

# **VERIFICATION & VALIDATION AND UNCERTAINTY ANALYSIS IN MULTI-PHYSICS MODELING FOR NUCLEAR REACTOR DESIGN AND SAFETY**

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## **ABSTRACT**

Multi-level approach has been utilized in verification and validation of coupled neutronics/thermal-hydraulics (multi-physics) codes in international standard problems. Appropriate benchmarks have been developed in international co-operation led by the Nuclear Energy Agency (NEA) of the Organization for Economic Cooperation and Development (OECD) that permits testing the neutronics/thermal-hydraulics coupling, and verifying the capability of the coupled codes to analyze complex transients with coupled core/plant interactions. The paper summarizes these activities conducted by the Expert Group on Reactor Stability and Transient Benchmarks at the Nuclear Science Committee (NSC) of NEA/OECD. The Expert Group deals with modeling and benchmarking issues in the field of Three-Dimensional (3-D) coupled neutronics/thermal-hydraulics transients for nuclear cores and coupling of core phenomena and system dynamics for nuclear reactor core design and safety analysis. In recent years there has been an increasing demand from nuclear research, industry, safety and regulation for best estimate predictions to be provided with their confidence bounds. The ongoing OECD Light Water Reactor (LWR) Uncertainty Analysis in Modeling (UAM) benchmark activities contribute to establishing such unified framework to estimate safety margins, which would provide more realistic, complete and logical measure of reactor safety. The paper describes the activities of the NSC Expert Group on Uncertainty Analysis in Modeling as well as discusses the progress of the OECD LWR UAM benchmark. The efforts of both NSC Expert Groups could be only undertaken within the framework of a program of international co-operation which have benefited from the coordination of the NEA/NSC and from interfacing with the CSNI activities. The authors wish to express their sincere appreciation for the outstanding support offered by Dr. E. Sartori, who has provided efficient administration, organization and valuable technical advice of both NSC Expert Groups.

*Key Words:* Verification, Validation, Uncertainty Analysis, International Cooperation, Coupled Calculations

## **1. INTRODUCTION**

The qualification procedure of coupled multi-physics code systems is based on the qualification framework (verification & validation) of separate physics models/codes, and includes in addition verification and validation of the coupling methodologies of the different physics models. The extended verification procedure involves testing the functionality, the data exchange between different physics models, and their coupling, which is designed to model combined effects determined by the interaction of models. The extended validation procedure compares the

predictions from coupled multi-physics code systems to available measured data and reference results. It is important to emphasize that such validation should be based on a multi-level approach similar to the one utilized in validating coupled neutronics/thermal-hydraulics codes in international standard problems. Appropriate benchmarks have been developed in international co-operation led by the Nuclear Energy Agency (NEA) of the Organization for Economic Cooperation and Development (OECD) that permits testing the neutronics/thermal-hydraulics coupling, and verifying the capability of the coupled codes to analyze complex transients with coupled core/plant interactions. The paper summarizes these activities conducted by the Expert Group on Reactor Stability and LWR Transient Benchmarks at the Nuclear Science Committee (NSC) of NEA/OECD. The Expert Group deals with modeling and benchmarking issues in the field of Three-Dimensional (3-D) coupled neutronics/thermal-hydraulics transients for nuclear cores and coupling of core phenomena and system dynamics for nuclear reactor core design and safety analysis. In recent years there has been an increasing demand from nuclear research, industry, safety and regulation for best estimate predictions to be provided with their confidence bounds. The ongoing OECD Light Water Reactor (LWR) Uncertainty Analysis in Modeling (UAM) benchmark activities contribute to establishing such unified framework to estimate safety margins, which would provide more realistic, complete and logical measure of reactor safety. The paper describes the activities of the NSC Expert Group on Uncertainty Analysis in Modeling as well as will discuss the progress of the OECD LWR UAM benchmark. Both activities are designed to address current regulation needs and issues related to practical implementation of risk informed regulation. Establishing such internationally accepted LWR UAM benchmark framework offers the possibility to accelerate the licensing process when using best estimate methods. The efforts of both NSC Expert Groups could be only undertaken within the framework of a program of international co-operation which have benefited from the coordination of the NEA/NSC and from interfacing with the Committee of Safety of Nuclear Installations (CSNI) activities.

## **2. EXPERT GROUP ON REACTOR STABILITY AND LWR TRANSIENT BENCHMARKS**

The objectives of the NSC in the field of coupled neutronics/thermal-hydraulics computing are to advance scientific knowledge needed for the development of advanced modeling techniques for new nuclear technologies and concepts, as well as for current nuclear applications. This includes:

- a) Driving recent development of coupled 3-D neutronics/thermal-hydraulic (multi-physics) codes;
- b) Validation and benchmarking of their performance through comparison with experiments;
- c) Verifying the correctness of methods and computer codes, building confidence in areas where research is very expensive or lacking;
- d) Determination of model uncertainties;
- e) Promotion of their use in production runs and safety analysis.

The Expert Group on Reactor Stability and LWR Transient Benchmarks deals with modeling and benchmarking issues in the field of 3-D coupled neutronics/thermal-hydraulics transients for

nuclear cores and coupling of core phenomena and system dynamics (PWR, BWR, VVER). The transients considered include:

- a) Rod Ejection (PWR);
- b) Uncontrolled Withdrawal of Control Rods (PWR);
- c) Main Steam-Line Breaks (PWR);
- d) BWR Stability, time series and frequency analysis;
- e) Cold water injection and core pressurisation (BWR);
- f) Turbine Trips (BWR) benchmark;
- g) VVER-1000 Coolant Transient Benchmark (V1000-CT);
- h) BWR Full-size Fine-mesh Bundle Test (BFBT);
- i) Critical Issues in Nuclear Reactor Technology (CRISSUE-S).

Appropriate benchmarks have been developed in international co-operation led by the Nuclear Energy Agency (NEA) of the Organization for Economic Cooperation and Development (OECD) that permits testing the neutronics/thermal-hydraulics coupling, and verifying the capability of the coupled codes to analyze complex transients with coupled core/plant interactions [1]. Such benchmarks are the OECD/NRC PWR Main Steam Line (MSLB) benchmark, the OECD/NRC BWR Turbine Trip (TT) benchmark, and the OECD/DOE/CEA VVER-1000 Coolant Transient (V1000CT) benchmark. In order to meet the objectives of the validation of “best-estimate” coupled codes, a multi-level methodology has been introduced to evaluate systematically the transients. Since these benchmarks are based on both code-to-code and code-to-data comparisons further guidance for presenting and evaluating results has been developed. These benchmarks are developed in an international co-operation to provide a validation basis for the new generation of best-estimate codes. Based on the previous experience, several benchmark exercises were defined for each benchmark consisting of different steady-states and transient cases, which allow for a consistent and comprehensive validation process. The introduction of extreme transient scenarios contributes to the study of different numerical and computational aspects of coupled simulations. The participants use a cross-section library, generated by the benchmark team, which removes the uncertainties introduced with using different cross-section generation and modeling procedures. The defined benchmark cross-section modeling approach is a direct interpolation in multi-dimensional tables with complete representation of the instantaneous cross-section cross-term dependencies. In this way the benchmarks provides the opportunity to study the impact of different thermal-hydraulics and neutronics models as well as the coupling between them on code predictions and to identify the key parameters for modeling important transients for different types of power reactors. This in turn allowed the evaluation of these key parameters, through the performance of sensitivity studies, which led the participants to develop a more in-depth knowledge of the capabilities of the current generation best estimate thermal-hydraulic system codes. The results of the OECD/NEA LWR benchmark activities are discussed in the Sub-section 2.1 on the example of Exercise 3 (coupled neutronics/thermal-hydraulic system modeling) for the OECD/NRC BWR TT benchmark.

These benchmarks have stimulated also follow up developments and benchmark activities such as the OECD/NRC BFBT benchmark [2]. The models utilized have been improved when moving from one benchmark to the next one – for example the need for more accurate prediction of void fraction in the BWR TT benchmark led to establishing the BFBT benchmark, and the need for more accurate vessel mixing in MSLB simulations led to formulation of the V1000CT benchmark. The needs to refine models for best-estimate calculations based on good-quality experimental data should not be limited to currently available macroscopic approaches but should be extended to next-generation approaches that focus on more microscopic processes. An international benchmark has been initiated based on data made available from the NUPEC (Nuclear Power Engineering Corporation) database. From 1987 to 1995, NUPEC performed a series of void measurements using full-size mock-up tests for both BWRs and PWRs. Based on state-of-the-art computer tomography (CT) technology, the void distribution was visualized at the mesh size smaller than the sub-channel under actual plant conditions. NUPEC also performed a steady-state and transient critical power test series based on the equivalent full-size mock-ups. Considering the reliability not only of the measured data, but also of other relevant parameters such as the system pressure, inlet sub-cooling and rod surface temperature, these test series supply the first substantial database for the development of truly mechanistic and consistent models for void distribution and boiling transition. The international OECD/NRC Benchmark based on the NUPEC BWR Full-size Fine-mesh Bundle Tests (BFBT) has been established and is underway. This benchmark encourages advancement in this uninvestigated field of two-phase flow theory with very important relevance to the nuclear reactors' safety margins evaluation. Another important contribution of this benchmark is the uncertainty analysis of void distribution and critical power predictions, which are added as additional exercises. These exercises take into account uncertainties on input data (boundary conditions, geometry, etc. provided by the Specifications) and on models and produce results with “errors”, which are compared with measurement uncertainties. The results of the OECD/NRC BFBT benchmark are presented and discussed in Sub-section 2.2 .

### **2.1. OECD/NRC BWR TT benchmark**

The results of the OECD/NEA LWR benchmark activities are discussed in this section on the example of Exercise 3 (coupled neutronics/thermal-hydraulic system modeling) for the OECD/NRC BWR TT benchmark. Turbine trip transients in a BWR are pressurization events in which the coupling between core space-dependent neutronics phenomena and system dynamics plays an important role. The data made available from actual experiments carried out at the Peach Bottom 2 plant make the present benchmark particularly valuable. The Exercise 3 consists of the base test case (the so-called Best Estimate Case) and hypothetical cases (the so-called Extreme Scenarios). The purpose of Exercise 3 Best Estimate Case is to provide comprehensive assessment of all the participating coupled codes in analyzing complex transients. In order to validate such assessments, available measured plant data are utilized for this case during the comparative analyses presented in this report. In addition to the base case, the analysis of the Extreme Scenarios provides a further understanding of modeling limitations of coupled codes and the interplays between different feedback mechanisms as well as testing the coupled code capabilities at extreme situations. The following four extreme scenarios are analyzed by the participants in the course of this exercise:

- a) Extreme Scenario 1: Turbine trip (TT) with steam bypass relief system failure;
- b) Extreme Scenario 2: TT without reactor scram;
- c) Extreme Scenario 3: TT with steam bypass relief system failure without reactor scram;
- d) Extreme Scenario 4: TT with steam bypass system failure, without scram and without safety relief valves (SRV) opening.

The key elements of Exercise 3 are illustrated in the simple BWR schematic given in Figure 1. Extreme Scenario 1 (TT without bypass system relief opening) and Extreme Scenario 2 (TT without scram) can be considered as single failures and therefore provide information from the perspective of the safety of the plant. Extreme Scenario 3 (combination of Extreme Scenarios 1 and 2), which considers the coincidence of two independent failures, and Extreme Scenario 4 (in addition to Extreme Scenario 3 no opening of safety relief valves), which considers the coincidence of three independent failures are extremely unlikely from a safety perspective, while they help with the understanding of the short-time dynamics of the reactor system. In the base case, SRVs are not opening during the transient while this happens in the Extreme Scenarios 1, 2, and 3. In hypothetical cases, the dynamical response of the system due to the interaction of the flow in the steam line with the dynamics of the safety relief valves (SRVs) happens to be more challenging for the coupled codes. Hence, the Extreme Scenario 4 serves as clear comparison of physical models of the participants' codes. It should be noted that no comparison with measured data is possible for the extreme cases since they are hypothetical scenarios. Therefore, submitted extreme scenario results are compared with an "average" of the results of the benchmark participants.

The averaged spatial and time-history distributions over 15 participants' results (using different coupled code systems) are presented in Fig. 2 and Fig. 3 and discussed in order to outline common modeling tendencies. The most challenging part of the BWR steady state analysis is the prediction of the void fraction distribution. From Fig. 2 it can be seen that the standard deviation increases in the lower (bottom) part of the core which indicates differences in the void modeling in terms of sub-cooled boiling and vapor slip. Subsequently these deviations are also reflected in the comparison of the axial power profile predictions due to the void feedback mechanism - see Fig. 3.

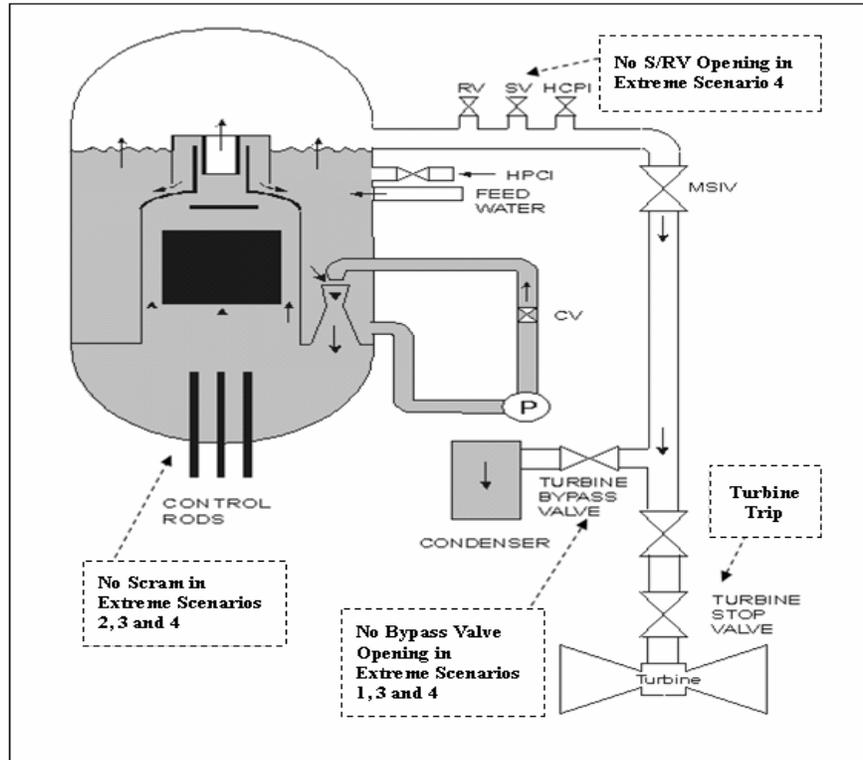


Figure 1. Key elements of Exercise 3 Best Estimate Case and Extreme Scenarios

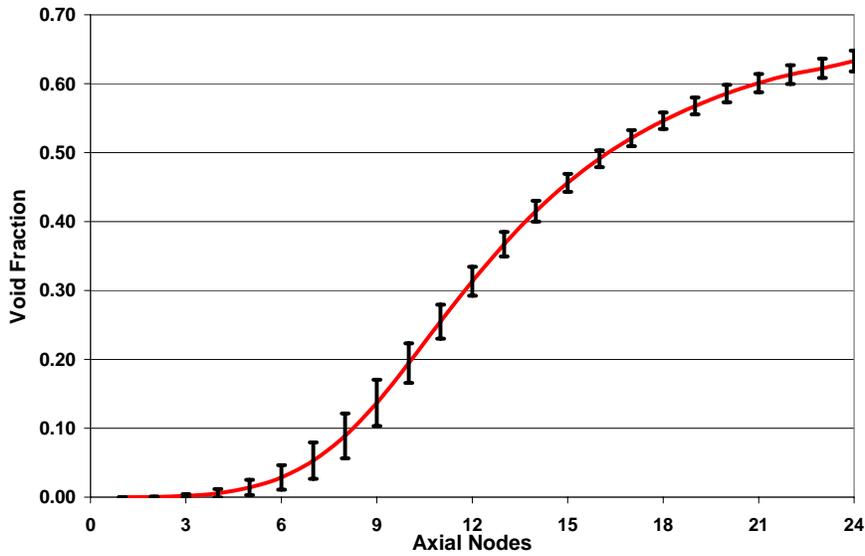
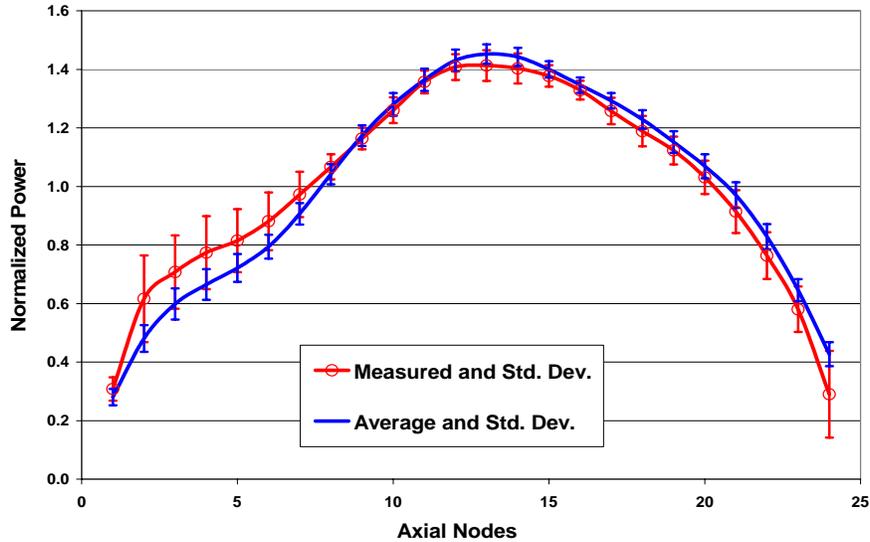


Figure 2. Steady state core average axial void fraction (mean and std. deviation)



**Figure 3. Steady state core average normalized axial power distribution (measured vs. mean and standard deviations)**

When analyzing the power history results in Fig. 4, it has to be taken into account that in the TT2 test, the thermal-hydraulic feedback alone limited the power peak and initiated the power reduction. The void feedback plays the major role while the Doppler feedback plays a subordinate role. The reactor scram then inserted additional negative reactivity and completed the power reduction and eventual core shutdown. The accurate prediction of void feedback during the transient depends on the modeling of the pressure wave propagation into the vessel. The indication of how successful is this modeling is the prediction of dome pressure time history – see Fig. 5. The participants’ results compared very satisfactory with measured data for the parameters dome pressure time history and power time history. These results increased the trustworthiness of the coupled code capabilities

As it was mentioned before the fourth extreme scenario is a turbine trip with no scram, no bypass system and no activation of SRVs. It provides both - a basis for better comparison of the physical models of the participants’ codes without external perturbations and a possibility to determine the eigenfrequency of the system. Such comparison for the fission power time history of the benchmark participants who have submitted results for this parameter is shown in Fig. 6.

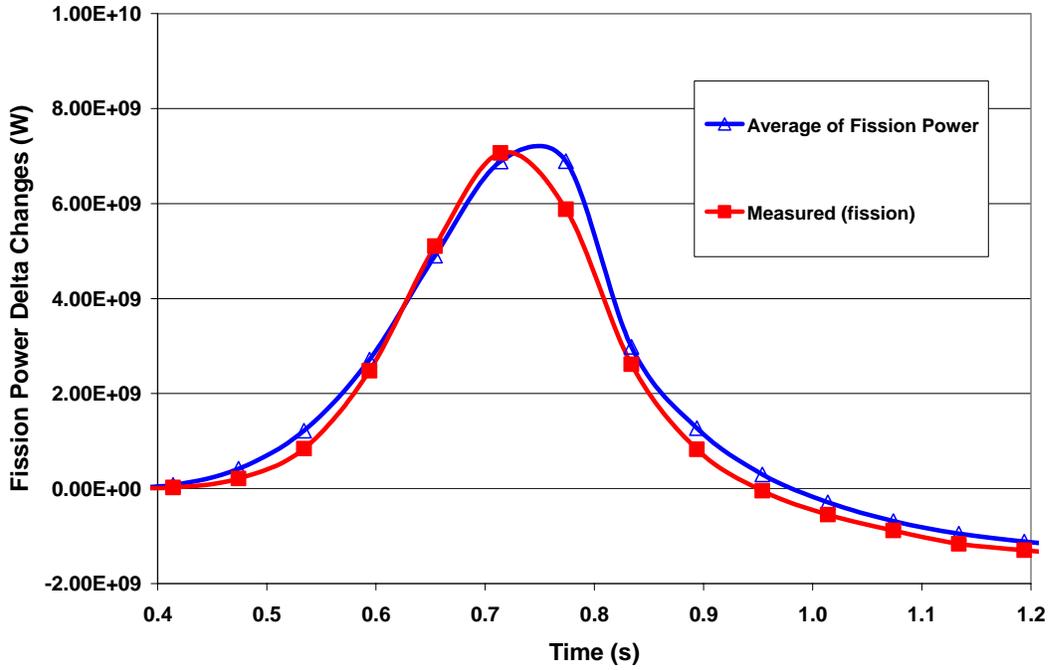


Figure 4. Best Estimate Case - Transient Fission Power Comparison (Average vs. Measured – zoom)

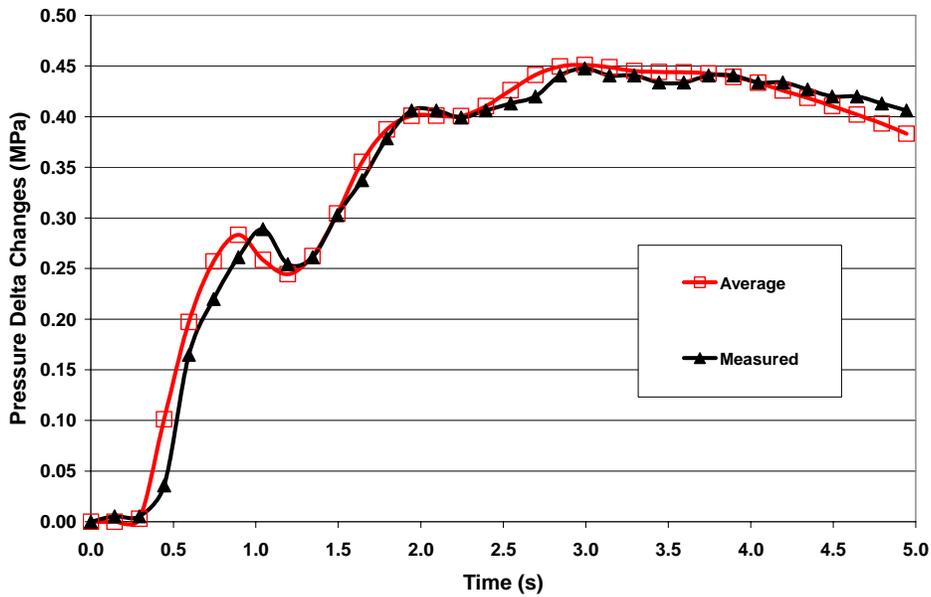
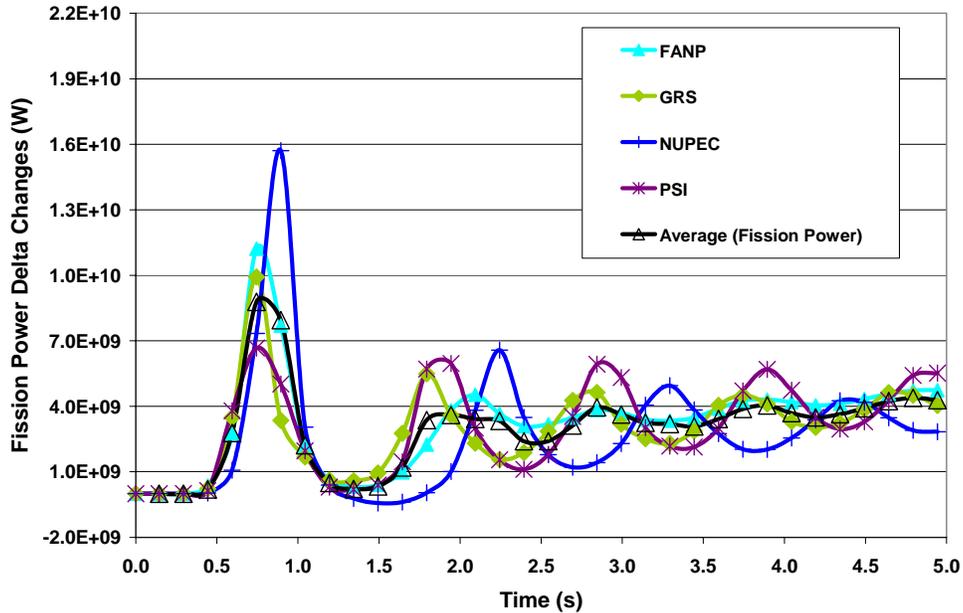


Figure 5. Best Estimate Case – Transient Dome Pressure (Average vs. Measured)



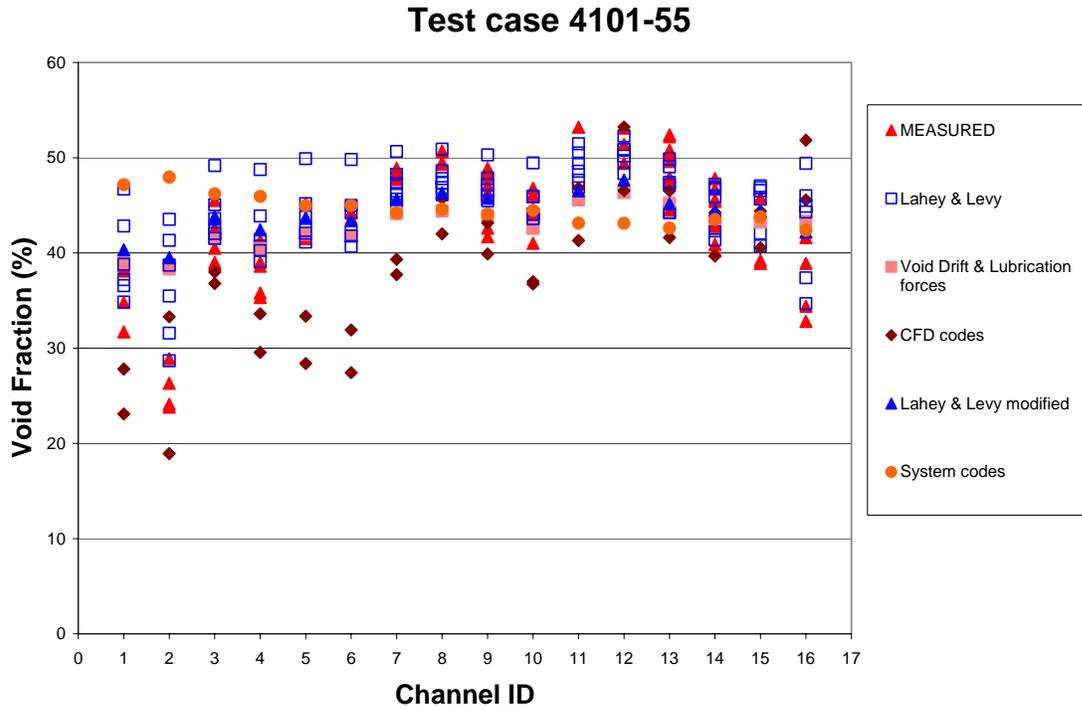
**Figure 6. Extreme Scenario 4 - Transient Power (Fission)**

## 2.2. OECD/NRC BFBT benchmark

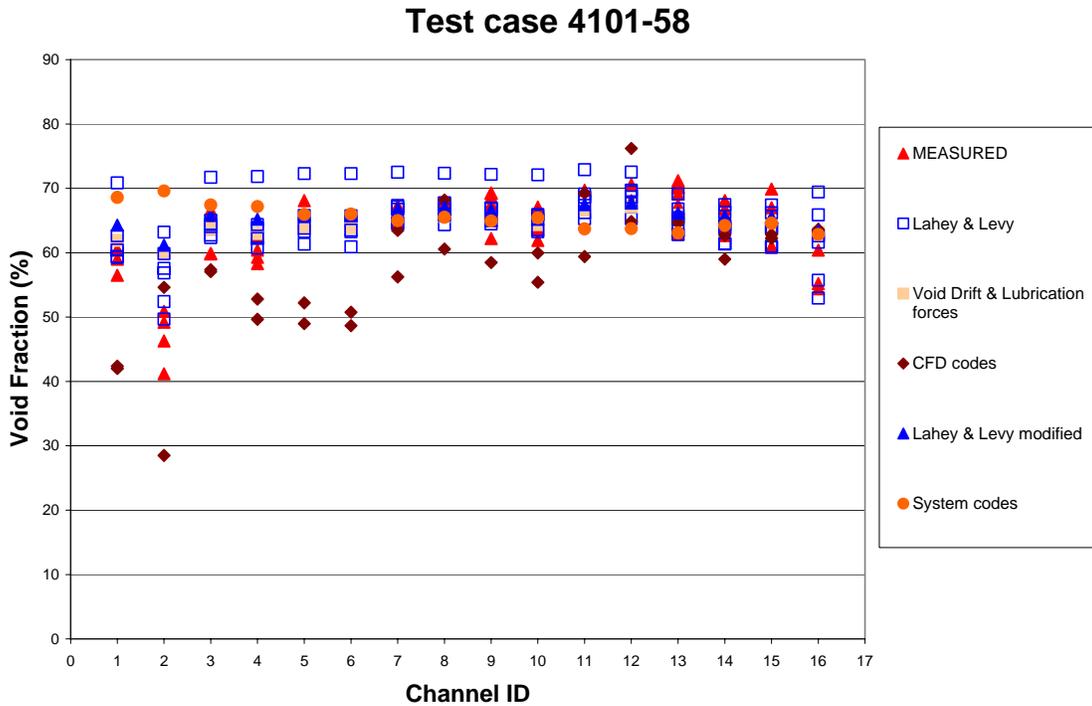
The BFBT benchmark is made up of two parts (phases), each part consisting of different exercises:

- Phase I – Void Distribution Benchmark
  - Exercise 1 (I-1) – Steady-state sub-channel grade benchmark
  - Exercise 2 (I-2) – Steady-state microscopic grade benchmark
  - Exercise 3 (I-3) – Transient macroscopic grade benchmark
  - Exercise 4 (I-4) – Uncertainty analysis of the steady state sub-channel benchmark
- Phase II – Critical Power Benchmark
  - Exercise 0 (II-0) – Pressure drop benchmark
  - Exercise 1 (II-1) – Steady-state benchmark
  - Exercise 2 (II-2) – Transient benchmark
  - Exercise 3 (II-3) – Uncertainty analysis of the steady critical power benchmark

It should be recognized that the purpose of this benchmark is not only to compare currently available macroscopic approaches but above-all to encourage the development of novel next-generation approaches that focus on more microscopic processes. Thus, the benchmark problem includes both macroscopic and microscopic measurement data. In this context, the sub-channel grade void fraction data are regarded as the macroscopic data and the digitized computer graphic images are the microscopic data. There are three types of codes participating in the benchmark – CFD, sub-channel and system codes. The results of the OECD/NRC BFBT benchmark activities are discussed in this section on the example of Exercise I-1.



**Figure 7. Turbulent mixing models and their effect on void distribution based on a sub-channel type for test case 4101-55**



**Figure 8. Turbulent mixing models and their effect on void distribution based on a sub-channel type for test case 4101-58**

When comparing the performance of the cross-flow models in Fig. 7 and Fig 8 (for two test cases within the benchmark framework of Exercise I-1), it could be concluded that the mixing length approach gives the best prediction of the measured data. The porous media approach (including CFD predictions) generally underestimates the void fraction.

The comparative analysis of all test cases of Exercise I-1 indicated the following tendencies:

- a) The scatter in code predictions is less for higher void fractions (greater than 70% - annular flow);
- b) Most scatter in calculations is observed for lower void fractions - bubbly to large bubble/slugging flow void fraction range (void fraction less than 40%);
- c) Significant scatter is seen in churn-turbulent void fraction range (approximately 40%);
- d) Most of the codes have difficulty predicting the void distribution near unheated structures (housing and water rods).

### **3. EXPERT GROUP ON UNCERTAINTY ANALYSIS IN MODELING**

In recent years there has been an increasing demand from nuclear research, industry, safety and regulation for best estimate predictions to be provided with their confidence bounds. Consequently an "in-depth" discussion on "Uncertainty Analysis in Modeling" was organized at the 2005 OECD/NEA NSC meetings, which led to a proposal for launching an Expert Group on "Uncertainty Analysis in Modeling" and the endorsement to hold a workshop with the aim of defining: future actions and a program of work.

As a result the OECD/NEA Workshop on Uncertainty Analysis in Modeling took place in Pisa, Italy, on April 28-29, 2006 (UAM-2006). The major outcome of the workshop was to prepare a benchmark work program with steps (exercises) that would be needed to define the uncertainty and modeling task. The other proposals made during the meeting would be incorporated under the different steps (exercises) within the overall benchmark framework for the development of uncertainty analysis methodologies for multi-physics (coupled) and multi-scale simulations.

Following the results from the UAM-2006 Workshop the OECD/NEA NSC at its June 2006 meeting endorsed the creation of an Expert Group on Uncertainty Analysis methods in Modeling [3]. This Expert Group will report to the Working Party on Scientific issues in Reactor Systems (WPRS). Since it addresses multi-scale/multi-physics aspects of uncertainty analysis, it will work in close co-ordination with the benchmark groups on coupled neutronics/thermal-hydraulics simulations and on coupled core-plant problems. The Expert Group will also coordinate its activities with the Group on Analysis and Management of Accidents (GAMA) of the Committee on Safety of Nuclear Installations (CSNI). The Expert Group has the following mandate:

1. To elaborate a state-of-the-art report on current status and needs of sensitivity and uncertainty analysis (SA/UA) in modeling, with emphasis on multi-physics (coupled) and multi-scale simulations.

2. To identify the opportunities for international co-operation in the uncertainty analysis area that would benefit from coordination by the NEA/NSC.
3. To create a roadmap along with schedule and organization for the development and validation of methods and codes required for uncertainty analysis including the benchmarks adequate to meet those goals.

The NEA/NSC has endorsed that this activity be undertaken with the Pennsylvania State University (PSU) as the main coordinator and host with the assistance of the Scientific Board. To summarize, in addition to LWR best-estimate calculations for design and safety analysis, the different aspects of uncertainty analysis in modeling are to be further developed and validated on scientific grounds in support of its performance. There is a need for efficient and powerful analysis methods suitable for such complex coupled multi-physics and multi-scale simulations. The proposed benchmark sequence addresses this need by integrating the expertise in reactor physics, thermal-hydraulics and reactor system modeling as well as uncertainty and sensitivity analysis, and will contribute to the development and assessment of advanced/optimized uncertainty methods for use in best-estimate reactor simulations.

### **3.1. OECD LWR UAM benchmark**

In the proposed comprehensive international LWR Uncertainty Analysis in Modeling benchmark activity different uncertainty analysis methods for coupled codes will be compared, and their value assessed including the validation of the methodologies for uncertainty propagation [4]. For the first time the uncertainty propagation will be estimated through the whole simulation process on a unified benchmark frame-work to provide credible coupled code predictions with defensible uncertainty estimations of safety margins at the full core/system level. The benchmark will allow not only to compare and to assess the current UA methods on representative applications but also will stimulate the further development of efficient and powerful UA methods suit-able for complex coupled code simulations and will help to formulate recommendations and guidelines on how to utilize advanced and optimized sensitivity analysis and UA methods in “best estimate” coupled reactor simulations in licensing practices.

The above-described approach is based on the introduction of nine steps (Exercises), which allows for developing a benchmark framework which mixes information from the available integral facility and NPP experimental data with analytical and numerical benchmarking. Such an approach compares and assesses current and new uncertainty methods on representative applications and simultaneously benefits from different methodologies to arrive at recommendations and guidelines. These nine steps (Exercises) are carried out in three phases.

### **3.1. Safety Implications**

The expected impact and benefits of the OECD LWR UAM benchmark activity for LWR safety and licensing are summarized in [5]. This benchmark project is challenging and responds to the needs of estimating confidence bounds for results from simulations and analysis in real applications. Among the expected results of this project are:

- a) Systematic identification of uncertainty sources;

- b) Systematic consideration of uncertainty and sensitivity methods in all steps. This approach will generate a new level of accuracy and will improve transparency of complex dependencies;
- c) All results will be represented by reference results and variances and suitable tolerance limits;
- d) The dominant parameters will be identified for all physical processes;
- e) Support of the quantification of safety margins;
- f) The experiences of validation will be explicitly and quantitatively documented;
- g) Recommendations and guidelines for the application of the new methodologies will be established.

The OECD LWR UAM activity will establish an internationally accepted benchmark framework to compare, assess and further develop different uncertainty analysis methods associated with the design, operation and safety of LWRs. As a result the LWR UAM benchmark will help to address current nuclear power generation industry and regulation needs and issues related to practical implementation of risk informed regulation such as:

- a) Incorporating an assessment of safety significance or relative risk in US NRC regulatory actions;
- b) Making sure that the regulatory burden imposed by individual regulations or processes is commensurate with the importance of that regulation or process to protecting public health and safety and the environment.

The realistic evaluation of consequences must be made with best estimate coupled codes, but to be meaningful, such results should be supplemented by an uncertainty analysis. The use of coupled codes allows to avoid unnecessary penalties due to incoherent approximations in the traditional decoupled calculations, and to obtain more accurate evaluation of margins regarding licensing limit. This becomes important for licensing power upgrades, improved fuel assembly and control rod designs, higher burn-up and others issues related to operating LWRs as well as to the new Generation 3+ designs being licensed now (ESBWR, AP-1000, EPR-1600 and etc.). Establishing such internationally accepted LWR UAM benchmark framework offers the possibility to accelerate the licensing process when using best estimate methods and contributes to establishing a unified framework to estimate safety margins, which would provide more realistic, complete and logical measures of reactor safety.

### 3. CONCLUSIONS

It is expected that the application of coupled multi-physics codes for safety analyses will be continuously growing. In fact, they are the only means to perform best-estimate calculations for accident conditions with a tight coupling of neutronics and thermal-hydraulics effects. Developing multi-level benchmarks, which utilize the available experimental data (such as the described in this paper OECD/NRC BWR TT Benchmark) for consistent validation and

verification of coupled multi-physics codes in international co-operation is of significant importance.

Recently the NEA/NSC has decided to introduce a new OECD benchmark based on NUPEC PWR Sub-channel and Bundle Tests (PSBT) as follow-up benchmark activities of the OECD/NRC BFBT benchmark.

The current tendencies in coupled code developments are towards systematic integration of uncertainty and sensitivity analysis with simulations for safety analysis. Sensitivity and uncertainty analysis capabilities must be further developed for comprehensive coupled code simulations with nonlinear feedback mechanisms as well as tested for uncertainty propagation through multi-physics multi-scale calculations on comprehensive benchmark frameworks as the described in this paper OECD LWR UAM benchmark.

### ACKNOWLEDGMENTS

The authors wish to express their sincere appreciation for the outstanding support offered by Dr. E. Sartori, who has provided efficient administration, organization and valuable technical advice of the NSC Expert Groups. This paper is devoted to Dr. Sartori and his contributions in verification & validation and uncertainty analysis in multi-physics modeling for nuclear reactor design and safety analysis.

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