensional approximation for modelling real plant systems. However, in the nuclear area there are issues for which traditional treatment using one dimensional system codes is considered inadequate for modelling local flow and heat transfer phenomena. There is therefore increasing interest in the application of three dimensional computational fluid dynamics (CFD) codes as a supplement to or in combination with system codes. There are a number of both commercial (general purpose) CFD codes as well as special codes for nuclear safety applications available.

With further progress in safety analysis techniques, the increasing use of CFD codes for nuclear applications is expected. At present, the main objective with respect to CFD codes is generally to improve confidence in the available analysis tools and to achieve a more reliable approach to safety relevant issues. An exchange of views and experience can facilitate and speed up progress in the implementation of this objective. Both the International Atomic Energy Agency (IAEA) and the Nuclear Energy Agency of the Organisation for Economic Co-operation and Development (OECD/NEA) believed that it would be advantageous to provide a forum for such an exchange. Therefore, within the framework of the Working Group on the Analysis and Management of Accidents of the NEA's Committee on the Safety of Nuclear Installations, the IAEA and the NEA agreed to jointly organize the Technical Meeting on the Use of Computational Fluid Dynamics Codes for Safety Analysis of Reactor Systems, including Containment. The meeting was held in Pisa, Italy, from 11 to 14 November 2002.

The present publication constitutes the report of the Technical Meeting. It includes short summaries of the presentations that were made and of the discussions as well as conclusions and recommendations for further work. A CD containing the entire collection of papers is provided as a supplement to this report.

The IAEA officer responsible for this publication, which was prepared in collaboration with J. Royen of OECD/NEA, was J. Mišák of the Division of Nuclear Installation Safety.

EDITORIAL NOTE

CONTENTS

1. INTRODUCTION

1.1. BACKGROUND

Computational fluid dynamics (CFD) codes are used to solve mass and energy conservation equations for different media. They do so with a high level of sophistication, averaging parameters of media under consideration over a scale smaller than a hydraulic diameter. CFD codes are capable of calculating local media parameters (velocities, concentrations, etc.), i.e. they provide a localized snapshot of the real situation.

CFD codes are typically used to model multi-component distribution and mixing phenomena. Although these codes were originally developed for non-nuclear applications, there are already many examples of the use of CFD codes in reactor safety related areas, such as:

- Analysis of heterogeneity in coolant temperature distribution and its effect on pressurized thermal shock;
- Transient boron dilution and other reactivity initiated accidents with non-homogenous core behaviour;
- Propagation and mixing of gases (hydrogen, air, steam) in the containment and the effect of gas distribution on the containment dynamics;
- Chemical reactions in the containment (combustion, flame propagation);
- Modelling of containment condensation;
- Transport and deposition of aerosols in severe accidents;
- Evaluation of performance of passive safety features;
- Investigation of local phenomena leading to cladding ruptures;
- Multidimensional thermal-hydraulics in various components;
- Liquid/gas stratification and interface tracking;
- Bubble dynamics in suppression pools.

As illustrated above, CFD codes have a very broad range of applicability; they provide detailed insight and offer a unique tool for analysis of local phenomena. However, their use is quite different from that of typical system codes and there are still limitations to their applicability as a routine tool for safety justification of nuclear power plants (NPPs).

1.2. OBJECTIVES AND ORGANIZATION OF THE MEETING

The purpose of the technical meeting was to provide an international forum for the presentation and discussion of selected topics related to the development and application of CFD codes to nuclear reactor safety problems. The information collected at the meeting will be useful as a basis for further activities in this area such as:

- Development of a guidance document for use of CFD codes in nuclear safety applications;
- Assessment of CFD codes for nuclear reactor safety problems;
- Development of CFD code benchmark problems (three benchmark problems foreseen);

- Evaluation aimed at extension of the applicability of CFD codes to cover two-phase flow problems.

The meeting was organized by the IAEA in co-operation with OECD/NEA and was hosted by the University of Pisa. One hundred participants from 24 Member States and two international organizations (NEA and IAEA) participated in the meeting.

The detailed programme of the meeting was prepared by an organizing committee, composed of the two scientific secretaries, J. Mišák and J. Royen, representing the IAEA and OECD/NEA, respectively, F. D'Auria representing the host organization, M. Durin and J.-C. Micaelli of the Institut de radioprotection et de sûreté nucléaire (IRSN), France, and J. H. Mahaffy of The Pennsylvania State University, USA. The meeting comprised thirty-one oral and 16 poster presentations. The presentations were split into seven oral and two poster sessions:

(1) Session 1. Introduction, chaired by Prof. E. Vitale, Dean of the Faculty of Engineering, University of Pisa

(2) Session 2. In-vessel boron mixing, chaired by O. Sandervåg, Sweden

(3) Session 3. In-vessel mixing and pressurized thermal shock, chaired by M. Scheuerer, Germany

(4) Session 4. In-vessel severe accidents, chaired by Z. Téchy, Hungary

(5) Session 5. Containment, chaired by M. Durin, France

(6) Session 6. Combustion, chaired by B. Smith, Switzerland

(7) Session 7. Two-phase modelling and other advanced methods, chaired by F. D'Auria, Italy

(8) Poster Session 1. Primary system applications, chaired by J.-C. Micaelli, France

(9) Poster Session 2. Containment and severe accident applications, chaired by J. Mahaffy, United States of Ameria

(10) General discussion, chaired by M. Réocreux and F. D'Auria.

A number of CFD computer codes, the status of their development and validation, the approaches used, and a variety of applications were presented. A summary of the presentations and the ensuing discussions in the individual sessions is provided in Section 2 of this report. These summaries were prepared by the chairpersons of the sessions and afterwards agreed upon at a meeting of the organizing committee and the session chairpersons. The full papers from the meeting are provided separately on a CD as a supplement to this report.

2. SUMMARY OF MEETING SESSIONS

2.1. SESSION 1: INTRODUCTION

Introducing the meeting, M. Réocreux, in his invited paper, presented several issues related to the use of CFD codes for nuclear reactor safety (NRS) applications. He noted that in various situations relevant to NRS, CFD codes could contribute to significant progress in present practices. However, to be accepted for safety justification, these codes needed to satisfy several requirements. These were listed in the presentation. Present approaches in the use of numerical simulation tools were described. They included different calculation methodologies (single direct, conservative, best estimate), the merits and limitations of which were summarized. Specific features of the CFD codes related to physical modelling, assessment and numerical schemes were listed and compared to the requirements for acceptability in safety justification. In conclusion, it was recognized that interesting results had already been produced by CFD codes, especially for use in design studies. For nuclear safety purposes, further needs for development were identified in the area of modelling improvements, control of numerical schemes, minimization of user effects, code assessment, and evaluation of uncertainties.

2.2. SESSION 2: IN-VESSEL BORON MIXING

Boron is added to the water in pressurized water reactors to control power and to maintain subcriticality under shutdown conditions. The safety issue is whether a slug of water that is depleted of boron may, under certain circumstances, accumulate in the circuits and be transported to the core where it can cause a reactivity excursion.

Several mechanisms with the potential to accumulate boron-free volumes have already been identified and investigated. Such mechanisms include, for instance, inadvertent dilution during maintenance and accumulation of condensate under certain conditions during small break loss of coolant accident (SBLOCA). The accumulation mechanisms are well established and were only very briefly discussed in the session. The response of the reactor to a diluted slug was also briefly discussed. However, the major focus was on the transportation of the diluted slug into the core. It has been recognized that various mechanisms associated with the transportation and mixing of the boron will significantly modify, and even possibly eliminate the safety concerns. CFD technology is used to assess these mechanisms. There are essentially two major classes of transportation. One involves startup of a reactor coolant pump in the diluted loop and the other is the onset of natural circulation that may occur when the water inventory is restored after an accident. Experimental and theoretical work has been carried out on both of these classes.

The following four papers were presented in Session 2:

- *Simulation of OECD/NEA International Standard Problem No. 43 on Boron Mixing Transients in a Pressurized Water Reactor*, by M. Scheuerer, Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, Germany;
- *Simulation with CFX-4.3 of Steady State Conditions in a 1/5th-Scale Model of a Typical 3-Loop PWR in the Context of Boron-Dilution Events*, by T.V. Dury, presented by B.L. Smith, Paul Scherrer Institut (PSI), Switzerland;
- *Utilisation of CFD-Type Computer Code FLUENT for Safety Related Purposes of Nuclear Power Plants with VVER Reactors*, by J. Macek, J. Schmid and P. Mühlbauer, Nuclear Research Institute Řež plc, Czech Republic;

- *Experiments and CFD Calculations on Coolant Mixing in PWR – Application to Boron Dilution Transient Analysis*, by G. Grunwald et al., Forschungszentrum Rossendorf e.V., Germany.

The paper by Scheuerer dealt with simulation of boron mixing transients that were addressed in International Standard Problem 43 (ISP-43), which was a boron mixing experiment in a loop at the University of Maryland. The objective of the experiment was to provide data for CFD code assessment. Sensitivity studies were carried out with respect to numerical schemes, buoyancy effects and reactor core models.

Both Smith and Mühlbauer presented papers describing simulations of boron dilution, one for a scaled test facility using the CFX computer code, and the other, for a WWER-1000 reactor using the FLUENT computer code. The paper by Grunwald et al., presented by co-author Höhne, described experiments addressing relevant mixing phenomena in the ROCOM facility in Rossendorf. CFD calculations and reactor dynamics calculations were performed using the CFX-4 code and the DYN3D code, respectively. Favourable agreement between measurements and CFD results was claimed. The reactor dynamics calculations using data from the validated CFD calculations indicated that significant amounts of diluted water would be necessary to cause a large reactivity accident.

The potential to address the boron mixing phenomena using CFD technology was emphasized in the discussion that followed. The question of how uncertainties could be addressed was raised and the importance of having developed guidelines was pointed out. It was also emphasized that more data for validation of the CFD technology was needed to establish confidence in its use for nuclear applications. In this regard, very long computation times could prove to be a limiting factor. Assessment is needed for nuclear applications in order to reduce significant user effects.

2.3. SESSION 3: IN-VESSEL MIXING AND PRESSURIZED THERMAL SHOCK

Seven papers were presented in Session 3:

- *Experiences with Validation of CFD Methods for Pressure Vessel Downcomer Mixing Analyses*, by T.S. Toppila, Fortum Nuclear Services Ltd. Finland;
- *Comparisons of Non-stationary Convective Mixing Process between Turbulence Models*, by N. Kimura, M. Igarashi and H. Kamide, Japan Nuclear Cycle Development Institute (JNC), Japan;
- *Numerical Analysis of Coolant Mixing in the RPV of VVER-440 Type Reactors with the Code CFX-5.5.1*, by I. Boros and A. Aszódi, Budapest University of Technology and Economics, Hungary;
- *Three dimensional Analysis of Flow Characteristics in the Reactor Vessel Downcomer during the Late Reflood Phase of a Postulated LBLOCA*, by T.-S. Kwon et al., Korea Atomic Research Institute, Republic of Korea;
- *Three dimensional Hydrodynamics and Heat Transfer in WWER Reactor Units*, by E.M. Fedorov, E.I. Levin and Yu.G. Dragunov, Experimental and Design Organization "Gidropress", Russian Federation;
- *Simulation of Turbulent Fluid–Structure Interaction using Large Eddy Simulation (LES), Arbitrary Lagrangian–Eulerian (ALE) Co-ordinates and Adaptive Time–Space Refinement*, by P.A.B. De Sampaio (Instituto de Engenharia Nuclear, Comissão

Nacional de Energia Nuclear), P.H. Hallak, A.L.G.A. Coutinho and M.S. Pfeil (Instituto Alberto Luiz Coimbra, Federal University of Rio de Janeiro), Brazil;

- *Efficient Nodal Schemes for CFD in Nuclear Engineering Applications*, by R. Uddin, University of Illinois at Urbana-Champaign, USA.

Five of the papers dealt with flows in reactor pressure vessels and related geometry. Commercial CFD codes, namely STAR-CD, CFX and FLUENT, were used for these simulations. The paper by Kimura, Igarashi and Kamide concerned the comparison of turbulence models for a triple jet configuration. Proprietary codes developed at the Japan Nuclear Cycle Development Institute were employed for this study. Sampaio and Uddin presented the development of numerical methods.

The objectives of the presentation by Toppila were to define and develop 'optimum' ways to use CFD at Fortum Nuclear Services. The optimum was defined as a set of objectives including satisfactory reproduction of data and a calculation time of less than 10–20 days. The flows in three downcomer test facilities (Vattenfall, UMCP (University of Maryland) and Fortum) were simulated with FLUENT. Hybrid and hexahedral grids with 150,000–285,000 nodes were used. The mathematical model consisted of the averaged Navier-Stokes equations and the k-ε two-equation turbulence model in several variations. Logarithmic wall functions were used to calculate wall fluxes. The results showed satisfactory agreement with available data.

Boros and Aszódi applied the CFX-5.5 software to a full-scale pressure vessel of the WWER-440 reactor. The striking feature of this presentation was the detail of geometry modelling and the assessment of the influence of this modelling on the flow in the reactor pressure vessel. In particular, sub-models were developed for simulating the effect of the alignment drifts, the hydro-accumulators, the control rod chamber and the elliptical perforated plate at the core inlet. Tetrahedral grids with up to 2,700,000 nodes were applied. As in the previous presentation, the mathematical model consisted of the averaged Navier-Stokes equations and the k-ε two-equation turbulence model with logarithmic wall functions. Time dependent boundary conditions were taken from the APROS system code. Agreement with experimental data was satisfactory.

Kwon et al. used FLUENT in the downcomer geometry of an APR1400 reactor to corroborate the applicability of empirical linear scaling laws by three dimensional CFD calculations. This was done by simulating the flows in full-scale and scaled-down geometries and by comparing results for global parameters such as pressure losses, velocity distributions and streak lines, to data from the MIDAS test facility and to computational results from the MARS and RELAP system codes. Hexahedral grids were employed for the CFD calculations. The mathematical model consisted of the averaged Navier-Stokes equations together with the k-ε two-equation turbulence model with logarithmic wall functions. In the second part of the presentation, calculations of an emergency core cooling two-phase water jet were shown. These were performed with a Volume-of-Fluid model. The results were qualitatively similar to those obtained from experiments.

Fedorov et al. demonstrated applications of STAR-CD to flows in the reactor pressure chamber and the reactor collection chamber of a WWER-440 reactor. In all cases, 90° sections of the geometry were discretized with hybrid grids using local refinement. The number of grid elements was typically 300,000. Averaged Navier-Stokes equations were employed in combination with the k-ε two-equation turbulence model and logarithmic wall functions. In addition, a conjugate heat transfer model was used to simulate energy transfer within the structural elements. The emphasis of the presentation was to demonstrate the complexity of the ensuing flow fields and, consequently, the necessity to use methods based on three dimensional Navier-Stokes equations. A comparison with experimental data was not performed. At the end of the presentation, the need for free surface and two-phase flow models, as well as a systematic approach to code validation and verification, was pointed out.

Kimura et al. showed the comparison of three different turbulence models for a triple jet configuration. The models were the k-ε two-equation turbulence model, a low Reynolds number version of a second moment closure model, and 'direct numerical simulations (DNS)'. 'DNS' appears in quotes because Kimura et al. performed a two dimensional unsteady state calculation of the jet flow without turbulence model, whereas the term DNS is usually reserved for simulations of the full three dimensional flow pattern of turbulent flow. They showed the superiority of their 'DNS' approach over the statistical models in terms of temperature fluctuations and the spectrum of the temperature fluctuations. However, in the case of the statistical models, it remained unclear how the turbulence spectrum was reconstructed from the solution of an equation for the temperature variance. It also remained unclear how the turbulence characteristics of the jet were captured so well in the 'DNS' in spite of only two of the three fluctuating components having been resolved.

Sampaio et al. presented the development of an unsteady state two dimensional method using a Petrov-Galerkin finite element method on a Lagrangian (i.e. moving) grid. The method was combined with a grid adaptation scheme and allows for the solution of fluid–structure interaction problems. 'Large eddy simulation (LES)' is used for turbulence modelling. 'LES' appears in quotes because it was applied in a two dimensional context, whereas traditionally LES is reserved for simulations of three dimensional turbulence simulations. Validation of the method was performed for the laminar and turbulent flow behind cylinders. Fluid–structure interaction results were presented by showing the flow over the two dimensional cross-section of a bridge.

Uddin presented the development of a 'nodal scheme' for the Navier-Stokes equations. Such schemes are successfully used in neutronics calculations. Currently the method is available for two dimensions and Cartesian co-ordinates. It has recently been extended to non-rectangular, two dimensional geometries. In addition, a local mesh refinement method has been introduced. So far, the method is only applicable to laminar flows. Various laminar test problems, such as the flow in lid driven cavities, were presented as verification test cases.

In conclusion, the following observations can be made:

- The five industrial test cases were simulated with commercial CFD software and simple turbulence and near-wall models. They showed a comparable, satisfactory level of agreement with experimental data.
- Investigation and quantification of numerical errors and uncertainties before the assessment of turbulence models is not generally performed. There is apparently no use of Best Practice Guidelines in the community to facilitate this task. A more systematic approach to this subject will be essential for increased acceptance of CFD results in the NRS community.
- The applied turbulence models are of the standard types. New approaches like the SST turbulence model, second moment closure models, or more modern wall function approaches with automatic switches between linear and logarithmic wall functions are scarcely, if at all, applied.

- The numerical method development presented in the session covered interesting aspects. In particular the method shown by Sampaio et al. touched on components like dynamic mesh adaptation and fluid–structure interaction that may be of interest for future calculations. However, both methods presented in the session seem still to be in their infancy, and require further validation and the extension to three dimensions before being of practical use in NRS.

The discussion at the end of the session focused on the necessity to apply safety standards in order to assess the uncertainty margins of CFD software. The actual objectives of CFD in NRS were also discussed. It was generally agreed that CFD cannot replace experiments because of the uncertainty of the empirical models for turbulence, multiphase flow and chemical reactions in the codes. However, CFD can reduce the number of experiments necessary to validate designs. It can also provide a deeper understanding of the flow physics and thus lead to better designs and/or more adequate safety margins. For system analysis, CFD is complementary to system codes and experiments. With increasing computer power and improved modelling, the usage and application of CFD in NRS is likely to increase.

The participants agreed that there were now methods to quantify numerical errors and uncertainties arising from boundary conditions. A description of such procedures is partly available for non-nuclear applications (for instance from the European Research Community on Flow, Turbulence and Combustion (ERCOFTAC)). Quantification of the influence of the physical models is more intricate. It should only be performed after numerical errors and uncertainties have been quantified. It requires reliable experimental data for comparison and validation. Several participants in the discussion commented on the lack of such data for the important field of multiphase flows in NRS.

2.4. SESSION 4: IN-VESSEL SEVERE ACCIDENTS

The following four papers were presented in Session 4:

- *The Development of SIMMER-III, An Advanced Computer Program for LMFR Safety Analysis*, by Y. Tobita et al. (Japan Nuclear Cycle Development Institute, Japan), K. Morita (Kyushu University, Japan), W. Maschek (Forschungszentrum Karlsruhe (FZK) Germany), P. Coste et al. (Commissariat à l'énergie atomique (CEA), France) ;
- *Analyses of Non-condensable Gas Accumulation and Hydrogen Combustion in Pipe using IMPACT Code*, by R. Kubota (Fuji Research Institute Corporation), M. Naitoh, F. Kasahara (Nuclear Power Engineering Corporation) and I. Ohshima (Nuclear and Industrial Safety Agency, Ministry of Economy, Trade and Industry), Japan;
- *CFD Analysis of Air Ingress Distribution during Mid-Loop Accident Sequences*, by F. Oriolo, G. Fruttuoso (University of Pisa) and M. Leonardi (THEMAS S.r.l.), Italy;
- *Study with the CFD Code TRIO_U of Natural Gas Convection for PWR Severe Accidents*, by H. Mutelle (CEA) and U. Bieder (IRSN), France.

The first paper, presented by Tobita, provided information about SIMMER-III, a 2-D multiphase and multi-component fluid dynamics code. The code is tailored to the liquid metal fast breeder (LMFR) materials, but its thermophysical properties and equation of state functions are sufficiently flexible to include other (non-LMFR) applications. The code includes coupling with a space–time and energy dependent neutron transport kinetics model. Code validation is ongoing in two phases. Phase 1 involves a fundamental code assessment of individual models Phase 2 is an integral assessment for key phenomena relevant to LMFR safety. Individual test problems and the major results of the validation were presented. The main advantage of the SIMMER-III code is its integrated and consistent approach to fluid dynamics and neutronics.

In response to a question concerning the application of the SIMMER-III code to light water reactor problems, Tobita referred to other presentations at this meeting addressing the issue.

The paper by Kubota et al. addressed the pipe rupture accident in the residual heat removal steam condensing line at Hamaoka NPP, Unit 1 (Japan) on 7 November 2001. The cause of the accident was identified as the detonation of hydrogen. Hydrogen was generated through radiolysis of the coolant. Fluid conditions in the pipe and the accumulated amount of hydrogen and oxygen were calculated with IMPACT, a 3-D multiphase CFD code. The hydrogen combustion module of the IMPACT code was used for the analysis of the pressure in the pipe generated by the detonation wave. The results were roughly in agreement with a theoretical Chapman-Jouguet solution. As a next step, a pipe deformation analysis was performed based on the transient 3-D pressure distribution obtained. The analysis showed that the pipe strains exceeded critical values in the elbow region, causing a pipe rupture. The results were consistent with the actual pipe deformation observed in the accident.

Because of the safety importance of the topic, the presentation was followed by a lively discussion. The authors answered the questions addressing the details of the pipeline and the accident conditions.

In the paper presented by Leonardi, the authors analysed mid-loop scenarios of a two-loop, 980 MWe pressurized water reactor (PWR) reactor with possible air ingress were analysed. The FLUENT-V5.0 CFD code was used for the calculations. The analysis involved a diffusive description of the air bubble spreading in a radial direction towards the peripheral area zones. As a consequence, peripheral fuel rods, which are generally less likely to be oxidized during an accident, may be exposed to air–fuel interaction. On the other hand, air–fuel interaction may aggravate local degradation phenomena occurring predominantly in the central regions; from this point of view, the radial spreading of the air bubble may alleviate the situation.

Mutelle reported on studies with the TRIO_U CFD code of natural circulation conditions in the primary system of a PWR during a high pressure scenario. In one case, the gas flow in the hot leg was investigated with a simplified representation of the reactor vessel and the steam generator tube. Calculations were performed for structured and unstructured meshing with and without the thermal radiation model between the walls and the gas. In the second case, calculations were performed for natural circulation in the steam generator. The results are in good agreement with the available experimental data. Further work is ongoing to involve other parts of the circuit, including the pressurizer.

The questions raised during the discussion addressed details of the model and calculations. Comments encouraged further progress and continuation of the work.

2.5. SESSION 5: CONTAINMENT

Eight papers were presented in this session:

- *Application of CFD Codes STAR-CD and FDS for addressing Hydrogen Distribution and Mitigation Issues in the Containments of Indian NPPs*, by S.G. Markandeya et al., Bhabha Atomic Research Centre, India;
- *Status of Development, Validation, and Application of the 3D CFD Code GASFLOW at FZK*, by P. Royl et al., FZK, Germany;
- *Aspects of Nuclear Reactor Simulation requiring the Use of Advanced CFD Models*, by B.L. Smith, M. Milelli and S. Shepel, PSI, Switzerland;
- *3D Calculations for Bubbler Condenser Experimental Qualification*, by Z. Téchy and P. Kostka, VEIKI Institute for Electric Power Research, Hungary;
- *Hydrogen Distribution in a Ventilated Room*, by S. Keijers, W. Vanhove and D. Aelbrecht, Tractebel Energy Engineering, Belgium;
- *Development of Fluid Dynamic Codes (MISAP, PCCSAC/3D) for Passive Safety Systems and Thermal Hydraulic Behavior of Qinshan-II under Severe Accident Conditions*, by S. Zhang, Nuclear Power Institute of China;
- *CFD Analyses of Hydrogen Risk within PWR Containments*, by J. M. Martín-Valdepeñas Yagüe and M. A. Jiménez García, Universidad Politécnica de Madrid (UPM), Spain;
- *CFD Analyses of Steam and Hydrogen Distribution in a Nuclear Power Plant*, by N.B. Siccama, M. Houkema and E.M.J. Komen, Nuclear Research and consultancy Group (NRG) Petten, Netherlands.

Four of the papers dealt with hydrogen and steam distribution in a containment, one with hydrogen distribution in a ventilated room, one described the 3-D calculation of a bubbler condenser, and one was on advanced modelling of condensation and bubble plume. Commercial CFD codes (CFX, STAR-CD, FDS) were employed for five studies, proprietary codes for three.

The objective of the presentation by Markandeya was the study of hydrogen distribution in the complex multi-compartment containment geometry. The two CFD codes employed for this purpose were STAR-CD and FDS (Fire Dynamics Simulator). Results from the HYMIS test facility were used to validate both the above mentioned CFD codes. Of the two codes, the FDS code was found to be superior, particularly for modelling the hydrogen dispersion phenomena, mainly due to its efficient numerical schemes and treatment of turbulence. The total CPU time requirement for the FDS code was noted to be much smaller compared to that required by the STAR-CD code for solving the same size of problem. Subsequently, the FDS code was chosen for conducting the hydrogen distribution studies. Following this, the code was further deployed to study the hydrogen dispersion phenomena in multi-compartment geometries. For this purpose, a hypothetical geometry comprising seven rooms of a two floor flat was chosen arbitrarily. Several parametric calculations were carried out to understand the effect of location, direction, and duration of hydrogen injection on its distribution. The code was then successfully used to conduct the pre-test calculations of hydrogen distribution in a multi-compartment containment studies facility, which is presently at an advanced stage of construction.

Royl gave a presentation on the status of development, validation and application of the 3-D CFD code GASFLOW. GASFLOW provides a finite volume solution of the 3-D Navier-Stokes equations on a staggered mesh with either Cartesian or cylindrical co-ordinates. The new model developments in GASFLOW concern radiation, hydrogen recombination, wall functions, a sump model and a spray model. Important validation work is ongoing with the new experiments on containment thermohydraulics that provide detailed and local data such as those tests that are currently being performed in the MISTRA, TOSQAN and ThAI Facilities as a new international standard problem (ISP-47). The applications in full 3-D containment simulations for a KWU type pressurized water reactor with a spherical containment were then presented. With an average cell volume of approximately 1 m^3, the number of fluid cells is of the order of 80,000. The GASFLOW simulation indicated a strong interaction between the source dynamics and the containment convection for all analysed scenarios and gave indications on the steam inertization as a function of the applied source term. In conclusion, the authors identified the need for a better validation of some generic effects identified in the 3-D simulation.

The paper presented by Smith described the development of advanced models to simulate complex phenomena occurring in light water reactors. The models are generic and general purpose, but in the context of the paper relate directly to advanced containment designs featuring passive decay heat removal systems. The first example is the development and implementation into the CFX-4 code of a condensation model. The paper described the model, its validation against analytical and semi-empirical data, and its application to a finned tube containment condenser for which measured data are available. The second example concerns the dynamics of submerged bubble injection, breakup of the gas/liquid interface due to the action of hydrodynamic instabilities, and the ultimate condensation of the steam. The paper described the inclusion of an interface tracking methodology, based on the Level Set method, into CFX-4. After breakup of the principal discharge bubble into fragmentary smaller bubbles, the heat transfer area is increased, and detailed analysis shows that virtually complete steam condensation occurs. It is important to know how the resulting bubble plume interacts with the surrounding water to efficiently mix the pool. This issue has prompted a parallel study of bubble plumes involving the development of appropriate two-phase turbulence models and the use of LES techniques to dispersed two phase flow. This work was also reported in the paper.

The paper by Téchy and Kostka described an experimental and analytical study of the bubbler condenser behaviour during postulated loss-of-coolant accidents in WWER-440/213 nuclear power plants. Experiments were conducted on the EREC test facility, a scale model (1:100) of the containment of the Paks NPP, constructed at Elektrogorsk, Russia. Three large break loss of coolant accident (LBLOCA) tests were performed at the EREC test facility in 1999. As a follow-up, a study was carried out with the GASFLOW 2.1 three dimensional CFD code to assess the thermal-hydraulic conditions in the EREC test facility during a transient. The simulation model consisted of 14,250 cells. GASFLOW simulations provided flow velocity fields and thermal-hydraulic parameters in much greater detail compared to lumped parameter code modelling. The analyses predicted a rather complex flow pattern around the bubbler condenser. The fluid flow enters the bubbler condenser in different paths: the main part turns around at the rear end of the facility, and a relatively small part of the stream enters the facility from the front side. The reason for this is that the front flow is impacted and redirected by the condenser pedestal and front grid plate. The GASFLOW simulations agreed well with the measurement results.

Keijers presented a paper on the hydrogen distribution in a ventilated room performed within the framework of an explosion risk assessment. The storage tanks for the gaseous effluents and their piping were identified as a possible source of failure, leading to leakage of explosive mixtures. The storage tanks containing hydrogen/nitrogen mixtures were situated in different compartments of a dedicated building. The aim of this study was to determine the hydrogen distribution in the compartments due to a possible leak in the piping to the storage tanks. Forced ventilation ventilated the compartments. Two interconnected compartments were simulated: the upper compartment where the valves on the piping and the ventilation inlet were situated and the lower compartment where the storage tank and the ventilation extractions were situated. Different leak types (jet, plume) were investigated by mean of the CFD code CFX-5. The mixing in the compartments is a function of the Froude number. The CFD results are compared to simplified calculation methods on averaged concentrations.

Zhang presented a paper on the development and use of CFD codes for the evaluation of the passive residual heat removal system of a new generation of PWR nuclear power plant (AC600/1000). The fluid dynamics analysis codes MISAP and PCCSAC/3D have been developed and some related experiments have been done by NPIC to verify and improve the codes. This paper introduced the functions, physical modelling and behaviour for the passive residual heat removal systems computer code MISAP and the PCC system three dimensional computer code PCCSAC/3D, respectively. The comparisons between the calculation values of the codes and experimental results show that the codes are able to be used in the design for AC600/1000., A comparison between PCCSAC/3D and COMMIX was performed under the same conditions, giving similar results.

The paper presented by M. Valdepeñas dealt with hydrogen risk within PWR containments. The code used was CFX-4, with a specific condensation model. Experiments were simulated to validate CFD calculations for buoyancy driven plumes, stratification phenomena and local accumulation of hydrogen, steam and other light gases. The MICOCO benchmark was used to validate the condensation model. Finally, an application to an actual Spanish PWR plant was performed in two scales of accuracy: detailed studies in the release room and full-scale 3-D plant application. The detailed study included the steam generator, the pump and the shield plate. The model had 12,000 nodes in a 1900 m^3 room. The level of risk was assessed using the Flame Acceleration and the Deflagration to Detonation Transition criteria, which were implemented in CFX. The full-scale containment mesh had a characteristic cell size of approximately 1 m^3, amounting to a total of 90,000 cells. The author's conclusion was that …with the geometry and the conditions used in this study, there was a only a small possibility of flame acceleration for just a few seconds within the break room.

The paper presented by Siccama likewise addressed the problem of CFD analyses of steam and hydrogen distribution in a nuclear power plant. The containment that was the subject of this study was equipped with 22 passive autocatalytic recombiners (PARs). Lumped parameter codes were used to determine optimum PAR positions and hydrogen removal efficiency. In order to assess possible multidimensional effects, a detailed three dimensional CFD model of the containment of the NPP was prepared. The code used was CFX-4.4 with a body fitted mesh using 680,000 hexahedral cells. Specific models for wall condensation and recombiners were used. In a first code-to-code comparison step, the model was used to compute a reference accident scenario that had been analysed earlier with the lumped parameter code SPECTRA (NRG). If there was good qualitative agreement, a quantitative discrepancy was observed between the CFX 4-4 and the SPECTRA results, explained by the absence of an evaporation model in the CFD code. Subsequently, the actual steam jet was realistically modelled in CFX 4-4 in order to determine the hydrogen distribution within the compartments. The authors concluded that 3-D CFD was required to determine the existence of flammable gas mixtures during the initial phase of the accident scenario.

The following points were addressed in the discussion:

- Application of CFD codes for analysis of steam and hydrogen distribution in nuclear power plants is increasing (using both specific in-house codes as well as commercial codes).
- Ongoing experiments such as ISP-47 will increase confidence in the use of CFD codes, mainly in the area of condensation modelling and scaling effects.
- Regulatory bodies still rely more on lumped parameter codes to evaluate the efficiency of mitigation measures in the case of beyond design basis accidents.
- 'Best estimate' calculations performed with simplified codes should be associated with evaluation of uncertainties; this step is usually not performed.
- The demonstration of conservatism in a simplified approach using lumped parameter codes is not always convincing because local effects are neglected.
- At the present stage of development, CFD code results are mainly used for qualitative analysis.
- CFD analysis is very useful to identify specific issues that would need further detailed investigation.
- CFD codes could also be used to improve the simplified lumped parameter approaches used up to now.
- As a long term objective, the complementary use of system codes and CFD codes should be considered.

2.6. SESSION 6: COMBUSTION

The following three presentations were made in this session, although the subject of combustion had also appeared in earlier presentations:

- *Use of a Finite-Volume Scheme for the Simulation of Hydrogen Explosions*, by A. Beccantini (CEA) and P. Pailhories (IRSN), France;
- *CFD – Application to Reactor Safety Problems with Complex Flow Regimes*, by A.K. Rastogi, Becker Technologies GmbH, Germany;
- *Multi-level Modelling in CFD Coupled with Sodium Combustion and Aerosol Dynamics in Liquid Metal Reactor*, by A. Yamaguchi, T. Takata and Y. Okano, Japan Nuclear Cycle Development Institute, Japan.

Pailhories described in some detail the background to the combustion models embodied in the CREBCOM suite, developed originally at the Kurchatov Institute in Moscow and now implemented in the TONUS CFD code. The model equations are Eulerian, which makes them amenable to well developed numerical methods for hyperbolic equations. Some validation cases in the main combustion areas of interest were presented and a plant sized application described. Ongoing work proceeds within the framework of the HYCOM European Project.

The method was demonstrated to be trustworthy for detonation and for slow and fast deflagration regimes.

Rastogi described current work being undertaken using STAR-CD in the areas of combustion and condensation modelling. Simulations involving condensation were carried out in the context of the ThAI experimental facility, wall condensation being modelled by implementation of the Uchida correlation for the heat/mass condensation rate. Given the limitations of the computer hardware resources, only a coarse mesh simulation could be attempted; this did, however, demonstrate the potential of the approach, and its (again, potential) superiority over lumped parameter approaches. The presentation sparked off a lively discussion concerning the general lack of standard models for wall condensation in commercial CFD software. Application of combustion models incorporated in the in-house code BASSIM showed encouraging results compared with the experimental data obtained from the Battelle Model Containment tests. There was no audience discussion on this part of the presentation.

There is currently very little work on sodium fires outside of Japan; it was therefore encouraging to hear the presentation of Yamaguchi, who showed that such issues require the use of very sophisticated tools like CFD. Commercial CFD software did not feature in the approach, and the power of in-house, special-effect approaches was convincingly demonstrated. Sodium is chemically reactive with both hydrogen and oxygen, and the production and transport of hazardous aerosols also needs to be taken into account. The detailed modelling of the complex physics required to describe the phenomena, and the attention to detail, was impressive.

Overall, the potential of using CFD techniques to quantify containment combustion issues was reinforced, although there was clear evidence that there is a need for the physical models to be improved. Reactor containments are large, multi-compartment structures, so 3-D, often time-dependent, simulations are required, and simulation of combustion, of the type encountered in reactor containments, remains a challenging area for state of the art CFD codes. It should not be forgotten – and the point was made several times – that the codes are only as good as the models within them, and one should not be dazzled by spectacular successes of CFD in the automotive and aerospace industries, where the essential complication is geometric complexity rather than difficult physics. Application of CFD to reactor simulation is still very much in its infancy and there is a definite need to develop appropriate closure laws and to validate predictions against quality experimental data.

2.7. SESSION 7: TWO-PHASE MODELLING AND OTHER ADVANCED METHODS

Five papers were presented in this session:

- *Modelling of Local Two-phase Flow Parameters in Upward Subcooled Flow Boiling with the CFX-4.3 Code*, by B. Končar and B. Mavko (presented by I. Kljenak), Jožef Stefan Institute, Slovenia;

- *Coupling the RELAP-3D© Systems Analysis Code with Commercial and Advanced CFD Software*, by R.R. Schultz and W.L. Weaver, Idaho National Engineering and Environmental Laboratory, USA;

- *First Experience in Developing and Applying the NEPTUNE Code: A Two-phase CFD Tool for Reactor Safety Analysis*, by D. Bestion et al. (CEA), M. Boucker and A Laporta (Electricité de France), France ;

- *3D Unified CFD Approach to Thermalhydraulic Problems in Safety Analysis*, by V. Chudanov, A. Aksenova and V. Pervichko, Nuclear Safety Institute, Russian Academy of Sciences;

- *CFD Application in Canadian Nuclear Society*, by A. Delja, Canadian Nuclear Safety Commission.

The paper by Končar and Mavko described an example of the modification of a commercial CFD code with the aim of predicting nucleate boiling. The approach led to reasonable agreement with the experimental reality; however, it is not unrelated to the current approach used in system codes, where averaging and use of empirical constants is necessary. Therefore the advantage of a 'CFD approach' in such conditions is not evident.

Schultz and Weaver dealt with an attempt to connect a system code with a CFD code. The CFD was 'called into operation' only for restricted zones of the modelled system during assigned periods of times where greater prediction detail for the phenomenon concerned was needed. A preliminary assessment of the coupled code was presented.

Bestion et al. presented a summary of the current status of activities at CEA–Grenoble derived from a large scale effort in the area of 'advanced' two-phase modelling lasting several years and involving several researchers. The problems encountered were mentioned together with preliminary results achieved regarding the prediction of physical phenomena (e.g. pressurized thermal shock (PTS)) that are considered main targets for the development of the new techniques. It was clear that it will not be possible to reach a full solution to the problem of a two-phase CFD or two-phase open media approach for a few more decades.

Chudanov presented a paper summarizing the effort made by the Russian Academy of Sciences in the area of modelling multiphase systems. A wide range of applications and results were discussed, ranging from core melt progression to single-phase 3-D predictions. The limited connection with other Russian activities was emphasized during the discussion, and that different rather than 'unified' (as the title would imply) approaches were described in the presentation.

Delja presented the current status and intentions of the Canadian Nuclear Regulatory Body in the area of CFD applications.

The session was oriented towards future developments even though the first two papers presented current achievements. The authors of the second paper could not attend the meeting but, in addition to their paper, submitted a poster describing the activity performed. The chairman gave a short outline of the contents of the paper.

It is clear from the presentations that a mature method for two-phase CFD does not exist and is not envisaged in the near future. State of the art reports in the area have recently been completed; one such report, mentioned in the presentation by Bestion et al., is that of the European Union's EUROFASTNET project. It is suggested that, considering the long time scale expected for the development of a reasonable code in the area, a comprehensive list of open questions be formulated, rather than attempting to solve a myriad of 'separate effect phenomena' connected with specific 3-D situations.

2.8. POSTER SESSION 1: PRIMARY SYSTEM APPLICATIONS

Poster Session 1, devoted to primary system applications, was closely connected to Sessions 2 and 3 of the meeting. It provided some complementary information and, more particularly, investigated five areas:

- Mixing and/or convection problems in specific geometries (core, pools);
- The application of CFD codes to liquid metals;
- The extension of CFD codes to the detailed modelling of two-phase flows;
- The question of code assessment;
- The problem of CFD code coupling with system codes (generally based on 1-D approaches).

2.8.1. Mixing and/or convection in specific geometries

Participants from Hungary presented the following two posters related to applications of CFD codes to specific geometries encountered in NPPs:

- *Detailed CFD Analysis of Coolant Mixing in VVER-440 Fuel Assemblies with the Code CFX-5.5*, by A. Aszódi and G. Légrádi, Budapest University of Technology and Economics, Hungary;
- *Detailed CFD Analysis of Natural Circulation in the RPV and the Cooling Pond of VVER-440 Type Reactors in Incidental Conditions during Maintenance*, by G. Légrádi and A. Aszódi, Budapest University of Technology and Economics, Hungary.

Both were related to the WWER-440 and presented calculations that hade been carried out by using the commercial code CFX.

The study documented on the first poster by Aszódi and Légrádi was performed in connection with the power uprating of a WWER-440. The poster illustrated the capability of the CFD code to investigate in detail very complex situations such as the flow in a fuel assembly around spacer grids. The use of CFD codes allows predictive calculations of flow mixing between the core channels to be done. This represents significant progress since, up to now, the usual way to calculate the flow mixing in a core was to use a subchannel code with empirical mixing coefficients fitted on full-scale experiments. The question of the level of confidence in these calculations nevertheless remains open.

The subject of the second poster was related to safety improvements in shutdown situations during maintenance. The application consisted mainly of 3-D calculations of natural convection in ponds to define whether the reactor pond cooling system was capable or not of removing the reactor residual power. A significant point that deserves mention is that the negative answer provided by the calculations was used to decide (or at least contributed to the decision) on the modification of the reactor cooling system. This point clearly illustrates the fact that CFD calculations may be used in a safety related decision process. Nevertheless, we may assume that, had the CFD calculations predicted that the pond cooling system would be capable of removing the reactor residual power, experimental confirmation would have been sought.

2.8.2. Application of CFD codes to liquid metals

Two posters were related to the application of CFD codes to liquid metal:

- *Computational Fluid Dynamics applied to Heavy Liquid Metals*, by B. Arien, Centre d'Etude de l'Energie Nucléaire (CEN-SCK), Belgium;
- *Computational Fluid Dynamics Code System for Liquid Metal Cooled Reactor Safety Analysis*, by A. Yamaguchi (JNC) and H. Ninokata (Tokyo Institute of Technology), Japan.

Both brought to light the fact that, due to the low Peclet number, the usual turbulence models used in commercial CFD codes are not adequate for liquid metal applications.

The investigation presented by Arien was related to the development of new systems or concepts such as: accelerator driven systems (ADS) and new fast reactor design. The poster was composed of two parts. The first part presented an international effort initiated within the Fifth Framework Programme of the European Commission to assess the state of the art in the field of CFD applied to heavy metals. The work consisted mainly of benchmarks; the preliminary conclusions were that R&D was still necessary in three areas to improve the predictive capabilities of CFD codes:

– the first area concerns the turbulence models, which have to take into account the fact the Reynolds analogy is not valid for liquid metal;

– the second one is related to the calculation of free surface, which must be precisely performed for ADS;

– the last area regards the calculation of two-phase flows since gas injection is currently used as a pumping mechanism or to prevent pressure waves in ADS.

This work illustrates an assessment methodology that could be followed in other domains in which CFD codes are used.

The second part of the poster presented CFD calculations related to an experimental ADS project called MYRRHA. Two complementary messages were conveyed by the author:

– the first message was that, as for other applications, the question of coupling CFD codes to 1-D system codes had to be addressed;

– the second was that, in general, we were not yet in a position in which confidence in CFD calculation was great enough to assess the safety of a design without experimental confirmation.

The poster by Yamaguchi and Ninokata concerned the general safety of sodium fast-breeder reactors. The poster had two parts:

– The first part provided a general description of the code system developed and used by JNC for safety studies. This system contains about ten codes, of which at least three or four correspond to what we call CFD codes.

– The second part illustrated the capability of two CFD codes belonging to the above mentioned system to investigate reactor accidents or incidents that had occurred in operating plants.

A fluid structure analysis carried out with the SPLASH code showed the reason for the sodium leakage that occurred in the MONJU accident. A thermal stripping analysis carried out with the DINUS code explained the reason for cracks in the PHENIX reactor. Besides demonstrating the usefulness of CFD tools for investigating safety problems, the authors mentioned the initiation in Japan of co-ordinated deliberations and/or actions to evaluate CFD results, and recommended establishing international collaboration on these topics.

2.8.3. Extension of CFD to detailed two-phase flow

Two posters were devoted to detailed two-phase flow:

- *Modelling of the Multidimensional Phase Distribution in a BWR Fuel Assembly*, by H. Anglart, Westinghouse Atom AB, Sweden;
- *Constitutive Laws for Interaction of Gas Bubbles within the Liquid Flow Field – Modelling and Experimental Basis*, by D. Lucas et al., Forschungszentrum Rossendorf e.V., Germany.

These posters dealt with bubbly flows in near 1-D conditions; they illustrated the fact that current measurement capabilities allow work to progress in this area, and that some basic phenomena are now well understood. In addition, they demonstrated that some aspects of two-phase flow may be reasonably well predicted by advanced models. Nevertheless, it is clear that the level at which it will be possible to cover all phenomena in this field is far from having been reached. A lot of work in terms of experimentation, model development and assessment remains to be done before practical applications in safety studies can take place.

2.8.4. CFD code assessment

The following two posters from Italy were especially devoted to code assessment:

- *Application of TRIO_U Code to the Analysis of Stationary Flows in a Circular Pipe*, by F. Moretti, D. Mazzini and F. D'Auria, University of Pisa, Italy;
- *Study of Turbulent Heat Transfer in a Rectangular Channel by TRIO_U Code*, by D. Mazzini, F. D'Auria and P. Vigni, University of Pisa, Italy.

These did not define any general methodology, but illustrated the typical actions to be carried out in a CFD code assessment process. Both were related to problems of stratification, flow mixing and pressurized thermal shock, and in both cases the TRIO_U code was used (an in-house code developed in France by CEA).

Moretti et al. dealt with the solution of a basic benchmark problem for in-pipe flow in laminar and turbulent conditions. D. Mazzini et al. illustrated the kind of preliminary work that is required when handling a particular code for the first time and investigating its characteristics and capabilities, and the applications that it is best suited for. This work was initiated in the context of a PTS study. It consisted of calculations carried out with a very simplified reactor pressure vessel (RPV) geometry. This study further aimed at defining a suitable methodology for coupling TRIO_U with a 1-D system code (RELAP5).

2.8.5. CFD coupling to 1-D codes

One poster concentrated specifically on the topic of CFD coupling to 1-D codes, namely:

- *Benchmarking Simulations with CFD to 1-D Coupling*, by H. Gibeling, J. Mahaffy, The Pennsylvania State University, USA.

This poster was related to a question raised in connection with several applications presented in the other sessions. It addressed complex system calculations where only one part required a 3-D CFD calculation. The authors identified a list of questions to be addressed and provided recommendations to be followed in the process of assessing coupling techniques between a 3-D CFD code and a 1-D system code.

2.8.6. Concluding comments

Several messages can be directly or indirectly derived from Poster Session 1:

- CFD tools have large investigative capabilities (especially for detailed analyses).
- Both commercial and in-house tools are used in safety applications.
- In the case of complex situations encountered in safety applications, the definition of boundary conditions raises the problem of CFD code coupling with other codes (especially 1-D system codes).
- The extension of CFD approaches to two-phase flows is at a very preliminary stage.
- In general, the question of the validity of results, namely of the related qualification level, is not fully addressed (adequacy of turbulence model, adequacy of numerical scheme, adequacy of meshing).There is a need for a co-ordination of actions that have already been initiated in different contexts to provide CFD code users with state of the art reports and the latest developments in assessment methodologies.CFD codes are mature for use in physical investigations; their maturity for safety demonstration purposes remains an open question.

2.9. POSTER SESSION 2: CONTAINMENT AND SEVERE ACCIDENT APPLICATIONS

Six papers were presented in this session:

- *Coupled RELAP5/GOTHIC Model for Accident Analysis of the IRIS Reactor*, by D. Grgić, T. Bajs (University of Zagreb, Croatia), L. Oriani and L.E. Conway (Westinghouse Electric Company, USA);
- *SIMMER-III Applications to Reactor Accident Analysis*, by T. Cadiou (CEA, France), W. Maschek, and A. Rineiski (FZK, Germany);
- *Chemical Reaction Models in a Code of the SIMMER-Family*, by D. Wilhelm, FZK, Germany;
- *CFD Analysis of Passive Containment Cooling by Falling Film Evaporation*, by W. Ambrosini, N. Forgione and F. Oriolo, University of Pisa, Italy;
- *Safety Analyses using CFD Code and its Application to a System Code "IMPACT-SAMPSON" for Severe Accident Analysis*, by M. Naitoh, T. Ikeda, H. Ujita, T. Morii (Nuclear Power Engineering Corporation) and T. Mitsuhashi (Fuji Research Institute Corporation), Japan;
- *Experimental Results for Condensing Jets*, by T. Eden, J. Mahaffy, The Pennsylvania State University, USA.

These covered the following topics:

- Linkage between a system code and CFD code;
- Description of a code;
- Description of code validation;
- Experimental results for use in code validation.

In the long term, the most valuable result from these papers may be the references and direct data supplied for use in validation of future CFD codes.

Grgić et al. provided a brief description of the proposed IRIS (Generation IV) design, and a description of a method to link RELAP5 simulation of the plant with GOTHIC simulation of the containment. The methodology applied to an SBLOCA scenario. In this particular application GOTHIC was run in a lumped parameter rather than CFD mode.

The paper by Cadiou et al. provided a brief summary of the history and contents of SIMMER-III. It next gave a description of the fuel pin model and some heat transfer assessment. Finally, capabilities and validation tests were described for Sodium Cooled Reactors, Gas Cooled Reactors, a Critical Burner Reactor, Accelerator Driven Systems, and a Fusion Reactor Cooling Blanket.

The paper by Wilhelm described models implemented in AFDM, a predecessor of SIMMER-III. It provided a clear description of the four-step solution algorithm also used in SIMMER III, and the specific entrainment and oxidation models developed within AFDM. The modelling approach is justified through a review of the relevant physical phenomena in the DISCO experiment, and assessment against the DISCO experiment is presented. Hydrogen from oxidation was all burned in the containment, resulting in containment pressure predictions that matched well with the experiment.

M. Naitoh et al. summarized a suite of codes used for severe accident analysis. PLASHY, a 3-D CFD code, has an interesting combination of QUICK based momentum equations, and first order upwind mass and energy equations. It has been built for parallel computing, using domain decomposition. Validation was shown for ISP-43 (boron dilution). FLAVOR is a structural code that can be used in conjunction with PLASHY for fluid structure interactions. Validation was provided against core barrel and aluminium tube vibration data. CAPE calculates fuel bundle critical power for a boiling water reactor (BWR), and was validated against a large set of data. SAMPSON is a severe accident code with validation against ISP-45 (hydrogen generation) and ISP-46 (PHEPUS-FPT1, molten core relocation). VESUVIUS is a steam explosion code with validation against KROTOS-44.

Ambrosini et al. provided a description of a simple falling film evaporation experiment. Fluent analysis was described for the experiment, including a parametric study of inclination angle of inlet air flow.

The paper by Eden and Mahaffy described an under-expanded jet experiment, providing data at several flow rates and pressure ratios for the following jet configurations: air jet into air; air jet into water; and steam jet into water.

2.10. GENERAL DISCUSSION

Two main questions were addressed in the discussion:

- Which CFD applications are the most valuable at present?
- What are the most important tasks to be performed for improvement of computer codes?

It was generally stated that a ‘threshold’ time had been reached and CFD codes had become useful tools for reactor safety applications. It was stated in the discussion that CFD codes should be used as a complementary tool in addition to system (lumped parameter) computer codes.

A variety of applications and attempts to solve nuclear safety issues were presented and a number of additional CFD applications indicated. CFD codes provide a unique opportunity to analyse and explain reactor accidents that have occurred in the past. In particular, CFD technology may be used to assess criticality accidents. Such applications are important to prevent reoccurrence of the same events in the future. CFD codes can be used to identify plant vulnerabilities and possible risky operational regimes in NPPs, with the aim of warning operators to avoid such regimes. This kind of use may not require a special validation effort and is very cost effective. Another area for CFD applications is the investigation of loads on structures in the water pools of BWR containments. A detailed study of fission product transport in the vicinity of leakages from a confinement could possibly also be performed by means of CFD codes. CFD codes can also be used to study natural circulation phenomena, for example in the case of severe accidents. Another CFD application is the study of temperature fluctuations in nuclear components, which is important for analysis of thermal fatigue.

The use of commercial (general purpose) codes for nuclear safety applications is not always straightforward since complicated fluid–structure interactions are often not adequately taken into account. Closer co-operation between experimentalists and code developers with a view to further improving the codes would be useful. To accelerate the progress, it is necessary to utilize experience from non-nuclear applications of CFD codes and to build up specific ‘nuclear’ experience. The distinction should be made in CFD applications between design basis and beyond design basis accidents. However, it should be taken into account that many issues that originated in the beyond design basis accident area are becoming a part of design issues, such as hydrogen distribution and treatment. All issues related to design basis accidents are of higher importance; these include analysis of reactivity initiated accidents of a 3-D nature (boron mixing) and pressurized thermal shock. More experimental data are needed for further validation of the codes for this area.

Since computer power is increasing, more powerful tools can be envisaged in the near future. It is important in the use of CFD codes to distinguish between physical mixing (diffusion) and numerical diffusion; numerical diffusion is, in general, a big issue. There are methods available to quantify numerical diffusion; in this respect, lessons should be learned from non-nuclear applications. The options available to the user should be eliminated to the extent possible. A possible way to avoid numerical problems would be the broader use of adaptive techniques: the first task would be to eliminate numerical errors and, thereafter, to improve physical models. For CFD codes, it is necessary to demonstrate convergence of the solution with a reduced mesh size.

For the future, it is important to take actions towards minimizing user effects (for example, by means of user guidelines), to control numerical schemes (numerical schemes should be ‘neutral’) and to address scaling effects. Guidelines from non-nuclear applications can be used. The use of CFD codes in the single-phase domain is quite mature. There is still a long way to go before the use of CFD codes for two-phase application is mature; however, the remaining problems related to their use in single-phase applications should be resolved first.

The application of CFD codes for steam/hydrogen distribution has been improved significantly, but validation is not as extensive as for boron dilution and the results are more of a qualitative value, useful for the identification of needs for further analysis.

An effort is now needed to take steps towards more reliable applications, including experimental validation of codes and improvement of models. Specification of further steps towards the qualified use of CFD codes is needed. A strategy needs to be developed for CFD code assessment. The development of guidelines would help to maintain competence. It is advisable for CFD applications to be associated with a statement regarding the code assessment and the uncertainties. Also in the use of CFD codes, the problem of scaling remains; this is problem dependent, and only in some specific cases (for example, for combustion) has it been adequately addressed. In the specific case of combustion, experience from non-nuclear (off-shore) industry can be utilized to some extent. For code assessment, lessons learned from system codes should be used; for example, validation matrices should be specified for all applications.

3. CONCLUSIONS AND RECOMMENDATIONS

3.1. CONCLUSIONS

(1) CFD codes are being applied increasingly for various purposes; it was demonstrated that these codes have a broad potential for qualitative assessment in areas in which traditional methods (lumped-parameter or 1-D simulations) are inadequate.

(2) CFD codes are capable of calculating local parameters. Due to this capability they provide insights into many problems, contribute to a deeper understanding of flow physics, and thus lead to better designs at reduced cost and/or to more precisely quantified safety margins. In nuclear safety, CFD codes thus have a complementary role to play in combination with system (lumped parameter) computer codes, particularly in those areas where multidimensional aspects are important. Combined applications, supported by proper experiments, may guarantee a more precise evaluation of safety margins.

(3) CFD applications have gained significantly from increased computer power but, in the case of some nuclear applications, very long computation times are still limiting the use of the technology. With the further increase of computer power and improved numerical methods, the usage and application of CFD in nuclear safety can be expected to increase.

(4) Single-phase CFD applications are already reasonably mature. Nevertheless, some models (for example, for turbulence and combustion) require improvement. Two-phase CFD modelling is still rudimentary and requires a considerable research effort even though some aspects of two-phase flow may already be reasonably well predicted by advanced models. Nevertheless, it is clear that in this field much work in terms of experimentation, model development and assessment remains to be completed before practical applications in nuclear safety studies can be attempted.

(5) In order to be able to address uncertainties, careful validation of the CFD codes is necessary for any nuclear safety application. For an adequate validation, it is necessary to assess existing experiments with respect to the availability of local, three dimensional measurements and the definition of initial and boundary conditions. Furthermore, suitable verification and validation of two-phase flow models will most likely require a separate experimental programme tailored to nuclear reactor safety specific flow phenomena.

(6) CFD methodology has the potential to address safety concerns related to local boron dilution, pressurized thermal shock and other phenomena related to primary system mixing. A more systematic approach to this subject will be essential for increased acceptance of CFD results in the nuclear community.

(7) The number of applications of CFD codes for analysis of steam and hydrogen distribution in reactor containments is also increasing (using both specific in-house codes as well as commercial codes). These CFD applications are very useful to identify specific issues that would need further investigation; however, at the present stage of development, CFD code results are mainly used for qualitative analysis in this area.

(8) The applicability of CFD methodology to various aspects of severe accidents was convincingly demonstrated; continuation of this work and further progress are encouraged.

(9) In some cases, CFD code applications are more advanced in other areas than they are in the nuclear field.

3.2. RECOMMENDATIONS

(1) Commonly accepted quality and performance criteria for the assessment of CFD results, and methods for nuclear reactor safety applications have to be established. Such criteria are necessary to reliably demonstrate to end users, utilities and regulatory agencies the extent to which CFD can enhance the accuracy of safety analyses.

(2) To this end, Best Practice Guidelines on the consistent use of CFD methods for reactor safety problems have to be established. (A first step in this direction has already been undertaken in the context of the European Union's Fifth Framework Programme ECORA.) These guidelines should address geometry and grid generation, consistent boundary condition specification, the selection of physical models, and choice of solution algorithms.

(3) The Guidelines are necessary for the formalized judgement of experimental and numerical results, thus ensuring a consistent evaluation of CFD simulations. An essential aspect of the general quality assurance of CFD flow simulations is the quantification of iteration, solution and model errors as well as the determination of those software components (numerical grid, discretization schemes, or two-phase flow and turbulence models) responsible for disagreement between measured data and calculations.

(4) There is a need for the systematic assessment of CFD codes. In order to improve our knowledge of the capabilities and features of the CFD approach, it is recommended to organize code benchmarking, based on code-to-code and code-to-experiment comparisons, for generic situations related to nuclear safety problems. Moreover, this activity will provide input for the user guidelines and improve the expertise of CFD code users.

(5) Experience from code assessment and user guidelines from outside the nuclear field should be used for nuclear applications with the exception of neutronic feedback, which is specific to reactors. The exchange of information and collaboration with experts in other fields are recommended. In particular, single-phase applications, in which the geometric complexity is the only challenging issue, are dealt with quite successfully these days using commercial CFD software, although further improvements need to be made in the turbulence modelling area.

(6) Research efforts related to two-phase CFD applications should be continued as a long term task in order to extend the domain of applicability of the codes to typical accident conditions. For the near future, it is suggested that, considering the long time scale expected for the development of a reliable code, a comprehensive list of open questions be formulated, rather than attempting to solve a large number of 'separate-effect phenomena' connected with specific three dimensional situations.

(7) In the case of system codes, the problem of the lack of understanding of fundamental two-phase flow phenomena could, to a large extent, be resolved through the careful application of trustworthy correlations. For two-phase CFD modelling, instead of applying correlations, appropriate small-scale models that may be used in a multidimensional, multi-scale environment should be developed and be well validated against experimental data. The development of such models involves a very strong commitment on the part of the nuclear CFD community, but could be facilitated in part by examining similar activities in the chemical and process industries. A multi-disciplinary approach in this area is essential.

(8) On account of the intensive ongoing work in the area of CFD code development and applications, it is recommended that an international meeting on this subject be organized in about four years time to monitor progress specifically related to nuclear safety.

ABBREVIATIONS

ADS	Accelerator driven system
BWR	Boiling water reactor
CFD	Computational fluid dynamics
DNS	Direct numerical simulation
FDS	Fire Dynamics Simulator
ISP	International Standard Problem
LBLOCA	Large break loss of coolant accident
LES	Large eddy simulation
LMFR	Liquid metal fast reactor
NPP	Nuclear power plant
NRS	Nuclear reactor safety
PAR	Passive autocatalytic recombiner
PTS	Pressurized thermal shock
PWR	Pressurized water reactor
RPV	Reactor pressure vessel
SBLOCA	Small break loss of coolant accident
VVER or WWER	Water moderated, water cooled power reactor (Russian design)

ORGANIZING COMMITTEE AND SESSION CHAIRPERSONS

D'Auria, F.	University of Pisa, Italy
Durin, M.	Institut de radioprotection et de sûreté nucléaire, France
Mahaffy, J. H.	The Pennsylvania State University, United States of America
Micaelli, J.-C.	Institut de radioprotection et de sûreté nucléaire, France
Mišák, J.	International Atomic Energy Agency
Réocreux, M.	Institut de radioprotection et de sûreté nucléaire, France
Royen, J.	Nuclear Energy Agency of the Organisation for Economic Co-operation and Development
Sandervåg, O.	Swedish Nuclear Power Inspectorate (SKI), Sweden
Scheuerer, M.	Gesellschaft für Reaktor- und Anlagensicherheit (GRS) mbH, Germany
Smith, B.	Paul Scherrer Institut, Switzerland
Téchy, Z.	VEIKI Institute for Electric Power Research, Hungary
Vitale, E.	University of Pisa, Italy

LIST OF PARTICIPANTS

BELGIUM

M.B. Arien
CEN/SCK, Boeretang 200, B-2400 Mol
Tel.: (+32-14) 33 22 56
Fax: (+32-14) 31 89 36
E-mail: barien@sckcen.be

S. Keijers
Thermal-hydraulics and Severe Accidents,
Safety and Systems Department, Tractebel Energy Engineering,
Avenue Ariane, 7, B-1200 Brussels
Tel.: (+32-2) 773 98 41
Fax: (+23-2) 773 89 00
E-mail: steven.keijers@tractebel.com

BRAZIL

P.A.B. de Sampaio
Instituto de Engenharia Nuclear Comissão Nacional de Energia Nuclear (CNEN),
Via 5 s/n, Cidade Universtãria – Ilha do Fundão,
Caixa Postal 68550, 21945-970 Rio de Janeiro – RJ
Tel.: (+55-21) 25604113 ext. 2157
Fax: (+55-21) 22098059 *or* 25902692
E-mail: sampaio@ien.gov.br

CANADA

A. Delja
Plant Thermal Hydraulics Division,
Directorate of Assessment and Analysis,
Canadian Nuclear Safety Commission,
280 Slater Street, P.O. Box 1046, Station B,
Ottawa, Ontario, K1P5S9
Tel.: (+1-613) 947 6033
Fax: (+1-613) 995 5086
E-mail: Deljaa@cnsc-ccsn.gc.ca

M. Krause
Containment and Thermalhydraulics Branch,
Atomic Energy of Canada, Chalk River Laboratories,
Chalk River, Ontario, K0J 1J0
Tel.: (+1-613) 584 8811 (ext. 6515)
Fax: (+1-613) 584 4200
E-mail:krausem@aecl.ca

CHINA

S. Zhang
Nuclear Power Institute of China (NPIC),
P.O. Box 436, Chengdu, Sichuan
Tel.: (+86-28) 85582199 ext. 33171
Fax: (+86-28) 85903103 *or* 85903171
E-mail:zhangsr@npic.ac.cn *or* zhangsr_1@elong.com

CROATIA

T. Bajs
University of Zagreb,
Faculty of Electrical Engineering and Computing
Unska 3, HR-10000 Zagreb

Tel.: (+385-1) 6129 994
Fax: (+385-1) 61 29 890
E-mail:tomislav.bajs@fer.hr

D. Grgić
University of Zagreb,
Faculty of Electrical Engineering and Computing,
Unska 3, HR-10000 Zagreb

Tel.: (+385-1) 6129 994
Fax: (+385-1) 6129 890
E-mail:davor.grgic@fer.hr

CZECH REPUBLIC

P. Mühlbauer
Nuclear Research Institute Řež plc,
Department of Thermal-hydraulic Analyses,
CZ-250 68 Řež

Tel.: (+420-2) 6617 2376
Fax: (+420-2) 6617 2334
E-mail: muh@ujv.cz

FINLAND

T.S. Toppila
Fortum Nuclear Services Ltd,
Rajatorpantie 8, P.O. Box 10, FIN-00048 Fortum

Tel.: (+358-10) 453 2364
Fax: (+358-10) 453 3403
E-mail:timo.toppila@fortum.com

FRANCE

Y. Abou-Rjeily
Institut de Radioprotection et de Sûreté Nucléaire (IRSN),
B.P. 16, F-92262 Fontenay aux Roses Cedex

Tel.: (+33) 1 58 35 79 21
Fax: (+33) 1 58 35 95 99
E-mail:yves.abourjeily@irsn.fr

D.J. Bestion
Commissariat à l'Energie Atomique DEN/DTP/SMTH,
17 rue des Martyrs, F-38054 Grenoble Cedex 9

Tel.: (+33) 4 38 78 36 45
Fax: (+33) 4 38 78 94 53
E-mail:dominique.bestion@cea.fr

U. Bieder
Commissariat à l'Energie Atomique DTP/SMTH,
17 rue des Martyrs, F-38054 Grenoble Cedex 9

Tel.: (+33) 4 38 78 95 14
Fax: (+33) 4 38 78 50 36
E-mail: ulrich.bieder@cea.fr

T. Cadiou
Commissariat à l'Energie Atomique DER/SERI,
Centre d'Etudes de Cadarache, Bât. 212,
F-13108 St. Paul lez Durance Cedex

Tel.: (+33) 4 42 25 66 17
Fax: (+33) 4 42 25 71 87
E-mail: cadiou@drncad.cea.fr *or* cadiou@monet.cad.cea.fr

P. Dietrich
Institut de Radioprotection et de Sûreté Nucléaire (IRSN),
DPEA/SEAC, B.P. 6,F-92265 Fontenay-aux-Roses Cedex

Tel.: (+33) 1 58 35 81 99
Fax: (+33) 1 46 54 85 59
E-mail: philippe.dietrich@irsn.fr

P. Dolleans
Framatome–ANP SAS, Tour Framatome,
1 place de la Coupole, F-92084 Paris La Defense

Tel.: (+33) 1 47 96 50 99
Fax: (+33) 1 47 96 01 48
E-mail: pdolleans@framatome-anp.com

F. Dubois
Institut de Radioprotection et de Sûreté Nucléaire (IRSN),
B.P. 16, F-92262 Fontenay aux Roses Cedex

Tel.: (+33) 1 58 35 98 97
Fax: (+33) 1 47 46 86 76
E-mail: franck.dubois@irsn.fr

M. Durin
Institut de Radioprotection et de Sûreté Nucléaire (IRSN),
DPEA/SEAC, B.P. 6, F-92265 Fontenay-aux-Roses Cedex

Tel.: (+33) 1 58 35 81 83
Fax: (+33) 1 46 54 32 64
E-mail: michel.durin@irsn.fr

J.-C. Micaelli
Institut de Radioprotection et de Sûreté Nucléaire (IRSN),
Département de Recherches en Sécurité (DRS)/SEMAR,
B.P. 3, F-13115 Saint-Paul lez-Durance Cedex

Tel.: (+33) 4 42 25 72 49
Fax: (+33) 4 42 25 29 29
E-mail: jean-claude.micaelli@irsn.fr

H. Mutelle
Institut de Radioprotection et de Sûreté Nucléaire (IRSN),
Département de Prévention et d'Etude des Accidents,
Service d'Etudes sur les Accidents,
Laboratoire de Physique des Accidents Graves,
B.P. 17, F-92262 Fontenay-aux-Roses Cedex

Tel.: (+33) 1 46 54 83 99
Fax: (+33) 1 46 54 85 59
E-mail: herve.mutelle@irsn.fr

P. Pailhories
Institut de Radioprotection et de Sûreté Nucléaire (IRSN),
DPEA/SEAC, B.P. 6, F-92265 Fontenay-aux-Roses Cedex

Tel.: (+33) 1 58 35 80 32
Fax: (+33) 1 58 35 85 59
E-mail: pierre.pailhories@irsn.fr

M.L. Réocreux
Institut de Radioprotection et de Sûreté Nucléaire (IRSN),
Département de Recherches en Sécurité, Bt. 250, B.P. 3,
F-13115 Saint-Paul lez-Durance Cedex

Tel.: (+33) 4 42 25 31 48
Fax: (+33) 4 42 25 76 79
E-mail:michel.reocreux@irsn.fr

GERMANY

T. Höhne
Forschungszentrum Rossendorf e.V., Institute of Safety Research,
P.O. Box 51 01 19, D-01314 Dresden

Tel.: (+49-351) 260 24 25
Fax: (+49-351) 260 23 83
E-mail: hoehne@fz-rossendorf.de

D. Lucas
Forschungszentrum Rossendorf e.V., Institute of Safety Research,
P.O. Box 51 01 19, D-01314 Dresden

Tel.: (+49-351) 260 2047
Fax: (+49-351) 260 2383
E-mail:D.Lucas@fz-rossendorf.de

A.K. Rastogi
Becker Technologies GmbH,
Kölner Str. 6, D-65760 Eschborn

Tel.: (+49-6196) 936 115
Fax: (+49-6196) 936 199 *or* 100
E-mail:rastogi@becker-technologies.com

P.H.G. Royl
Forschungszentrum Karlsruhe GmbH,
Institut für Kern- und Energietechnik (IKET),
Bau 322, Zi. 164, Hermann-von-Helmholtz-Platz 1,
D-76344 Eggenstein-Leopoldshafen
Postal address:
Postfach 3640,
D-76021 Karlsruhe
Tel.: (+49-7247) 82 2578
Fax: (+49-7247) 82 4332
E-mail:royl@iket.fzk.de

G. Scheuerer
AEA Technology GmbH,
Staudenfeldweg 12, D-83624 Otterfing
Tel.: (+49-8024) 9054 11
Fax: (+49-8024) 9054 17
E-mail: Georg.Scheuerer@cfx-germany.com *or*
G.Scheuerer@t-online.de

M. Scheuerer
Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH
Forschungsgelände Garching, D-85748 Garching
Tel.: (+49-89) 32004-401
Fax: (+49-89) 32004-599
E-mail: Martina.Scheuerer@grs.de *or*
G.Scheuerer@t-online.de

D. Wilhelm
Forschungszentrum Karlsruhe GmbH,
Institut für Kern- und Energietechnik (IKET),
Hermann-von-Helmholtz-Platz 1,
D-76344 Eggenstein-Leopoldshafen
Postal address:
Postfach 3640,
D-76021 Karlsruhe
Tel.: (+49-7247) 826319
Fax: (+49-7247) 825987
E-mail:wilhelm@iket.fzk.de

HUNGARY

A. Aszódi
Budapest University of Technology and Economics,
Institute of Nuclear Techniques,
Műegyetem rakpart 9, H-1111 Budapest
Tel.: (+36) 1 463 1989
Fax: (+36) 1 463 1954
E-mail: aszodi@reak.bme.hu

I. Boros
Budapest University of Technology and Economics,
Institute of Nuclear Techniques,
Műegyetem rakpart 9, H-1111 Budapest

Tel.: (+36) 1 463 1633
Fax: (+36) 1 463 1954
E-mail: boris@reak.bme.hu

G. Légrádi
Budapest University of Technology and Economics,
Institute of Nuclear Techniques,
Műegyetem rakpart 9, H-1111 Budapest

Tel.: (+36) 1 463 1633
Fax: (+36) 1 463 1954
E-mail:legofiu@reak.bme.hu

Z. Téchy
Institute for Electric Power Research Co. (VEIKI),
Gellérthegy u. 17, H-1016 Budapest

Tel.: (+36-1) 457 8245
Fax: (+36-1) 457 8253
E-mail: techy@hella.hu *or*
techy@helka.iif.hu

P. Kostka
Institute for Electric Power Research Co. (VEIKI),
Gellérthegy u. 17, H-1016 Budapest

Tel.: (+36-1) 457 8275
Fax: (+36-1) 457 8253
E-mail:kostka@aed.veiki.hu

INDIA

S.G. Markandeya
Bhabha Atomic Research Centre, Reactor Safety Division,
Engg. Hall No. 7, Trombay, Mumbai 400 085

Tel.: (+91-22) 5593775
Fax: (+91-22) 5505151
E-mail: sgmarkan@magnum.barc.ernet.in

ISRAEL

T.G. Reisin
Soreq Nuclear Research Center, Applied Physics Division,
81800 Yavne

Tel.: (+972-8) 9434287
Fax: (+972-8) 9383157
E-mail: treisin@soreq.gov.il

ITALY

A. Alemberti
Ansaldo Energia, Nuclear Division,
Corso F.M. Perrone, 25, I-16161 Genova

Tel.: (+39-010) 655 8473
Fax: (+39-010) 6401 8473
E-mail: alemberti@ansaldo.it

S. Aliotta
Università di Palermo, Dipartimento di Ingegneria Nucleare,
Viale delle Scienze, I-90128 Palermo

Tel.: (+39-091) 232252
Fax: (+39-091) 232215
E-mail: saliotta@din.unipa.it

W. Ambrosini
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa

Tel.: (+39-050) 8366 73
Fax: (+39-050) 8366 65
E-mail: walter.ambrosini@ing.unipi.it

D. Araneo
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa

Tel.: (+39-050) 8366 57
Fax: (+39-050) 8366 65
E-mail: dino.araneo@studenti.ing.unipi.it

E. Baglietto
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione, Via Diotisalvi, 2,
I-56126 Pisa

At present at:
Tokyo Institute of Technology,
Research Institute of Technology,
2-12-1 O-okayama, Meguro-ku, Tokyo 152-8550,
Japan

Tel.: (+81-090) 6115-2395 *(mobile)*
E-mail:01D51276@nr.titech.ac.jp

B. Bordini
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa

Tel.: (+39-050) 8366 1
Fax: (+39-050) 8366 65

M. Casamirra
Università di Palermo,
Dipartimento di Ingegneria Nucleare,
Viale delle Scienze, I-90128 Palermo

Tel.: (+39-091) 232252
Fax: (+39-091) 232215
E-mail: mdcasamirra@din.unipa.it

A. Bousbia
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa

Tel.: (+39-050) 8366 1
Fax: (+39-050) 8366 65
E-mail: b.salah@ing.unipi.it

F.S. D'Auria
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa

Tel.: (+39-050) 8366 53
Fax: (+39-050) 8366 65
E-mail: dauria@ing.unipi.it

F. De Rosa
ENEA,
Italian National Agency for New Technologies,
Energy and the Environment, FIS/NUC
Via Martiri di Monte Sole 4, I-40129 Bologna

Tel.: (+39-051) 6098715
Fax: (+39-051) 6098279
E-mail: derosa@bologna.enea.it

F. Di Cuia
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione, Via Diotisalvi, 2, I-56126 Pisa

Tel.: (+39-333) 2977518
Fax: (+39-050) 8366 65
E-mail: calsollima@tiscali.it

B. Di Maro
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione, Via Diotisalvi, 2, I-56126 Pisa
Tel.: (+39-050) 8366 1
Fax: (+39-050) 8366 65
E-mail: 16604717@studenti.unipi.it

G. Forasassi
President of CIRTEN,
Università di Pisa, Via Diotisalvi,2, I-56126 Pisa
Tel: (+39-050) 8366 15
Fax: (+39-050) 8366 65
E-mail giuseppe.forasassi@ing.unipi.it

N. Forgione
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione, Via Diotisalvi, 2, I-56126 Pisa
Tel.: (+39-050) 8366 57
Fax: (+39-050) 8366 65
E-mail: nicola.forgione@ing.unipi.it

F. Franceschini
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa
Tel.: (+39-050) 8366 1
Fax: (+39-050) 8366 65
E-mail: f_franceschini@hotmail.com

L. Frustaci
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa
Tel.: (+39-050) 8366 1
Fax: (+39-050) 8366 65

F. Inzoli
Politecnico di Milano,
Dipartimento di Energetica,
Piazza Leonardo da Vinci, 32, I-20133 Milano
Tel.: (+39-02) 2399 3883
Fax: (+39-02) 2399 3940
E-mail: fabio.inzoli@polimi.it

M. Leonardi
THEMAS s.r.l.,
Via Rustichello, 8, I-56126 Pisa
Tel: (+39-050) 41384
Fax: (+39-050) 8366 65
E-mail leonardi@ing.unipi.it

G. Lomonaco
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa
Tel.: (+39-050) 8366 1
Fax: (+39-050) 8366 65
E-mail: Guglielmo.Lomonaco@studenti.ing.unipi.it

F. Maggini
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa
Tel.: (+39-050) 8366 1
Fax: (+39-050) 8366 65
E-mail: pollon76@katmail.com

N. Marconi
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa
Tel.: (+39-050) 8366 1
Fax: (+39-050) 8366 65

F. Mattioda
ENEA,
Italian National Agency for New Technologies,
Energy and the Environment, FIS/NUC,
Via Martiri di Monte Sole 4, I-40129 Bologna
Tel.: (+39-051) 6098592
Fax: (+39-051) 6098279
E-mail: mattioda@bologna.enea.it

D. Mazzini
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa
Tel.: (+39-050) 8366 57
Fax: (+39-050) 8366 65
E-mail: d.mazzini@ing.unipi.it

P. Meloni
ENEA,
Italian National Agency for New Technologies,
Energy and the Environment, FIS/NUC,
Via Martiri di Monte Sole 4, I-40129 Bologna

Tel.: (+39-051) 6098521
Fax: (+39-051) 6098279
E-mail: meloni@bologna.enea.it

A. Montazeri
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa

Tel.: (+39-050) 8366 1
Fax: (+39-050) 8366 65

K. Moosavian
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione, Via Diotisalvi, 2, I-56126 Pisa

Tel.: (+39-050) 8366 1
Fax: (+39-050) 8366 65

F. Moretti
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione, Via Diotisalvi, 2, I-56126 Pisa

Tel.: (+39-050) 8366 57
Fax: (+39-050) 8366 65
E-mail: d.mazzini@ing.unipi.it *or*
famo@interfree.it

F. Oriolo
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa

Tel.: (+39-050) 8366 52
Fax: (+39-050) 8366 65
E-mail: oriolo@ing.unipi.it

C. Parisi
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa

Tel.: (+39-050) 8366 1
Fax: (+39-050) 8366 65

F. Pierro
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa

Tel.: (+39-050) 8366 1
Fax: (+39-050) 8366 65
E-mail: 19182915@studenti.unipi.it

G. Pilone
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa

Tel.: (+39-050) 8366 1
Fax: (+39-050) 8366 65
E-mail: giupilone@tiscali.it

M.E. Ricotti
Politecnico di Milano,
Dipartimento di Ingegneria Nucleare,
Via Ponzio, 34/3, I-20133 Milano

Tel.: (+39-02) 2399 6325
Fax: (+39-02) 2399 6309
E-mail: marco.ricotti@polimi.it

A. Rilli
Società Gestione Impianti Nucleari, SOGIN,
Via Torino 6, I-00184 Roma

Tel.: (+39-06) 83040348
Fax: (+39-06) 83040474
E-mail: rilli@sogin.it

G. Saiu
Ansaldo Energia, Nuclear Division,
Corso F.M. Perrone, 25, I-16161 Genova

Tel.: (+39-010) 655 8591
Fax: (+39-010) 6401 8591
E-mail: saiu@ansaldo.it

C. Sollima
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa

Tel.: (+39-333) 2977518
Fax: (+39-050) 8366 65
E-mail: calsollima@tiscali.it

A. Spadoni
Società Gestione Impianti Nucleari, SOGIN,
Via Torino 6, I-00184 Roma

Tel.: (+39-06) 83040468
Fax: (+39-06) 83040474
E-mail: spadoni@sogin.it

J. Vedovi
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa

Tel.: (+39-050) 8366 1
Fax: (+39-050) 8366 65

N. Zaccari
Università di Pisa,
Dipartimento di Ingegneria Meccanica,
Nucleare e della Produzione,
Via Diotisalvi, 2, I-56126 Pisa

Tel.: (+39-050) 8366 1
Fax: (+39-050) 8366 65
E-mail: 19611431@studenti.unipi.it

JAPAN

N. Kimura
New Technology Development Group,
Advanced Technology Division,
Japan Nuclear Cycle Development Institute (JNC),
O-arai Engineering Center, 4002, Narita,
O-arai, Higashi-Ibaraki, Ibaraki 311-1393

Tel.: (+81-29) 267 4141 ext. 5834
Fax: (+81-29) 266 3867
E-mail: kimura@oec.jnc.go.jp

R. Kubota
Industrial Safety Section, Research and Science Division,
Fuji Research Institute Corporation,
2-3 Kandanishiki-Cho, Chiyoda-ku, Tokyo 101-8443

Tel.: (+81-3) 5281 5324
Fax: (+81-3) 5281 5331
E-mail: rkubota@star.fuji-ric.co.jp

M. Naitoh
Advanced Simulation Systems Department,
Nuclear Power Engineering Corporation (NUPEC),
Fujitakanko Toranomon Bldg. 6F, 3-17-1 Toranomon,
Minato-ku, Tokyo 105-0001

Tel.: (+81-3) 4512 2655
Fax: (+81-3) 4512 2699
E-mail: ms-naito@nupec.or.jp

Y. Tobita
Nuclear System Safety Research Group,
Advanced Technology Division, O-arai Engineering Center,
Japan Nuclear Cycle Development Institute,
4002, Narita, O-arai, Higashi-Ibaraki-gun, Ibaraki 311-1393

Tel.: (+81-29) 267 4141 ext. 5662
Fax: (+81-29) 266 3675
E-mail: tobita@oec.jnc.go.jp

A. Yamaguchi
Thermal-hydraulic Research Group,
Advanced Technology Division,
Japan Nuclear Cycle Development Institute (JNC),
O-arai Engineering Center, 4002, Narita,
O-arai, Higashi-Ibaraki-gun, Ibaraki 311-1393

Tel.: (+81-29) 267 4141 ext. 5680
Fax: (+81-29) 266 3675
E-mail:yamaguti@oec.jnc.go.jp

REPUBLIC OF KOREA

T. Kwon
Department of Thermal-hydraulic Safety Research,
Korea Atomic Energy Research Institute (KAERI),
150 Dukjin-Dong, Yuseong-Gu, Taejeon, 305-353

Tel.: (+82-42) 868 8717
Fax: (+82-42) 868 8362
E-mail:tskwon@kaeri.re.kr

LITHUANIA

E. Ušpuras
Lithuanian Energy Institute,
3 Breslaujos, LT-3035 Kaunas

Tel.: (+370-37) 401926
Fax: (+370-37) 351271
E-mail:eugeniju@isag.lei.lt

NETHERLANDS

N.B. Siccama
Nuclear Research and consultancy Group (NRG),
P.O. Box 25, NL-1755 ZG Petten

Tel.: (+31-224) 56 40 34
Fax: (+31-224) 56 84 90
E-mail: siccama@nrg-nl.com

G.L.C.M. Vayssier
Ministry of Housing, Spatial Planning and the Environment,
Nuclear Safety Department,
P.O. Box 16191, NL-2500 BD The Hague

Tel.: (+31-70) 339 2447 *or*
(+31-71) 523 2345
Fax: (+33-71) 523 2341
E-mail:vayssier@hetnet.nl

RUSSIAN FEDERATION

V.V. Chudanov
Nuclear Safety Institute, Russian Academy of Sciences,
52, Bolshaya Tulskaya, RU-113191 Moscow

Tel.: (+7-095) 955 22 34
Fax: (+7-095) 958 00 40
E-mail: chud@ibrae.ac.ru

E.M. Fedorov
Experimental and Design Organization OKB 'Gidropress',
21 Ordzhonikidze street, Podolsk, RU-142103 Moscow Region

Tel.: (+7-0967) 54 25 16 *or*
(+7-095) 502 79 10
Fax: (+7-095) 715 97 83 *or*
(+7-0967) 69 97 83
E-mail: levin@grpress.podolsk.ru *or*
fil@grpress.podolsk.ru

SLOVAKIA

Ľ. Kubišová
Nuclear Regulatory Authority of the Slovak Republic,
Bajkalská 27, P.O. Box 24, SK-820 07 Bratislava 27

Tel.: (+421-2) 58248223
Fax: (+421-2) 53421015
E-mail: kubisova@ujd.gov.sk

M. Krištof
Nuclear Regulatory Authorityof the Slovak Republic,
Okružná 5, SK-918 64 Trnava

Tel.: (+421-33) 5992005
Fax: (+421-33) 5991190
E-mail: kristof@ujd.gov.sk

J. Remiš
VÚJE Trnava, Inc. – Engineering, Design
and Research Organization,
Okružná 5, SK-918 64 Trnava

Tel.: (+421-33) 599 1168
Fax: (+421-33) 599 1708
E-mail:remis@vuje.sk

SLOVENIA

I. Kljenak
Reactor Engineering Division, Jožef Stefan Institute,
Jamova 39, SI-1000 Ljubljana

Tel.: (+386-1) 5885 332
Fax: (+386-1) 5612 335
E-mail: Ivo.Kljenak@ijs.si

SPAIN

M.A. Jiménez García
Universidad Politécnica de Madrid (UPM),
Departamento de Ingeniería Nuclear, ETSI Industriales UPM,
José Gutiérrez Abascal 2, E-28006 Madrid

Tel.: (+34-91) 336 3112
Fax: (+34-91) 336 3002
E-mail: cfdnuc@ctn.din.upm.es

J.M. Martín-Valdepeñas Yagüe
Universidad Politécnica de Madrid (UPM),
Departamento de Ingeniería Nuclear, ETSI Industriales UPM,
José Gutiérrez Abascal 2, E-28006 Madrid

Tel.: (+34-91) 336 3112
Fax: (+34-91) 336 3002
E-mail:cfdnuc@ctn.din.upm.es

SWEDEN

H. Anglart
Westinghouse Atom AB,
Finnslätten, Bränslegatan,
SE-721 63 Väterås

Tel.: (+46-21) 34 7920
Fax: (+46-21) 34 8299
E-mail: henryk.anglart@se.westinghouse.com

W. Frid
Department of Reactor Technology,
Swedish Nuclear Power Inspectorate (SKI),
SE-106 58 Stockholm

Tel.: (+46-8) 698 84 60
Fax: (+46-8) 661 90 86 *or*
(+46-8) 206 454
E-mail: wiktor.frid@ski.se

M.E. Henriksson
Vattenfall Utveckling AB,
SE-814 26 Älvkarleby

Tel.: (+46-26) 835 40
Fax: (+46-26) 836 70
E-mail: mats.henriksson@vattenfall.com

T.A. Probert
Barsebäck Kraft AB,
Box 524, SE-246 25 Lödderköpinge

Tel.: (+46-46) 72 44 56
Fax: (+46-46) 77 58 48
E-mail: Thomas.Probert@barsebackkraft.se

O. Sandervåg
Swedish Nuclear Power Inspectorate (SKI),
Klarabergsviadukten 90, SE-106 58 Stockholm

Tel.: (+46-8) 698 84 63
Fax: (+46-8) 661 90 86
E-mail: oddbjorn.sandervag@ski.se

Z. Yitbarek
Studsvik Eco & Safety AB,
SE-611 82 Nyköping

Tel.: (+46-155) 221600
Fax: (+46-155) 221616
E-mail: zemichael.yitbarek@studsvik.se

SWITZERLAND

B.L. Smith
Paul Scherrer Institut (PSI),
CH-5232 Villigen PSI

Tel.: (+41-56) 310 2726
Fax: (+41-56) 310 4481
E-mail:Brian.Smith@psi.ch

UNITED STATES OF AMERICA

J.H. Mahaffy
Applied Research Laboratory, Penn State University,
P.O. Box 30, State College, PA 16804

Tel.: (+1-814) 863 4018
Fax: (+1-814) 863 8896
E-mail: jhm@psu.edu

R. Uddin
Department of Nuclear Plasma and Radiological Engineering,
University of Illinois at Urbana-Champaign,
103 S. Goodwin Ave., Urbana, IL 61801

Tel.: (+1-217) 244 4944
Fax: (+1-217) 333 2906
E-mail: rizwan@uiuc.edu

ORGANIZATIONS

INTERNATIONAL ATOMIC ENERGY AGENCY

J. Mišák
Safety Development Unit, Safety Assessment Section,
Division of Nuclear Installation Safety,
Vienna International Centre, P.O. Box 200, A-1400 Vienna, Austria

Tel.: (+1-43) 2600-22007
Fax: (+1-43) 26007-22007
E-mail: J.Misak@iaea.org

OECD NUCLEAR ENERGY AGENCY

J. Royen
Nuclear Safety Division,
Le Seine St.-Germain, 12, Boulevard des Îles,
F-92130 Issy-les-Moulineaux, France

Tel.: (+33) 1 45 24 10 52
Fax: (+33) 1 45 24 11 29
E-mail:jacques.royen@oecd.org

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