Computational Fluid Dynamics for Nuclear Reactor Safety Applications-6 (CFD4NRS-6)  
Workshop Proceedings, 13-15 September 2016, Cambridge, United States
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– to provide authoritative assessments and to forge common understandings on key issues as input to government decisions on nuclear energy policy and to broader OECD analyses in areas such as energy and the sustainable development of low-carbon economies.

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

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

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

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>BPGs</td>
<td>Best practice guidelines</td>
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<tr>
<td>BWR</td>
<td>Boiling water reactor</td>
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<tr>
<td>CFD</td>
<td>Computational fluid dynamics</td>
</tr>
<tr>
<td>CHF</td>
<td>Critical heat flux</td>
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<td>CMFD</td>
<td>Computational multifluid dynamics</td>
</tr>
<tr>
<td>CSNI</td>
<td>Committee on the Safety of Nuclear Installations (NEA) Departure</td>
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<tr>
<td>DNB</td>
<td>Departure from nucleate boiling</td>
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<tr>
<td>DNS</td>
<td>Direct numerical simulation</td>
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<tr>
<td>FEM</td>
<td>Finite elements method</td>
</tr>
<tr>
<td>FVM</td>
<td>Finite volume methods</td>
</tr>
<tr>
<td>IAEA</td>
<td>International Atomic Energy Agency</td>
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<tr>
<td>IQN-ILS</td>
<td>Interface quasi-Newton inverse Jacobian from a least-squares</td>
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<tr>
<td>IRM</td>
<td>Interface resolving methods</td>
</tr>
<tr>
<td>ITM</td>
<td>Interface tracking methods</td>
</tr>
<tr>
<td>LDV</td>
<td>Laser-Doppler velocimetry</td>
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<tr>
<td>LIF</td>
<td>Laser-induced fluorescence</td>
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<tr>
<td>LES</td>
<td>Large-eddy simulation</td>
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<tr>
<td>NPP</td>
<td>Nuclear power plant</td>
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<tr>
<td>PIV</td>
<td>Particle image velocimetry</td>
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<td>PTS</td>
<td>Pressurised thermal shock</td>
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<tr>
<td>UQ</td>
<td>Uncertainty quantification</td>
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EXECUTIVE SUMMARY

Background

The present report summarises the 6th workshop on Computational Fluid Dynamics for Nuclear Reactor Safety Applications (CFD4NRS-6) in the biennial series, supported by the Nuclear Energy Agency Working Group on the Analysis and Management of Accidents (NEA/WGAMA) and the International Atomic Energy Agency (IAEA). The tradition began in Garching in 2006, and this workshop followed the format and objectives of its predecessors in creating a forum whereby numerical analysts and experimentalists exchange information in the application of computational fluid dynamics (CFD) to nuclear power plant (NPP) safety and future design issues. The emphasis, as always, was to ensure a congenial atmosphere, to offer exposure to state-of-the-art (single-phase and multi-phase) CFD applications reflecting topical issues arising in NPP design and safety and to promote the release of high-resolution experimental data to continue the CFD validation process in this application area.

The reason for the increased use of multi-dimensional CFD methods is that a number of important thermal-hydraulic phenomena occurring in NPPs cannot be adequately predicted using traditional one-dimensional system hydraulics codes with the required accuracy and spatial resolution when strong threedimensional motions prevail. Established CFD codes already contain empirical models for simulating turbulence, heat transfer, multi-phase interaction and chemical reactions. Nonetheless, such models must be validated against test data before they can be used with confidence.

The necessary validation procedure is performed by comparing model predictions against trustworthy experimental data. However, reliable model assessment requires CFD simulations to be undertaken with full control over numerical errors and input uncertainties. The writing groups originally set up by the NEA have been consistently promoting the use of best practice guidelines (BPGs) in the application of CFD for just this purpose, and BPGs remain a central pillar of the simulation material accepted at this current workshop, as was the case for its predecessors. In order to assess the maturity of CFD codes for use in reactor safety and design, it is necessary to establish a database of CFD-grade experimental material. This remains the second pillar of the CFD4NRS series of workshops.

The third pillar is advancing the use of CFD modelling in multi-phase applications. Here, the challenges are considerable. Not only are the governing equations an order of magnitude more complex than for single-phase applications, but validation databases for which there is genuine three-dimensional involvement remain quite sparse. Multi-phase CFD is of course not the sole province of NPP applications, and important developments are taking place in other industrial arenas, such as in the chemical and processing industries, and in environmental studies. Prudence dictates that the CFD4NRS series of workshops should not provide reporting space for such non-nuclear CFD applications, but should recognise that links with diverse application areas exist and need to be maintained.
Scope

A recent IAEA initiative declared the intention to merge the twin technologies of NPP safety and NPP design within the context of the advancement and application of CFD in nuclear technology. Both of these application areas rely on validation procedures to keep the science trustworthy, and the validation procedures underpinning their reliability have been jointly recognised.

Emphasis in this workshop was placed in the following areas:

- Single-phase and multi-phase CFD simulations with a focus on validation areas such as: single-phase and multi-phase heat transfer, free-surface flows, direct contact condensation and critical heat flux, pool heat exchangers, boron dilution, hydrogen distribution in containments, thermal striping and fatigue, and/or advanced design concepts, such as tight-lattice fuel configurations, passive safety options and design optimisation. Many papers were indeed devoted to these issues. The uses of systematic error quantification, and the application of BPGs, were as strongly encouraged as in previous workshops in this series, leading to the rejection of some papers that did not adequately address these issues. Papers submitted related principally to NPP-relevant safety issues, such as pressurised thermal shock, critical heat flux, boron dilution, hydrogen distribution in containments, thermal striping and fatigue, and/or advanced design concepts, such as tight-lattice fuel configurations, and passive safety options. Continuing to advance the CFD4NRS-5 discussion of uncertainty quantification (UQ) in CFD was strongly encouraged. The first keynote speech presented the synthesis of NEA-GEMIX Benchmark Results on UQ.

- Experiments providing data suitable for computational fluid dynamics (CFD) or computational multifluid dynamics (CMFD) validation were particularly recommended, though these should include local measurements using multi-sensor probes, laser-based techniques (laser-Doppler velocimetry, particle image velocimetry, laser-induced fluorescence), hot-film/wire anemometry, imaging or other advanced measuring techniques for local measurements. It is now rapidly becoming an obligation for papers describing experiments to include a discussion of measurement uncertainties.
**Results and their significance**

There were 126 registered attendees at the CFD4NRS-6 workshop, up by about 15% from the previous meeting. Remarkably, the workshop had zero no-shows, evidence of the success of requiring registration before inclusion of the papers in the proceedings. A balanced attendance was registered from the three world regions, and representatives from 16 different countries attended the event. It is noted that the unfortunate coincidence with the “Problems of verification and application of CFD codes to the nuclear industry” conference in Russia justifies the reduced presence of Russian attendees. Future events should be co-ordinated to eliminate such overlap.

![Regional Distribution of attendees of the CFD4NRS-6 Workshop](image)

A total of 91 extended abstracts were received for evaluation following the initial announcements. This represents an 18% increase from the previous workshop, but in line with the typical numbers in this series of events. All the abstracts were evaluated for suitability by at least two reviewers, and invitations to write a full paper sent out at three hierarchical levels:

- **Unconditional** (favourable reviews had been received from all the reviewers)
- **Conditional** (at least one reviewer was unsure of the final acceptance of the paper)
- **Guarded** (it was anticipated that major revision of the paper would be necessary)

The number of technical papers finally received for evaluation was 60. All technical papers received were evaluated by 2-4 reviewers, each according to journal standards, for a total of 160 reviews. Of these, 44 were accepted for oral presentation, and 14 to be presented in poster form. The remaining two papers were withdrawn by their authors. Four keynote lectures and one plenary lecture were given, each to introduce the morning/afternoon sessions, as appropriate. In addition, one poster was displayed relating to the NEA-GEMIX benchmark exercise (for which no accompanying paper was requested).

Following numerous requests, it was decided to add an additional special “Student Poster Competition” for which no accompanying paper was requested. The call for posters was sent out 1 month before the meeting and 14 posters were presented. The attendance at the Student Poster session was fantastic, the quality of the posters was very high and the feedback from the attendees very positive. Three awards were assigned at the competition:

- Best Presentation: Jai Oan Cho (KAIST)
- Most Innovative: Daniel Nunez (UMich)
- Best Research: Andrew Richenderfer (MIT)

The use of best practice guidelines for performing high-quality CFD computations has clearly advanced in the single-phase applications area, where it is now almost universally applied. On the other hand, multiphase CFD applications still evidence insufficient verification of the methods and of the
implementation of the modelling closures, leading at times to conflicting conclusions. The still incomplete maturity of the multiphase methods further underlines the importance of further extending the experimental programmes in order to continue to produce CFD-grade data for validation purposes. The need for top quality experimental data for improving the multiphase closure laws remains essential, but the enhanced maturity of the multiphase direct numerical simulation (DNS) methods appears to be able to provide important contributions to the area. It is noted that on the experimental side as well, the pursuit of providing precise details of measurement error (i.e. error bounds on the data) capable of accounting also for measurement biases, needs to be further enforced.

It was announced that the next workshop in the series, in 2018, would take place on the campus of the Shanghai Jiao Tong University (SJTU), and Professor Jinbiao Xiong had already accepted the responsibility for organising this event. In the panel session at the close of CFD4NRS-6, delegates confirmed their interest in attending this follow-up workshop, if possible, and considered the two-year interval between workshops to be appropriate. The two and a half day duration of formal presentations, with a fieldtrip on the afternoon of the third day, was also accepted as an acceptable format.

As is customary at the panel session, which in this case was led by D. Bestion (CEA) and E. Baglietto (MIT), summaries were made by the respective session chairpersons of the presentations that were given during the oral sessions, and general comments were invited from the audience. These session summaries are now embodied into the present document.

Conclusions and recommendations

The session topics, as expected, were wide and various, including such issues as flow mixing, fluid structures interaction, boiling and condensation modelling, multi-phase and multi-physics problems, plant application, hydrogen transport in containments, advanced measuring techniques, and single and multi-phase flow in reactor cores and sub-channels.

On the organisational side, the conference presented the usual challenges in predicting the number of attendees, but overall the number of attendees was consistent with the early predictions. A suggestion for future organisers is to carefully plan the contracts for room rates at hotels since new accommodation means (e.g. Airbnb) seem to be slowly replacing the classic conference hotel approach. The experience of the previous meeting, where a large number of very late withdrawals from the official programme created serious challenges, was leveraged to enforce the registration of all speakers before inclusion of their papers, and with systematic reminders to all the authors. The approach was extremely successful, and there were no withdrawals from the programme. The rigorous and strict review of the abstract probably also played a very important role, as only one author who was invited to submit the full paper had to withdraw early and did not attend the meeting. The support from gold sponsors – CEA and Elysium Industries – and silver sponsors – ANSYS and CD-adapco – played a relevant role in the success of the event, and supported the conference banquet at the MIT museum.

A suggestion for future workshops is that the session summaries should also provide an overall summary of progress and key conclusions rather than just a summary of the individual papers.

General conclusions

The technical presentations and related discussion at the CFD4NRS-6 workshop evidenced significant progress in the adoption of CFD for safety related applications. CFD plays a growing role in the industrial community, which shows the immediate value of the method. Some of the applications, for example those related to nuclear fuel, have reached a good level of maturity thanks to the fundamental support of CFD-grade experiments, as demonstrated by successful international blind and open benchmarks. In this regard, the role of the NEA benchmarks has been fundamental in driving much larger involvement of the
international community. Following the previous NEA benchmark on containment analysis, four sessions were held at the present event where a large number of high-quality papers demonstrated a further important step in the understanding of the phenomena and provided valuable guidelines for CFD application to support safety evaluation. While the maturity of the CFD methods has grown considerably, the community will benefit from further advances in the area of uncertainty quantification in support of reactor licensing. The conclusion presented for the NEA-GEMIX blind benchmark exercise represented a good first step, and allowed for the pinpointing of some fundamental challenges that the community will work on addressing. The next NEA benchmark will be an excellent opportunity to evaluate progress, and there is hope to see more complete methodologies presented and discussed at the next CFD4NRS event.

Delegates appeared satisfied that the subject areas covered by the workshop were comprehensive within the nuclear CFD community, and that leading experts in the field adequately covered the present state of the art, or projected future trends, as appropriate. The message was received that “small is good”, and that the workshop should remain rigidly focused on CFD issues, and should not broaden its boundaries beyond this. While a longer discussion time would have been valuable, it would seem to be incompatible with the workshop duration since the number of papers would need to be further reduced.

- The current format, length and intervals between CFD4NRS workshops were generally considered to remain appropriate, as was the rotation of venues worldwide. Hence no changes are proposed in this regard.
- The formula of combining the blind CFD benchmark activity with the occasion of the workshop was appreciated. Participants have the possibility to display their work (as posters without accompanying papers), and discuss their experiences. This practice will therefore be continued, as far as possible, in the future, and an earlier communication to the benchmark participants will encourage an increase in the number of posters at future meetings.
- It was generally considered that the level of quality of the papers was sufficient, at a similar level with the previous events. The high rejection rate of the abstracts (35%) was an important contributor in providing high-quality papers and presentations.

Specific recommendations

- The value and challenges of applying uncertainty quantification (UQ) methods were clearly evidenced by the NEA-GEMIX benchmark. A second round of analysis of the NEA-GEMIX benchmark could be valuable as it would allow for the incorporation of lessons learnt, both in terms of the measurement uncertainty and methodologies application. Discussion of the updated benchmark at the next workshop would be certainly welcome.
- The nuclear CFD community should be encouraged to extend the application of UQ to their simulations, including uncertainties arising from the numerical solution procedure, the physical models employed, and in the application of initial and boundary conditions.
- The discussion demonstrated an improved use of best practice guidelines (BPGs) in producing single-phase CFD simulations. The community is further calling for similar guidelines applicable to large-eddy simulation (LES) and hybrid methods.
- The use of BPGs in the multiphase CFD applications is still insufficient and should be further encouraged, in particular to verify the implementation of the multiphase closures.
- The need for error bars on experimental data should continue to be reinforced. In the design and analysis of experiments, efforts should be made to make the uncertainty estimates complete and not simply limited to the linear addition of the known instrument uncertainties. The lack of understanding of measurement biases can render the validation almost worthless.
- It is recommended that future test data offered to this series of workshops should continue to improve the quantification of measurement error. As noted in previous meetings, best practice guidelines on the presentation of experimental data currently do not exist. In the context of further workshops in this series, a strong message of correction must be sent in this regard.

### Keynote lectures

1. Arnoldo Badillo; Paul Scherrer Institut (PSI), Switzerland  
   *Synthesis of results of the OECD-GEMIX blind benchmark exercise.*

2. David W. Pointer; ORNL, USA  
   *Progress and Challenges in Predictive Simulation of Thermal Hydraulic Phenomena.*

3. Jan-Patrice Simoneau; EDF, France  
   *CFD practices at EDF for nuclear safety - current applications and future challenges.*

4. Philippe Bardet; George Washington University, USA  
   *Laser diagnostic development for code benchmark and validation.*

### Plenary lecture

1. Dominique Bestion; CEA, France  
   *Review of Uncertainty methods for CFD application to nuclear reactor thermalhydraulics.*

### Poster papers on the NEA-GEMIX Benchmark

1. Christopher Boyd; Nuclear Regulatory Commission, USA  
   *OECD-GEMIX Benchmark Results*
Session 1: FUEL APPLICATIONS 1
Co-Chairs: R. Brewster (WEC, USA), E. Baglietto (MIT, USA)

   *New Insights Into The Flow Inside Nuclear Reactor Fuel Bundles Using Magnetic Resonance Velocimetry*

2. M. E. Conner, C. E. Estrada Perez, E. Dominguez-Ontiveros and Y. Hassan
   *Demonstration of Advanced Hydraulic Benchmark Data for PWR Mixing Vane Grid*

   *CFD Simulation of Flow Mixing and Heat Transfer in 4x4 Rod Bundle with Twist-Vane Grid*

   *Experimental and Computational Investigations of Flow By-Pass in a 37-Element CANDU Fuel Bundle in a Crept Pressure Tube*

Session 2: CONTAINMENT 1
Co-Chairs: M. Andreani (PSI, Switzerland), E. Laurien (UniStuttgart, Germany)

1. M. Freitag and E. Schmidt
   *Double Blind Simulation Benchmark Based on Initial Operation Test of the Extended THAI+ Facility on Steam Condensation and Light Gas Mixing by Natural Convection*

2. P. Royl, J. Xiao and T. Jordan
   *Blind Simulations of THAI Test TH27 with GASFLOW-MPI for Participation in the International Benchmark Conducted within the German THAI Program*

3. C. Kaltenbach and E. Laurien
   *Numerical Simulation of Droplet Flows in the Model Containment THAI*

   *URANS Analysis of the Erosion of a Stably Stratified Layer*
Session 3: MULTIPHASE GENERAL 1
Co-Chairs: D. Bestion (CEA, France), A. Uchibori (JAEA, Japan)
1. D. Lucas, E. Krepper and R. Rzehak
   Validation of the Baseline Model for Poly-Disperse Bubbly Flows
2. S. Mimouni, D. Lucas and I. Tiselj
   CFD Calculations of Multiphase Flows with a Multifield Approach
3. J. Fang, J. Feng and I. Bolotnov
   Integral and Separate Effect Simulations of Bubbly Flows Using Interface Tracking Approach

Session 4: PLANT - PTS
Co-Chairs: J.P. Simoneau (EDF, France), M. Tanaka (JAEA, Japan)
1. T. Höhne and S. Kliem
   IAEA CRP Benchmark of ROCOM Boron Dilution and PTS Test Cases for the Use of CFD in Reactor Design
2. D. Rosa, A. Shams and E.M.J. Komen
   Towards the Benchmarking Direct Numerical Simulations of a Single Phase Pressurized Thermal Shock
   Methodology Development of CFD/PFM for PTS Analysis on Nuclear Reactor Safety

Session 5: BOILING 1
Co-Chairs: S. Mimouni (EDF, France), S. Lo (CD-adapco, UK)
1. S. Vahaji, L. Deju, S.C.P. Cheung, J.Y. Tu and Yeoh
   Evaluation of Coalescence and Break-Up Kernels of Subcooled Boiling Flows in Vertical Channels
2. Guion, J. Buongiorno, S. Zaleski, S. Afkhami and C. Narayanan
   Numerical Simulation of Nucleate Boiling Using Dynamic Models of Microlayer Formation and Evaporation
3. M. Sonntag and X. Cheng
   CFD Model for Simulation of Subcooled Nucleate Flow Boiling – Implementation and Validation

Session 6: FLUID STRUCTURE INTERACTION 1
Co-Chairs: K. Miyoshi (INSS, Japan), T. Hoehne (HZDR, Germany)
1. J. Berland, E. Deri, A. Adobes
   Investigation of Cross-Flow Induced Vibrations in a Normal Square Tube Array by Means of Large-Eddy Simulations for Tube Damage Risk Assessment
2. E. ter Hofstede, S. Kottapalli and A. Shams
   *Numerical Prediction of Flow Induced Vibrations for Safety in Nuclear Reactor Applications*

3. R.A. Brewster and Y. Aleshin
   *Validation of Beam Vibration Simulations in Axial Flow*

**Session 7: FUEL APPLICATIONS 2**

Co-Chairs: X. Cheng (SJTU, China), W-K. In (KAERI, Korea)

1. P. E. Angeli and M. P. Peybernes
   *CFD Analysis of the Turbulent Flow in a PWR 5x5 Rod Bundle with Staggered Structural Grids*

2. M. Bottcher and R. Gomez
   *CFD Studies of Heat and Momentum Transfer at a Structured Fuel Rod Surface*

   *Departure From Nucleate Boiling Simulations Using Computational Fluid Dynamics*

**Session 8: CONTAINMENT 2**

Co-Chairs: G. Zigh (USNRC, USA), S. Kelm (FZJ, Germany)

1. K. Hall and C. Boyd
   *CFD Simulation of Cooler Tests in the MISTRA Facility: A Focus on Liquid Condensate Re-evaporation*

2. H. Müller, J. Lehmkuhl, S. Kelm, A. Hundausen, A. Belt and H.-J. Allelain
   *Development of a Wall Condensation Model for Coarse Mesh Containment Scale Applications*

3. M. Pellegrini and M. Naitoh
   *Application of Two-Phase Flow CFD to the Phenomena Expected in the Fukushima Daiichi S/C*

**Session 9: BOILING 2**

Co-Chairs: G. H. Yeoh (UNSW, Australia), D. Lucas (HZDR. Germany)

   *Recent Advances in Nucleate Boiling Modelling and Application to DNB*

2. S.J. Kim, D.V. Rao, B. Okhuysen, R. Johns and E. Baglietto
   *A CFD Simulation Effort on the Departure from Nucleate Boiling (DNB) in Subcooled Flow*

   *State-of-the-Art Hydraulic Pressure Drop and Lift Force Analysis for a PWR Fuel Assembly by Using CFD as Compared to the Classical One-Dimensional Approach*
**Session 10: FLUID STRUCTURE INTERACTION 2**

Co-Chairs: E. Komen (NRG, Netherlands), Gaurav Kewlani (MIT, USA)

1. M. Tanaka, J. Kobayashi and K. Nagasawa  
   *Fundamental Validation of Fluid-Structure Thermal Interaction Simulation Code for Thermal Stripping in Sodium-Cooled Fast Reactors with Parallel Triple Jets Mixing Experiments*

2. M. Jeltsov, W. Villanueva and P. Kudinov  
   *Effects of Seismically Induced Sloshing in ELSY Reactors*

3. K. Miyoshi, Y. Utanohara and A. Nakamura  
   *Measurement of Wall Temperature with 148 Thermocouples to Improve Simulation Methods for Thermal Fatigue Evaluation at a Mixing Tee*

**Session 11: MULTIPHASE GENERAL 2**

Co-Chairs: A. Tentner (ANL, USA), J. Xiong (SJTU, China)

1. N. Mérigoux, J. Laviéville, S. Mimouni, M. Guingo and C. Baudry  
   *A Generalized Large Interface to Dispersed Bubbly Flow Approach to Model Two-Phase Flows in a Nuclear Power Plant*

2. E. Krepper, D. Lucas and F. Zidouni  
   *Analysis and Applications of a Multi-Field Approach for Plunging Jet Configurations*

3. G. Montoya and E. Baglietto  
   *Resolved Interface Taylor Bubble Simulations to Support Eulerian Multiphase Closures Derivation*

**Session 12: CONTAINMENT 3**

Co-Chairs: M. Pellegrini (IAE, Japan), K. Hall (ALDEN, USA)

   *Synthesis of a Blind CFD Benchmark Exercise Based on a Test in the PANDA Facility Addressing the Stratification Erosion by a Vertical Jet in Presence of a Flow Obstruction*

2. S. Kelm, H. Müller, H.-J. Allelein  
   *Importance of Thermal Radiation Heat Transfer Modeling in Containment Typical Flows*

   *Modeling of Thermal Stratification and Mixing Induced by Steam Injection Through Spargers into a Large Water Pool*
Session 13: BEST ESTIMATE / VUQ
Co-Chairs: J. Laviéville, (EDF, France), Matteo Bucci (MIT, USA)
1. S. Koshizuka, M. Tanaka and K. Nakada
   *AESJ Guideline for Computer Simulation in Nuclear Engineering*

2. K. Hall and C. Boyd
   *Uncertainty Quantification and Validation of a CFD Simulation of Surface Condensation in the Presence of Non-Condensable Gas*

3. A. Papukchiev, C. Geffray, D. Grischenko and P. Kudinov
   *Application and Validation of the Multiscale Code ATHLET-ANSYS CFX for Transient Flows in Next Generation Reactors*

Session 14: CONTAINMENT 4
Co-Chairs: H. Müller (RWTH, Germany), C. Boyd (NRC, USA)
1. A. Mansour and E. Laurien
   Simulation of a Natural Convection Flow with Humid Air in a Two-Room Geometry

2. A. Dehbi and J. Kalilainen
   Large Eddy Simulations of Free Convection Particle Transport Inside Cavities at Rayleigh Numbers up to 1010

   Investigations on Steam Condensation with Air at the Exterior Surface of a Circular Tube for Passive Containment Cooling System Design

Poster Session 1: PLANT AND MIXING APPLICATIONS
1. H.Xu, R.F. Wright
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RESEARCH ON SUBCHANNEL RESISTANCE COEFFICIENT CALCULATION BASED ON CFD METHODOLOGY
Session 1: FUEL APPLICATIONS 1

The papers in this session were good examples of the intersection between computational fluid dynamics (CFD) and experimentation. A variety of experimental and CFD were used in the session papers.

The first and fourth papers together provided a combined experimental and computational investigation of bypass flow in a CANDU fuel bundle. The experimental use of MRV was quite novel. The fourth paper provided LES results using Hydra-TH with comparison to experimental data.

The second paper presented new lateral Particle image velocimetry (PIV) measurements of the entire field downstream of the grid in a 5x5 simulated fuel bundle. Results were compared to previous PIV measurements in another facility and to CFD results using STAR-CCM+. This technique promises to yield high-quality, whole field transient validation data.

The third paper presented PIV measurements and CFD results for a simulated assembly with twist-vane grids. Results were provided for two P/D ratios (1.35 and 1.08). Rod wall temperatures were also measured. CFD results agreed generally well for P/D = 1.35, but not as well for P/D = 1.08. Discussion included the possibility that unsteadiness may play an important role for P/D = 1.08.

While no generally agreed standard CFD approach exists for modelling flow in fuel bundles, industry benchmarks such as the EPRI NESTOR and IAEA CRP may help address this aspect. In addition, best practices need to evolve over time as CFD technology develops.

Session 2: CONTAINMENT 1

The session included four papers. Three of the papers addressed gas mixing, and one spray cooling. In the first paper the double-blind phase of an international benchmark including 12 participants was evaluated using data from the THAI facility. The basis for the benchmark was test TH27, which was performed as the commissioning test for the extended THAI+ facility. The new THAI configuration consists of the THAI Test Vessel (TTV) and the smaller parallel attachable drum (PAD) which are connected at the top and at the bottom by two pipes. The challenge of the benchmark was to generate two models and simulate two long transients without previous model calibration. Overall the benchmark demonstrated the high prediction quality of the CFD codes, especially taking into account that the operating behaviour of the THAI+ is yet unknown. For CFD codes the increase in CPU cost was up to 1000 times in comparison to Lumped Parameters (LP) codes.

In the second paper, both the double-blind and the blind calculations of the benchmark test TH27 were well interpreted with the GASFLOW-MPI code. The blind simulation with updated boundary conditions was performed after the double blind simulation. The code simulates the transient helium distribution very well. A significant new effort was spent for controlling the boundary conditions of the slab structures. The user can now define these structures in a very flexible way. The solution algorithm of GASFLOW-MPI has shown improved numerically stability. The calculation covers a time of 38 hours and applies a 3D Cartesian single block model with 349000 cells. Such large problems had not been calculated before with GASFLOW-MPI. The calculation with GASFLOW-MPI required 14 days with 8 CPUs on a modern LINUX cluster.

In the third paper presented a spray model, which was implemented in the code ANSYS CFX 16.1 in the framework of the Eulerian-Eulerian approach. Since models for spray are not included in the ANSYS code these must be developed by users interested in considering its effect in containment
analysis. In particular, the paper emphasises the importance of transient heat-up of droplets for properly calculating the condensation rate and thus the depressurization produced by the spray. The limited success on the selected validation case indicates that more work is necessary in this direction.

The fourth paper presented an in-depth investigation on simulation of turbulent jets. In particular, the dependence of the jet behaviour on the geometry of the source, nozzle or pipe, was discussed. It was shown that the geometrical dependency of the jets could be recovered by modifying the turbulence model coefficients. Although the approach of modifying model constants in eddy viscosity model is generally not acceptable, the study has the merit to identify the effect of the coefficients on the predictions and most importantly to demonstrate that the adequate representation of the free jet is a pre-requisite for the successful prediction of stratification build-up, erosion and break-up.

Session 3 and Session 11: MULTIPHASE GENERAL 1 and 2

In sessions 3 and 11 “Multiphase General”, new approaches of numerical simulation on two-phase flow were presented, together with several validation efforts. A polydispersed bubbly flow model was validated on a large variety of bubbly flows. Numerical approaches based on the interface tracking method were applied to complex flows. Approaches towards a modelling of all flow regimes and validation simulations were presented.

The word “general” may refer to several things:

1. A two-phase flow model may be called general if it is able to model all flow regimes - We have seen attempts to develop such models which combine ITM or IRM methods for large interfaces (paper 3.2) with phase averaging for dispersed fields while keeping reasonable CPU time. This is a recent trend and models are developed such as the GENTOP model in CFX or a multifield model in NEPTUNE-CFD. Initially CFD models focused on pure dispersed flow or separate-phase flow; now they go to the most complex flow regimes and good new results were shown on gas injection in a tank, on a transition to slug flow, on churn flow, on transition from bubbly to stratified flow, and on bubbly flow injected in liquid with a possible free surface. This extension is mandatory for CFD to be used in all flow conditions even before knowing what the flow regime will be and for CFD to become a reference for 1D models. The very challenging case of gas entrainment by a plunging jet was investigated (paper 11.2) using the GENTOP model and showed good global capabilities with still some difficulties for quantitative predictions. A simplified “all flow regime approach” was also presented (paper 11.1) using the two-fluid model and proved also good capabilities at a lower cost.

2. A two-phase flow model can be said general when a same set of models can obtain good or reasonable results in a large validation data base - This was the objective of a paper on a baseline polydispersion modelling of bubbly flow (paper 3.1). Polydispersion was found as one of the main difficulties and here a single model is validated on three sets of data and obtains a good agreement. It is rather easy to find a model which agrees with an experiment but when we want to evaluate the predictive capabilities and the maturity of a model we should go in this direction to define a baseline model confronted to a large data base.

3. A two-phase flow model may be called general if it can model all flow processes even at a very local scale for which very limited experimental information is available - In such case DNS or LES type simulations with ITM may provide an additional source of information. We have seen applications of such methods to bubbly (paper 3.3) flow with information of interfacial forces and we may expect that such techniques will be progressively more used for modelling purpose. This requires some development of adequate data analysis methods to take full advantage of the information provided. We also have seen LES application to slug flow with good agreement with data (paper 11.3).
So the sessions 3 & 11 definitely demonstrated there is a very good trend to go towards a “general multiphase CFD” which is good news:

- General in the sense that it covers all modelling scales from DNS to LES and RANS
- General in the sense that it models all flow regimes
- General in the sense that it is validated in a wide range of experimental data.

**Session 4: PLANT – PTS**

Three papers were presented in this session discussing validation data, modelling and development of methods for application of computational methods to the issue of plant mixing and pressurised thermal shock (PTS).

The first paper discussed two sets of ROCOM CFD-grade test data that were made available for an IAEA benchmark, relating to boron dilution (pump start-up) and PTS. While the topic of mixing in the reactor vessel has been under investigation for some time, the availability of an open benchmark and involvement of a larger industry community could further extend the understanding and help support the assessment and life extension of operating reactors. The second paper discussed a valuable activity ongoing to assemble DNS data to further support the turbulence modelling advancement and validation for PTS related applications. The code NEK5000 was adopted and demonstrated at reduced order of accuracy, and will be leveraged to produce high-quality data on a representative PTS geometry. The availability of the DNS data will greatly supplement integral tests such as ROCOM in assembling modelling approaches with well quantified uncertainty. The third paper looked at the application challenges of CFD to PTS. The CFD calculation were coupled a Probabilistic Fracture Mechanic (PFM) method and attempted to leverage the BPGs and the ASME V&V guidances to evaluate the uncertainty of the prediction. The proposed methodology aims at addressing the NRC limit demonstration for Taiwan’s operating PWR reactors.

**Session 5 and Session 9: BOILING 1 and 2**

In sessions 5 and 9, five papers covered a range of aspect related to modelling boiling in CFD, starting from the fundamental aspects and covering application and assessment up to critical heat flux. The last paper departed from the boiling aspects and was related to the adoption of CFD to predict the pressure drop and the lift force exercised by the flow on a fuel assembly.

The sessions evidenced that subcooled boiling remains a challenging field. While current models can be adapted to predict specific regimes and sets of conditions, more work is required on the very fundamental aspect of both wall and bulk behaviour. Attempts to calibrate the models demonstrate that it is necessary to start from the fundamentals, and leverage and advance the measurements and DNS capabilities to quantify the microscopic boiling behaviour and incorporate into a more general representation. At the same time the adoption of calibrated models to predict DNB shows promises and could very soon extend the current modelling capabilities for safety analysis of reactor fuel.

The first paper of session 5 focused on the analysis of coalescence and break-up kernels for population balance models, and in particular on their influence on the prediction of boiling heat transfer. Useful comparisons and assessments are provided and indicate that further evaluation is necessary, where no one specific approach bears clear advantage on a large set of cases. The second paper presented an extensive research related to the development of dynamic submodels for microlayer formation and evaporation to advance the capabilities of directly simulating nucleate boiling in DNS. The ability to model the microlayer at low cost could finally bring the DNS capabilities to be able to support improved understanding and modelling of subcooled flow boiling.

The third and fourth papers interestingly presented two different model formulations with the common idea of adopting a boiling correlation to the partition boiling at the wall rather than the classic mechanistic partitioning. The direction attempted demonstrates the challenge in the community to
calibrate the existing partitioning models to cover a large range of application. The fourth paper aims at extending the modelling up to departure from nucleate boiling (DNB) and couple the experience of previous assessments with the new correlation based boiling. The fifth paper also focused on the aspect of predicting DNB with CFD. A baseline first generation boiling approach was assessed on the single tube high pressure CHF data from Weatherhead, demonstrating reasonable predictions at all tested conditions.

Session 6: FLUID STRUCTURE INTERACTION 1

Three papers were presented in this session, covering both fundamental FSI methods evaluation and practical applications. The papers overall indicate a generally good understanding of the challenge and best practices, and demonstrate the important role of simulations in this area of application.

The first paper focused on the investigation of cross flow induced vibrations in a squared lattice tube array, adopting a resolved LES method. The method was assessed against experimental reference data in terms of tube oscillation amplitudes and comparing the measured and calculated force spectra. The main findings of the work are related to evidencing that the tube motion excites clear tones at constant frequencies in the flow, corresponding to the vibrational models of the solid structure. The second paper provided an extensive validation of fluid structure coupling methods, namely the IQN-ILS and the Gauss Seidel methods were tested on a series of strongly coupled FSI problem, both for FVM-FVM and FVM-FEM implementations. The findings evidenced a computational advantage for the FVM-FEM solution while both IQN-ILS and Gauss Seidel methods are capable of solving FSI problems with strong coupling. The last paper discussed the validation of FSI methods for application to fuel rods vibration in the core during seismic events. A fundamental benchmark for a single beam was performed and demonstrated good predictions both for stagnant and flowing water. Work will still be necessary to extend and validate the applicability of the approach to prototypical reactor dimensions and flow conditions.

Session 7: FUEL APPLICATIONS 2

All three papers in the session Fuel Applications 2 focused on CFD studies related to fuel modelling, for different configurations and having different objectives. In one case new experimental findings were also discussed together with the CFD results.

The first two papers presented somewhat classic studies, of validation of turbulence models applicability to specific flow configurations and adapting their own set of test data. The first study adopted a classic PWR fuel configuration and available LDV measurements for a 5x5 bundle configuration to evaluate the applicability of the reworked TRIO-CFD code (formerly TRIO-U). Results presented are very consistent with the previous literature and underline the importance of including anisotropic effects to correctly represent flow away from the spacer region. The second paper compared the CFD predictions against single heated rod data for smooth as well as structured rod surfaces. While the flow configuration is different, conclusions are similar to the previous and evidence the importance of modelling anisotropy to improve the CFD predictions. Further, both papers also apply LES simulations which provide the optimal agreement, as expected, but also carry extreme computational requirements.

The final paper presented a different topic related to modelling DNB in PWR assemblies. The work presented a preliminary evaluation of the capabilities of the approach against single tube data. The work discussed the need to calibrate the model parameters in order to produce consistently good agreement for the selected set of test data. The conclusions are in line with those presented on similar application in Session 1: FUEL APPLICATIONS 1.
Session 8: CONTAINMENT 2

All papers in this session were related to model development and validation. None of the papers could be considered “full-scale” applications. BPGs were not followed in a strict sense, but some ideas to reduce numerical error (e.g. mesh sensitivities) were discussed.

The developments presented in this session aimed at including more physics and at improving the numerical efficiency of the models. Both aspects are still considered to be gaps towards full-scale application.

Paper 8.1 presented the discussion of the MISTRA test MERCO-2 on containment atmosphere mixing due to wall cooling (condensation). The effect of re-evaporation of condensate in the late phase was identified and could explain previously characterized discrepancies in predicting temperature and pressure histories. The presentation underlined that discrepancies between simulation and experiment should not simply be attributed to general uncertainty but could be related to missing physical description.

Paper 8.2 discussed the development of wall functions for condensing boundary layers. The approach allows reducing the effect of insufficient resolution in the near wall mesh and thus to improve prediction of heat flux and condensation rate on coarse “practicable” mesh resolutions. The approach, being an extension of previously demonstrated methods, showed promising results when compared to the SETCOM data. Further work is still necessary to fully integrate the approach in the overall simulation framework and to demonstrate its application to integral effect tests (IET).

Paper 8.3 presented a new model based on Rayleigh-Taylor instability theory to model the interfacial area density during chugging in a suppression pool. Promising results were reported in comparison to experiments and classical approaches.

Session 10: FLUID STRUCTURE INTERACTION 2

The three presentations during this session covered, respectively, the validation of a fluid-structure thermal interaction simulation code, a CFD study of seismically induced sloshing, and the measurement of wall temperature distribution on the pipe inner surface at the mixing tee.

In the first presentation, a fluid-structure thermal interaction simulation code MUGTHES, which has been developed to investigate and estimate the thermal fatigue in structures, was discussed. The verification and validation plus uncertainty quantification and prediction (V2UP) framework was highlighted. Three benchmark simulations conducted for fundamental validation, corresponding to the sodium test data of PLAJEST for planar triple parallel jets mixing, were also discussed. The mesh details, the wall conditions, and the discretization schemes were mentioned briefly, and the conjugate heat transfer model was described in detail. This was followed by a discussion of the simulation results.

In the second presentation, a CFD study of seismic sloshing in the ELSY reactor was discussed. The different sloshing modes and the seismic risks in LFRs including risk of structural damage and reactivity initiated accident were described in brief, and this was followed by an overview of the ELSY reactor, and the seismic cases used in the analysis. The reactor representative 2D model -- including the solver, geometry, and mesh -- was highlighted, and results from a mesh study (corresponding to different mesh sizes) and a time-step study (corresponding to different constant time steps, as well as adaptive time steps) were shown. Subsequently, the 3D modelling and the results for the Inter SG region, both with and without the baffle, were presented.

In the third presentation, the measurements of the wall temperature distribution on the pipe inner surface at the mixing tee were discussed, aimed to extend and improve the validation of fluid-structure coupled numerical simulations for thermal fatigue evaluation at a mixing tee. The basic process of thermal striping at a mixing tee was described, and the test section setup was discussed in fair detail.
The test conditions, including the fluid temperature in the inlet, and the mean cross-sectional velocity in the inlet, for the main pipe and the branch pipe respectively, were presented. The time-averaged temperatures on the pipe inner surface were then shown, and the uncertainties of the time-averaged value, the standard deviation and the fluctuation range of the wall temperature were also presented.

In summary, the research work presented in this session used established methods, and evaluated the performance of the simulation and/or experimental setups under various conditions.

Session 12: CONTAINMENT 3

Three papers were presented in this session and cover a range of containment related CFD studies. The session started from the synthesis of the blind NEA benchmark exercise PANDA. In this exercise the challenging phenomenon of helium stratification erosion induced by a vertical steam jet into the containment is treated. The benchmark clearly evidenced how the complex physics of the tests, and in particular the unsteady jet behaviour, challenge the current BPGs applicability. Two sets of blind tests were provided, one using a common model, and a second using a best estimate model. For the common model a list of recommendations was given to limit the variability of the case comparison. The results indicated that even for the common model, the results covered a large band, and possibly the development of dedicated BPGs will be required to increase the confidence on the CFD codes predictive capabilities.

The second paper underlined the importance of modelling thermal radiation heat transfer in containment related simulations. The work reported the experience achieved in modelling gas radiation in humid atmospheres and quantified its influence on different available test cases. The results demonstrated that gas radiation has a significant far field effect on the gas temperature field and the resulting gas to wall heat transfer. The results also stress the need for future experimental characterization of gas radiation heat transfer. Once again it was noted that dedicated BPGs might be required to apply radiation models to containment flows.

The third paper investigated the risk of thermal stratification in the wetwell of a BWR containment. In order to efficiently reproduce steam injection into the pool a simplified model is proposed which replaces the two-phase flow with single-phase boundary conditions for the steam injectors under the assumption of complete condensation. The model is validated with good results against experiments performed in the PANDA facility under the HYMERES project. As noted in other work, results can be particularly sensitive to the turbulent production due to buoyancy and attention should be devoted to selecting the appropriate method.

Session 13: BEST ESTIMATE / VUQ

The first paper discussed AESJ guidelines for computer simulations in nuclear engineering. It was noted that is important to develop a well-structured and reliable verification and validation framework to improve the confidence on the results of CFD codes. This can be vital to inform decision making, in particular during situations of crisis like the Fukushima accident. In this aim, AESJ have developed a new V&V strategy, inspired by the existing US and European recommendations. Further improvement of this document will address a decision making strategy based on the results of simulations and the estimate of their uncertainty.

The second paper presented uncertainty quantification and validation of a CFD simulation of surface condensation in the presence of non-condensable gases. When one wants to use experiments for CFD codes validations, uncertainties in measurements required as boundary or initial conditions can be very problematic, in particular if the measurement and the associated uncertainties are difficult to estimate. Notably, when a parameter carries large uncertainties, numerical methods and models may also be questionable. To overcome this issue, scoping numerical simulations can be leveraged to
identify what kind of measurement should be improved or developed before the construction of an experimental setup aimed at the validation CFD tools.

Application and validation of the multiscale code Athlet-ANSYS CFX for transient flows in the next generation reactors was presented last. Uncertainties on calculations coupling CFD and system codes are quite unexplored. The work presented in this session give an example of how this kind of exercise can be performed. However, it is important to understand if the coupling between two or more codes does not introduce further sources of uncertainties, e.g. in coupling of physical variables and models at the interface regions between two codes.

**Session 14: CONTAINMENT 4**

Session 14: Containment 4, dealt with a variety of containment and related CFD issues. Topics includes the challenges with the application of the GCI method to quantify the grid error, a study of the issues surrounding the prediction of particle transport and settling, and a design study for PCCS systems that included prediction of wall condensation in an air-steam mixture.

The first paper by Abdennaceur Mansour and Eckart Laurien focused on the application of the grid convergence index (GCI) for a “Simulation of Natural Convection Flow with Humid Air in a Two-Room Geometry.” The GCI method was applied to an unstructured mesh and noisy convergence was observed. The problem is common with many CFD tools on unstructured meshes. A series of five mesh cases were considered and three methods were utilised to compute the order of convergence. Demonstrating consistent methods to compute the GCI is an important aspect of completing uncertainty studies for typical reactor safety problems that utilize unstructured meshing techniques. In addition to the grid study, the parallel performance of CFX 16.1 was demonstrated. Maximum speed up for this model was found at 1800 cores.

The second paper by A. Dehbi and J. Kalilainen titled “Large Eddy Simulations of Free Convection Particle Transport inside Cavities at Rayleigh Numbers up to 1010,” demonstrated the importance of turbulence effects on particle transport with implications for release fraction calculations. Current modelling approaches from system codes are found to be overly conservative for particles of interest in severe accident scenarios. A theme that was noted here and also mentioned in other papers during CFD4NRS-6 was the importance of radiation modelling even for cases with relatively modest temperature differences. The work here included a grid study and comparison with test data.

The third paper, “Investigations on Steam Condensation with Air at the Exterior Surface of a Circular Tube for Passive Containment Cooling System Design,” by Dong-Wook Jeong and J-Hwan Hwang focused on the application of the STAR-CCM+ code to optimise the tube diameter used for PCCS. A series of sensitivity studies were completed on turbulence and diffusion models as well as tube curvature. Comparisons were made with available data. Best practices for this type of modelling are discussed. The application of wall condensation modelling was a common theme for several of the papers in CFD4NRS-6.
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