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## Validation of coupled thermal-hydraulic and neutronics codes in international co-operation

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### **Abstract:**

Incorporating full three-dimensional models of the reactor core into system transient codes allows for a “best-estimate” calculation of interactions between the core behavior and plant dynamics. Considerable efforts have been made in various countries and organizations on the development of coupled thermal-hydraulic and neutronics codes. Appropriate benchmarks have been developed in international co-operation led by NEA/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. Three such benchmarks are presented in this paper – the OECD/NRC PWR MSLB benchmark, the OECD/NRC BWR TT benchmark, and the OECD/DOE/CEA V1000CT benchmark. In order to meet the objectives of the validation of best-estimate coupled codes a systematic approach has been introduced to evaluate the analyzed transients employing a multi-level methodology. 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. During the course of the benchmark activities a professional community has been established, which allowed carrying out in-depth discussions of different aspects considered in the validation process of the coupled codes. This positive output has certainly advanced the state-of the art in the area of coupling research.

## **1 INTRODUCTION**

Incorporating full three-dimensional (3D) models of the reactor core into system transient codes allows for a “best-estimate” calculation of interactions between the core behavior and plant dynamics. Recent progress in computer technology has made the development of coupled thermal-hydraulic (T-H) and neutron kinetics code systems feasible. Considerable efforts have been made in various countries and organizations in this direction. 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 of two particular aspects. One is to verify the capability of the coupled codes to analyze complex transients with coupled core-plant interactions. The second is to test fully the neutronics/thermal-hydraulics coupling. One such benchmark is the Pressurized Water Reactor (PWR) Main Steam Line Break (MSLB) benchmark problem [1]. It was sponsored by the NEA/OECD, the United States Nuclear Regulatory Commission (US NRC), and the Pennsylvania State University (PSU). The benchmark problem uses a three-dimensional neutronics core model and thermal-hydraulics core and system models that are based on real plant design and operational data for Three Mile Island – Unit 1 (TMI-1) Nuclear Power Plant (NPP). A similar coupled code benchmark has been developed for Boiling Water Reactors (BWR) also under the sponsorship of NEA/OECD, US NRC and PSU [2]. The

chosen plant transient is a turbine trip (TT) and the reference design is based on the Peach Bottom-2 (PB-2) NPP. Unlike the PWR MSLB benchmark, measured plant data is available, rendering this benchmark potentially very valuable. In the framework of a joint effort between the NEA/OECD, the United States Department of Energy (US DOE), and the Commissariat à l'Énergie Atomique (CEA), France a coupled 3D neutron kinetics/thermal hydraulics benchmark was defined for a VVER-1000 type reactor named VVER-1000 Coolant Transient (V1000CT) benchmark. The benchmark is based on data from the Unit 6 of the Bulgarian Kozloduy NPP (KNPP). In performing this work the PSU and CEA-Saclay have collaborated with Bulgarian organizations, in particular with the KNPP and the Institute for Nuclear Research and Nuclear Energy (INRNE). The benchmark consists of two phases - Phase 1 (V1000CT-1): Main Coolant Pump Switching On [3]; and Phase 2 (V1000CT-2): Coolant Mixing Tests and MSLB [4]. These three benchmarks are presented in this paper. In order to meet the objectives of the validation of best-estimate coupled codes, a systematic approach has been introduced to evaluate the analyzed transients. A multi-level methodology is employed including the application of different phases and exercises, evaluation of several steady states, and simulation of multiple transient scenarios. Since these benchmarks are based on both code to code and code to data comparisons further guidance for presenting and evaluating results has been established employing statistical techniques. The lessons learned while applying the aforementioned multi-level methodology in each benchmark are outlined and discussed in separate sections of the paper. In addition, these benchmarks have stimulated follow up developments and benchmark activities, which are briefly presented in the concluding section.

## **2 OECD/NRC PWR MSLB BENCHMARK**

This benchmark is based on real plant design and operational data for the TMI-1 NPP. The purpose of this benchmark is three-fold: to verify the capability of system codes for analyzing complex transients with coupled core-plant interactions; to test fully the 3D neutronics/thermal-hydraulics coupling; and to evaluate discrepancies among the predictions of coupled codes in best-estimate transient simulations. The purposes of the benchmark are met through the application of three exercises: a point kinetics plant simulation (Exercise 1), a coupled 3D neutronics/core thermal-hydraulics evaluation of core response (Exercise 2), and a best-estimate coupled core-plant transient model (Exercise 3).

### **2.1 Transient**

The initiating event of the MSLB is assumed to be a double-ended rupture of one steam line upstream of the main steam isolation valve (MSIV) at the cross-connect. The loss of the secondary coolant causes a decrease in steam pressure and an increase of steam flow through the steam generator (SG) connected to the ruptured steam line. The higher steam flow rate increases heat transfer from the primary to the secondary side and results in lower coolant temperature in the loop of the broken steam line. Because of the large negative moderator temperature coefficient, the lower coolant temperature in the core region causes a positive reactivity insertion in the core and consequently a power increase. The reactor is tripped because of either too low reactor coolant pressure or high neutron flux. Following the reactor trip, the turbine trips and the turbine stop valves and feedwater control valves close. The low steam line pressure initiates the automatic feedwater isolation, which causes the SG associated with the rupture to blow dry. The high-pressure injection (HPI) system may be activated by low reactor coolant system (RCS) pressure during the cooldown period following a large area steam line break.

One of the major concerns for the MSLB is the return to criticality and/or return to power in the second half of the transient. To maximize the conservative conditions for the return to power, the MSLB transient is assumed to take place at hot full power (HFP) operating conditions at the end of cycle (EOC). The limiting MSLB for TMI-1 is at HFP because the SG liquid inventory increases as the power level increases; the worst case overcooling occurs at the maximum power level, which corresponds to the maximum liquid inventory in the SG.

Another conservative assumption is that the control rod with the maximum worth is stuck in a fully withdrawn position throughout the transient. This is a limiting condition because it reduces the available scram worth even further, and increases the probability of a return to power.

## 2.2 Methodology

In order to meet the objectives of the validation of best-estimate coupled codes a systematic approach has been introduced to evaluate the PWR MSLB transient. Such coupled codes use separate temporal and spatial models and numerical methods for core neutronics, core thermal-hydraulics and system thermal-hydraulics simulations. Therefore, the validation of these codes should include testing of these models for the defined transient (in this case a MSLB) as a separate exercise of the overall benchmark. The ultimate goal is to enable participants to initiate and verify these models before focusing on the major objective – testing of coupling methodologies in terms of numerics, temporal and spatial mesh overlays. This systematic approach allows one to evaluate in a more consistent way the modeling of the combined effects (determined by neutronics/T-H as well as core/plant interactions) and removes the uncertainties introduced with the separate models. In order to perform such a comprehensive validation of coupled codes a multi-level methodology is employed. The methodology includes the application of three exercises, the evaluation of several steady states, and the simulation of multiple transient scenarios.

To allow better testing of 3D coupled-code predictions there are two versions of the MSLB transient scenario: one corresponding to the licensing practice scenario and another extreme scenario. In the second scenario the 3D models are expected to predict return to power because of the conservative assumptions. Both scenarios have the same initial conditions and follow the same sequence of events. The difference is the value of the tripped control rod worth, which for the coupled calculations is achieved through modifying the rod thermal absorption cross-sections for control rod groups.

Exercise 1 is defined as “point kinetics (PK) plant simulation”. The purpose of this exercise is to test the primary and secondary system model responses. Compatible PK model inputs, which preserve axial and radial power distributions and tripped rod reactivity, are taken from the coupled three-dimensional (3D) kinetics/system T-H calculations, and are provided in the Specification as input data. Exercise 2 is defined as an evaluation of the core response to imposed system T-H conditions. The Benchmark Specification provides a complete core description, a cross-section library, and also initial and transient boundary conditions (BC) for 18 T-H channels. The BCs include radial distribution of the mass flow rates, liquid temperatures at the core inlet, and pressure at the core outlet. Exercise 3 is defined as a best-estimate coupled-core plant transient modeling. This exercise provides the opportunity to study the impact of different neutronics and T-H models on code predictions, as well as the coupling between them.

Since the MSLB benchmark is based on code-to-code comparisons, a statistical methodology has been established for presenting and evaluating the results. The situation is complicated by the lack of experimental data. The reference values are calculated based on the statistical mean value of all submitted results except obviously outlying solutions. While

not perfect, this method provides a strong basis for a statistical analysis and comparison of the results. In all phases of the MSLB problem, several types of data had to be analyzed, and the results of all participants compared. The analyzed data types were: Type I - Time History Data; Type II - 2D Radial Distributions; Type III - 1D Axial Distributions; and Type IV – Singular Parameter Values.

## 2.3 Results

Overall, this benchmark has been well accepted internationally, with about 15 participants representing 11 countries in each exercise. The results submitted by the participants for each exercise are used to make code-to-code comparisons and a subsequent statistical analysis. The results encompass several types of data for both thermal-hydraulics and neutronics parameters at the initial steady state conditions and throughout the MSLB transient. The final reports on the first, second and third exercises [5, 6, 7] contain summaries of the comparison of the participants' results. This information is presented in plots graphically illustrating the agreement of different code predictions and tables containing relative differences for each of the participants' results for each parameter. First the mean values and standard deviations are calculated. Participants' deviations and figures of merit are calculated relative to the mean solution.

Based on the comparisons of participants' results for Exercise 1 it was concluded that the deviations in the predictions of system-parameters time histories are due to both the modeling differences and the different theoretical models of the codes. These modeling differences were identified as follows: the conservative initial steam generator (SG) masses, the modeling of the additional feed water to the broken SG, the steam line break flow modeling, the flow paths to the upper head of reactor vessel, and the different reactor vessel mixing models. The need of resolving these issues was addressed by carrying out parametric studies that demonstrated sensitivity of power response during the MSLB transient to key input parameters. This fact initiated a discussion in depth about the main effects during a MSLB transient and their sensitivity to the modeling assumptions. As a result, a three-step procedure was applied: additional information was provided, some modeling assumptions were specified explicitly (such as the additional feed water to the broken SG which was specified as feed water mass flow rate vs. time), and other assumptions were made consistent (such as the SG initial mass). The lessons learned in the Exercise 1 were applied also to the third exercise.

The power response and the magnitude of the return to power during the transient as predicted by different codes are functions of the total reactivity time evolution (see Figures 1 and 2). The differences arise from the different predictions of moderator feedback and Doppler feedback reactivity components, as well as the prediction of the inserted negative reactivity of the tripped rod during the dynamic scram simulation. The moderator reactivity component follows the cold leg temperature. The discrepancies in the cold leg temperature predictions are due mostly to differences in the secondary side models. It was observed that the major factors affecting the dynamics of the transient are the break flow modeling (critical flow model), the liquid entrainment, the modeling of the aspirator flow, and the nodalization of the SG down comer. These factors affect the SG mass parameter for both the broken and the intact SGs. This parameter shows the greatest deviation amongst participants' results, both in the value and behavior of the SG masses throughout the transient. In addition the disagreement can be attributed to differences in the heat-transfer correlations used within each code. This is especially true for the participants who use proprietary correlations that are specific to U-Tube SGs in their codes; the behavior of a Once Through SG (OTSG) is much different than a U-Tube SGs, and also involves superheat, something U-Tube SGs do not have. The Doppler feedback reactivity predictions are sensitive to the relation used for

Doppler fuel temperature as well as to the used radial and axial nodalization of the heat structure (fuel rod).

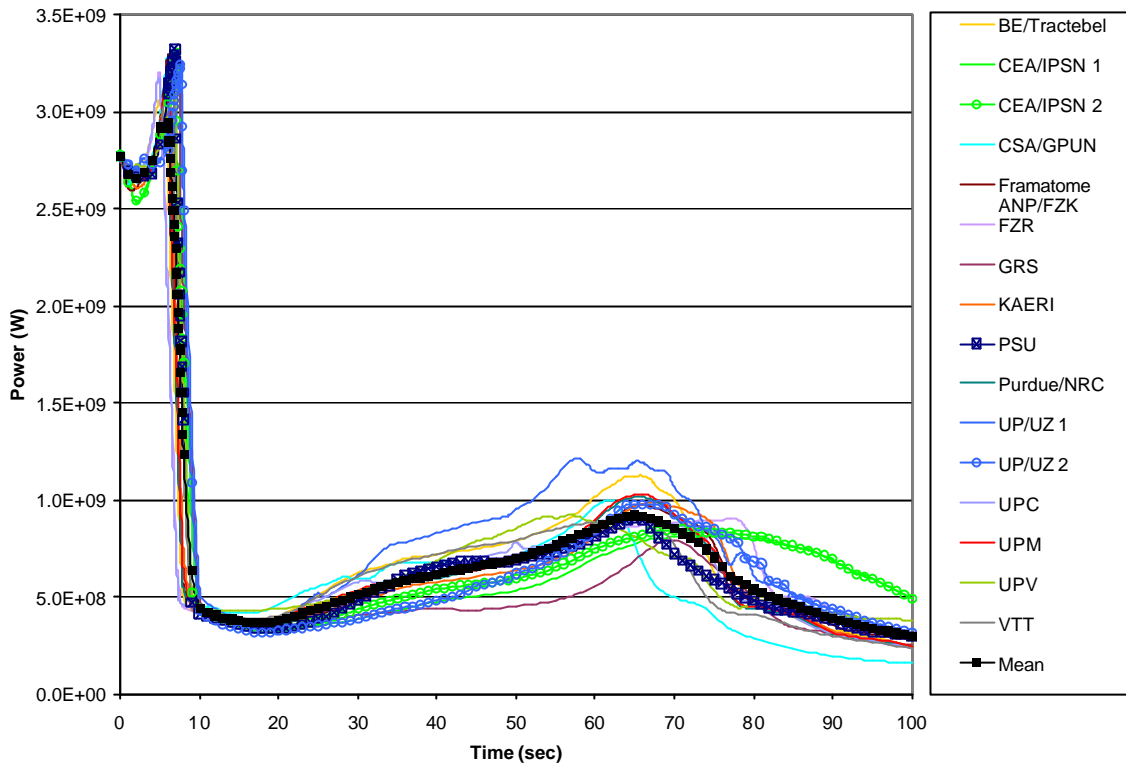


Figure 1. Core-Averaged Total Power Time History for Extreme Scenario, Exercise 3 of PWR MSLB Benchmark

Overall, it was determined that for the system behavior prediction in this benchmark, the key parameters were the SG masses, the break flow rates, the coolant and fuel temperatures, and the powers. The other parameters were valuable to analyze because they helped to determine what was causing the behavior of the key parameters. As expected, the break flow rates/modeling was very sensitive to the SG masses/modeling and vice versa. In addition, it was proven that the SG model has a great effect on the power throughout the transient. In particular, the way the additional feed water was introduced into the steam generator, the aspirator junction area, the down comer nodalization, and the OTSG model in general proved to be very important. During the Exercise 2 of this benchmark it was determined that the key parameters for coupled core modeling were the thermal-hydraulic core modeling and the spatial coupling schemes with the core neutronics model; the spatial decay heat modeling; and the Doppler temperatures and density correlations, used by the thermal-hydraulics codes. This conclusion was confirmed in the analysis of the Exercise 3. As expected, the axial distributions after the scram were very sensitive to the spatial decay heat modeling. In addition, it was proven that the detail of the core thermal-hydraulic models has a great effect on the radial power distribution throughout the transient. In particular, the differences can be up to 15 % for the snapshot at the time of highest return to power affecting local safety parameters such as maximum nodal fuel temperatures. Different code formulations/correlations for Doppler temperature and moderator density, affected both core average power and reactivity time histories and local distributions throughout the transient since these two parameters are the major feedback parameters for the cross-section modeling impacting in this way the neutronic predictions.

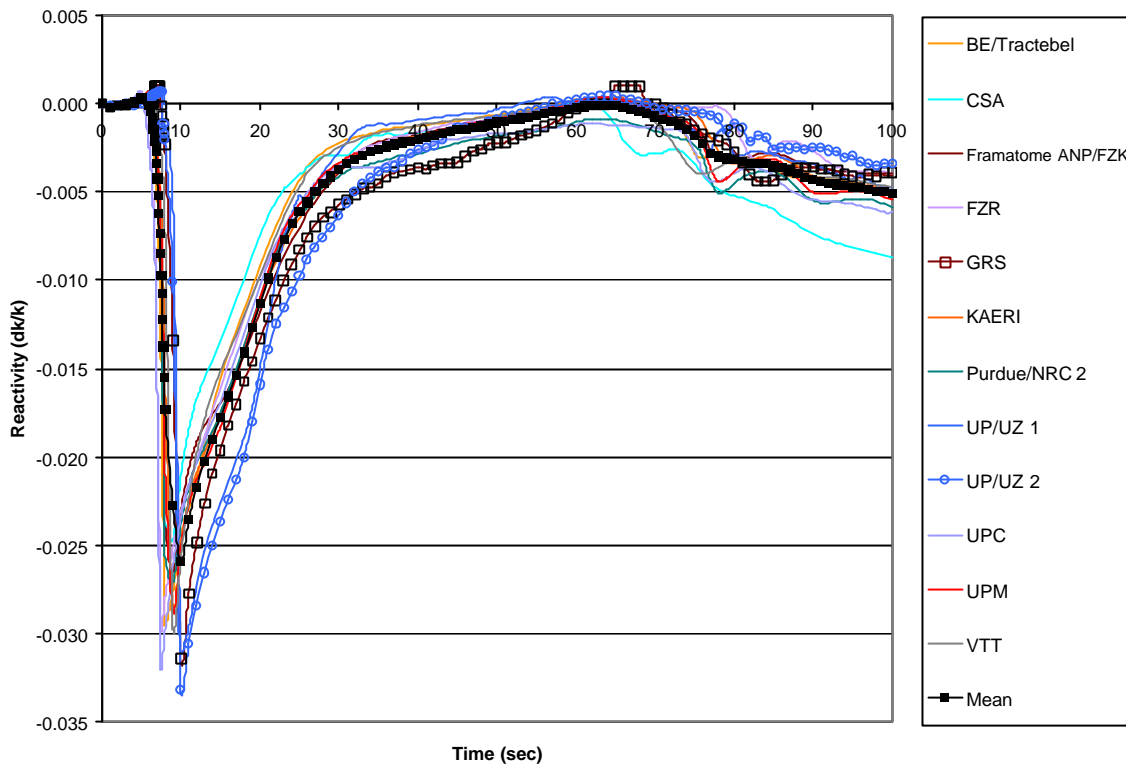


Figure 2. Core-Averaged Total Reactivity Time History for Extreme Scenario, Exercise 3 of OECD/NRC PWR

MSLB Benchmark

The observed discrepancies in the core averaged radial distributions, local axial distributions (in the position of the stuck rod), and maximum nodal Doppler temperature time history (especially for the return to power scenario) are mostly due to the detail of spatial coupling schemes: from very detailed spatial mesh overlays (one neutronics node per thermal-hydraulic cell/channel) to coarser mesh overlays (18-channel model). During the course of the MSLB transient, a power spike is seen at the position of the stuck rod. However, in the 18-channel model this assembly is averaged with several of the surrounding assemblies while mapping the neutronics model to the thermal-hydraulics model. This has the significant effect of underestimating the feedback in this part of the core. On the other hand, the 177-channel model (one neutronic assembly per T-H channel) is expected to more accurately predict the feedback (as a result of a better spatial feedback resolution), and therefore the relative power shape, near the stuck rod. This was seen very clearly from the comparisons of participants' results for the snapshot taken at time of highest return to power for transient scenario 2. The observed deviations (up to 15 %) in radial power distribution are due mostly to the different thermal-hydraulic (about 5 %) and heat structure (about 10 %) nodalization and mapping schemes. This result is very relevant since from a safety point of view, the possibility of a return to power in the later half of a MSLB transient is of great importance.

Participants' kinetics models for the benchmark utilized mostly a one node per assembly (npa) scheme in the radial plane. The benchmark team and some participants also developed a more detailed neutronic model using a 4-npa scheme in the radial plane and the subsequent mapping schemes. Comparative studies were performed for the extreme MSLB scenario with expected return to power. The obtained results demonstrated that the refinement of the neutronic model in the radial plane does not impact the total power transient evolution. The neutronic scheme refinement impacts local radial power distributions but not to the extent of the impact of the T-H nodalization. These parametric studies indicated that the MSLB calculations are mostly sensitive to the detail of the thermal-

hydraulic core modeling. The MSLB simulations are less sensitive to the radial refinements of the neutronic model, especially when coarser nodalization for the thermal-hydraulic core model is used. This reflects the feedback phenomena involved in the MSLB transient since the asymmetric cooling is the driving force of the transient.

Comparisons of the results of Exercise 1 (performed using point kinetics models) and Exercise 3 (performed using 3D neutronics models) demonstrate that the 3D analysis removes some of the conservatism inherent in point-kinetics analysis. The differences are believed to be caused by the inability of standard point-kinetics approaches to properly account for the moderator density feedback, dynamic scram simulation, local effects, and flux redistribution, which occur during the transient. As a result the 3D core transient modeling provides a margin to re-criticality over the point-kinetics approach during an MSLB analysis. Such a margin is desirable due to the extended refueling cycles and high burnups, which result in increasingly negative moderator temperature coefficients.

As mentioned previously, the simulated main steam line break transient results in asymmetric power and temperature distributions within the core region. As a result of this asymmetry, the assumption of 100% mixing within the core leads to non-conservative and non-realistic results. In order to determine the appropriate mixing percentage to be used when modeling such a transient several tests were performed at the Oconee Plant, which has a vessel identical to TMI-1. These tests were used to determine the amount of loop flow mixing that occurs within the reactor vessel when there is a large difference in the cold leg temperature behavior. For the MSLB benchmark problem, a ratio of 0.5 was chosen to limit the analysis at an upper value. In addition, the mixing was set to be 20% in the lower plenum and 80% in the upper plenum. The influence of the coolant mixing within the reactor pressure vessel on transient results was studied by some participants. They have observed that the coolant mixing ratio has an impact on the accident consequences. This is a drawback of the system codes using 1-D parallel channel models of the reactor core – the coolant mixing is input dependent and requires preliminary experimental knowledge. The codes, which have complete 3-D vessel T-H modeling information, do not need such input information but need to be validated for these applications.

### **3 OECD/NRC BWR TT BENCHMARK**

Following the success of the PWR MSLB benchmark another OECD/NRC sponsored coupled-code benchmark was defined for a BWR TT transient. Turbine trip transients in a BWR are pressurization events in which the coupling between core space-dependent neutronic phenomena and system dynamics plays an important role. In addition, the available real plant experimental data makes this benchmark problem very valuable. Over the course of defining and coordinating the BWR TT benchmark, the systematic validation approach, established during the PWR MSLB benchmark, was further developed to study different numerical and computational aspects of coupled best-estimate simulations.

#### **3.1 Transient**

Three TT transients at different power levels were performed at the PB-2 NPP (a GE BWR/4) prior to shutdown for re-fueling at the end of Cycle 2 in April 1977. The second test (TT2) has been selected for the benchmark problem since it has the highest quality measured dataset in order to investigate the effect of the pressurization transient (which follows the sudden closure of the turbine stop valve) on the neutron flux in the reactor core. The tests were designed to produce plant/core responses that approached the design basis conditions as closely as possible. The actual data were collected, including a compilation of reactor design

and operating data for Cycles 1 and 2 and the plant transient experimental data. This transient was selected for this benchmark study because it is a dynamically complex event with reactor variables changing very rapidly, and it constitutes a good problem to test the coupled codes on both levels: neutronics/thermal-hydraulics coupling, and core/plant system coupling. 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. Figure 3 illustrates the measured time history data of the core fission power and total reactivity. This provides a unique opportunity for a comprehensive feedback testing and examination of capability of advanced codes to analyze complex transients with coupled core/plant interactions through comparison with actual experimental data.

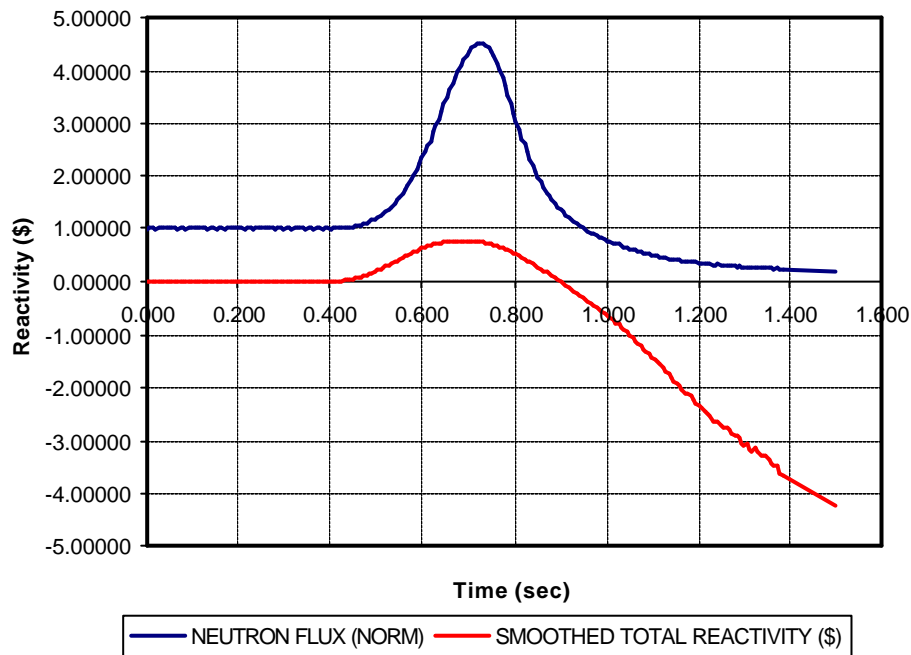


Figure 3. Neutron Flux and Reactivity Time Evolution for PB2 TT2

### 3.2 Methodology

The chosen benchmark transient – the turbine trip transient – is a rapid pressurization event in BWR reactors, which is characterized by tightly coupled thermal-hydraulic/neutronics phenomena. The core spatial effects are dominated by the axial changes; however, at the end-of-cycle 2, a slight radial non-symmetry exposure exists, which introduces radial spatial effects in the initial steady state. This radial non-symmetry has negligible impact on the transient response since the radial power distribution remains fairly uniform throughout the pre-scram portion of the transient. Previous Exelon (utility operating PB2 NPP) studies indicated that using a one-dimensional (1D) neutron kinetics model has limitations. First, a “single channel” core model with average power and flow does not respond dynamically in the same way as the average of all the channels – 3D average. Second, 1D cross-sections are dependent on the core thermal-hydraulic model used for their generation i.e. they are not universal and additional “normalization” procedures are needed to adjust these cross-

sections for specific code applications. The previous studies also demonstrated the major difficulty in validating coupled codes – it is difficult to determine if inaccurate thermal-hydraulic response is driving inaccurate neutronic response or vice versa. Similar relationships exist within the core/system interactions. In order to solve these problems the consistent benchmark approach, developed during the PWR MSLB benchmark, was utilized – the BWR TT benchmark consists of three separate exercises, two initial states and five transient scenarios. This approach provides opportunities for both a comprehensive validation and studying of the coupled codes and associated models.

The first exercise consists of performing a system thermal-hydraulic calculation with no neutron kinetics model involved – core power (or reactivity) is a fixed input for the PB-2 TT transient. The purpose of the first exercise is to test the thermal-hydraulic system response and to initialize the participants' system models. This approach is used to develop/refine key sub-models including steam lines, steam bypass system, jet pumps, steam separators and upper down-comer region where a distinct steam-water interface exists. The second exercise consists of performing coupled-core boundary conditions calculations. The purpose of the second exercise is to test and initiate the participants' core models. Thermal-hydraulic boundary conditions are provided to the participants from the benchmark team. The thermal-hydraulic core boundary conditions provided are the core inlet pressure, core exit pressure, core inlet temperature and core inlet flow. In summary the second exercise consists in performing a coupled 3D kinetics/T-H calculation for the reactor core using the boundary conditions provided at core inlet and exit. Three-dimensional two-group macroscopic cross-section libraries are provided to the participants. The core inlet flow is provided in two formats: total core flow as a function of time and radially distributed flow as a function of time for thirty-three channels. In addition, the benchmark team provided participants with normalized power vs. flow correlations for the different assembly types based on the detailed modeling in which each assembly represented by a thermal-hydraulic channel for the initial steady-state conditions. The studies performed by the benchmark team indicated that these correlations also apply reasonably well during the transient, which provided an opportunity for the participants to develop their own core coupled spatial mesh overlays. An additional steady state was defined in the framework of the second exercise – hot zero power (HZP) state with fixed thermal-hydraulic feedback. This allows for “clean” initialization of the core neutronics models and cross-section modeling algorithms. The third exercise consists of performing a coupled 3D kinetics/T-H calculation for the core and 1D thermal-hydraulics modeling for the balance of the plant. There are five transient scenarios – the best estimate scenario (the real test with available measured data) and four extreme versions. The extreme scenarios were introduced to provide the opportunity to better test the coupling and feedback modeling since they represent challenges for modeling the existing strong interactions between neutronics and thermal-hydraulics:

- Turbine trip without bypass system relief opening, which increases the peak pressure, and thus, the power peak and provides enough pressurization for safety/relief valve opening;
- Turbine trip without scram, which produces secondary power peaks, that are of particular relevance for testing the coupled code predictions;
- Combined extreme scenario – turbine trip with bypass system relief failure and without reactor scram. This is a very challenging case for code-to-code comparisons, Turbine trip with no scram, no bypass system and no activation of Safety Relief Valves (SRVs). The fourth extreme scenario was proposed by GRS, Germany. It provides both - a basis for better comparison of the physical models of the participants' codes without external perturbations since there is no need to model SRVs and their location, - and the possibility to determine the eigen-frequency of the system.

This benchmark involves both code-to-code and code-to-data comparative analyses of different levels: single values, 1D distributions, 2D distributions and time histories. The Automated Code Assessment Program (ACAP) [8] and the statistical methodology, established in the OECD/NRC PWR MSLB benchmark, have been used to perform these analyses. It should be noted that one issue has been re-solved by using ACAP, which is not incorporated into the statistical comparison techniques. In the case of time history data the overall curve shape should be compared as well. Several methods exist to complete such full curve analysis, and a number of these methods are implemented in the ACAP automatic assessment tool, which have been utilized for analysis of the BWR TT benchmark results.

### 3.3 Results

Overall, this benchmark also has been well accepted internationally, with about 15 participants representing 9 countries in each exercise. The results submitted by the participants are used to make comparisons, and a subsequent statistical analysis. This information encompasses several types of data for thermal-hydraulic parameters at the initial steady state conditions and throughout the turbine trip transient. The final report on Exercise 1 was published [9] and the other two reports are under preparation.

For the parameters for which the measured data is available the measured values are used as the reference. Such parameters are the core inlet enthalpy and core average pressure drop at the initial conditions of the TT2 test. The measured value for the core inlet enthalpy is 1209.055 KJ/kg, and participants' results display a standard deviation of  $\pm 3.149$  KJ/kg for Exercise 1. The measured value of the core pressure drop is 0.1136 MPa and the calculated standard deviation of the participants' results is  $\pm 0.0125$  MPa for Exercise 1. For the parameters for which measured data is not available (code to code comparisons) a mean solution is generated to serve as the reference. This can be seen in Figure 4, which shows the mean solution and standard deviations of the axial core averaged void fraction distribution. Overall, the participants' results for integral parameters, core-averaged axial distributions, and core-averaged time histories are in good agreement with reference solutions, considering some of the approximations in participants' models, uncertainties of some system parameters, and difficulties in interpreting some of the measured responses. In the void fraction results, deviations are mostly observed in the lower (bottom) part of the core, because of the differences in the participants' sub-cooled boiling models.

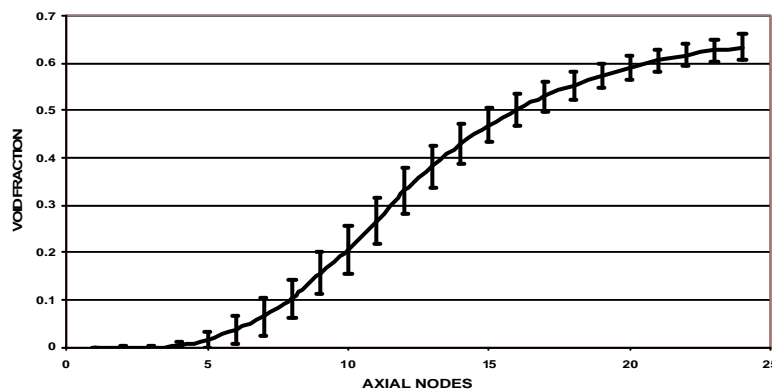


Figure 4. Exercise 1 – Core Average Axial Void Fraction Distribution – Mean Solution and Participants' Results

Deviations

In the time history comparisons, the deviations are mostly observed within the first 1.5 seconds after the transient starts. During the analysis of the results for the first exercise it became obvious that the sources of deviations in the participants' predictions stem from the differences in modeling of the two key parameters – pressure response and core flow response, which determine the void generation in the core channels. The accurate prediction of the pressure response depends on a number of models used by a given code: the steam line model, which requires adequate nodalization and treatment of momentum effects; the steam bypass system model; and the steam separator model since the steam separator inlet inertia and non-equilibrium effects at steam-water surfaces must be properly treated. As one of the very important models for this transient, the steam bypass system should be modeled consistently to accurately predict bypass flow response. The prediction of core flow response is sensitive to the jet pump model used since it must properly represent the dynamic response of flow to pressure, and the core exit/separator region model since it must properly represent the dynamic response of two-phase flow.

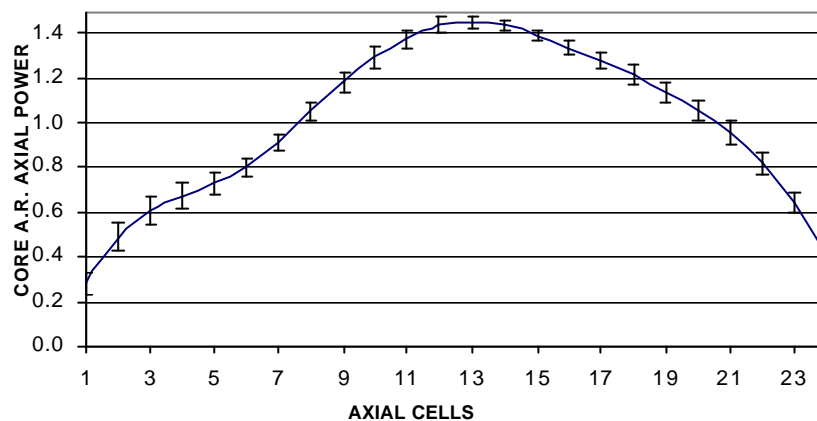


Figure 5. Exercise 2 - Core Average Relative Axial Power Distribution – Measured Data and Participants' Results

#### Deviations

During the comparative analysis of the participants' results for the second exercise (see Figure 5) the following sources of modeling uncertainties were identified: core pressure drop in terms of local losses and friction models, core bypass modeling and void feedback model in terms of sub-cooled boiling and vapor slip. The fuel heat transfer parameters such as the  $UO_2$  conductivity and gap conductivity and direct heating (2% to in-channel flow and 1.7 % to bypass flow) were specified. The scram initiation time and the speed of the rod insertion were also specified. The scram initiation time was specified since one of the objectives of the benchmark is to test coupled codes' capabilities to predict for TT2 that the thermal-hydraulic feedback alone limits the power peak and initiates the power reduction. Other important modeling issues were identified such as the impact of using assembly discontinuity factors, which are also provided to the participants in a similar table format as for the two group cross-sections; xenon correction to account for the actual xenon concentration distribution at the initial steady-state conditions of the turbine trip test 2; the number of thermal-hydraulic channels and spatial mapping schemes with the neutronics core model; and bypass density correction in the cross-section feedback modeling to account for the deviations of bypass density from the saturated value used in the cross-section homogenization since the cross-sections are generated by homogenizing the bypass region associated with the lattice.

In Exercise 3 the calculations of extreme scenarios 2, 3 and 4 indicated that the core power shows in-phase oscillations. While in scenarios 2 and 3 the dynamics of physical interactions between power and feedback mechanisms is interrupted by opening of the bypass valve and/or SRVs in scenario 4 the power oscillatory behavior continues until the end of the calculation – see Figure 6. Since the benchmark-measured data for the best-estimate (test) scenario also contain the Local Power Range Monitor (LPRM) measurements, the benchmark team provided the participants with the description of an appropriate algorithm to model LPRM response and the necessary associated data as microscopic detector cross-sections, flux factors, etc. The modeling of SRVs was identified as an important issue causing differences in the solutions.

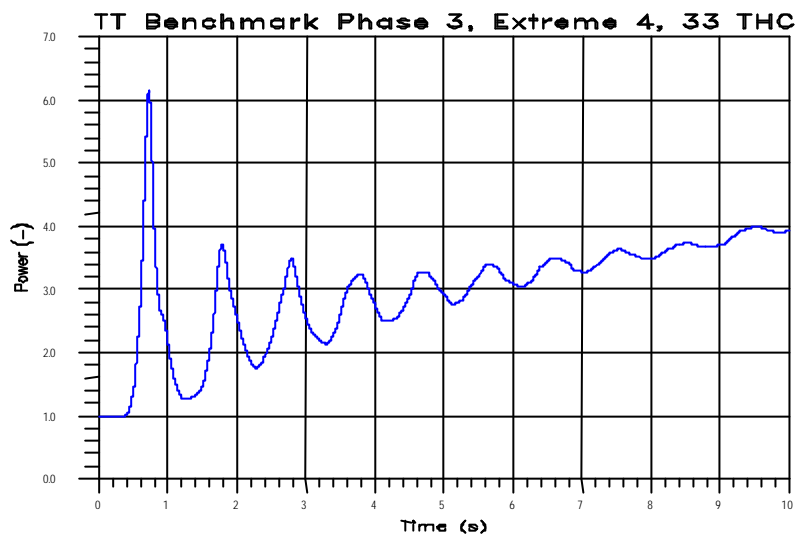


Figure 6. Exercise 3 – Extreme Scenario 4 Calculated with the GRS code ATHLET-QUABOX/CUBBOX

The BWR TT benchmark provided the opportunity to study the impact of different thermal-hydraulic and neutronics models on code predictions and to identify the key parameters for modeling a TT transient. The deviations of participants' results around the average solution can best be seen in the second extreme scenario of Exercise 3, which is without scram and thus allows to study the differences in modeling the feedback effects – see Figure 7. This in turn allowed the evaluation of these key parameters, through the performance of sensitivity studies. Such investigations were aimed toward evaluation of the impact of the following effects and parameters:

- Thermal-hydraulic modeling issues – turbine by-pass line modeling; nodalisation of vessel, steam line and steam separator region; the TSV position and steam mass flow modeling; thermal-hydraulic model – number of equations; void fraction model; steam-separator inertia; and jet-pump modeling, and SRVs modeling.
- Thermal-hydraulic key parameters – feedwater temperature; jet-pump parameters; void-fraction in the bulk water (carry-under); the core outlet pressure; the active core pressure loss; the core inlet temperature; the core inlet mass flow without bypass flow; sub-cooling; void generation rate; and gas gap conductance.
- Time step size – fixed time step of 6 ms vs. using a variable time step algorithm with a maximum time step size imposed.

- Cross-section modeling - cross-section history dependencies modeling, which is important for the initial steady state; instantaneous cross-section density dependence (void coefficient) – important for the transient modeling; xenon and bypass density correction in cross-section tables; ADF modeling; and refinement of cross-section library.
- Neutronics and coupling modeling - different neutronics methods, spatial coupling schemes between core neutronics and thermal-hydraulics in terms of number of the T-H channels, direct moderator heating; temporal coupling schemes and time step sizes; and scram initialization.

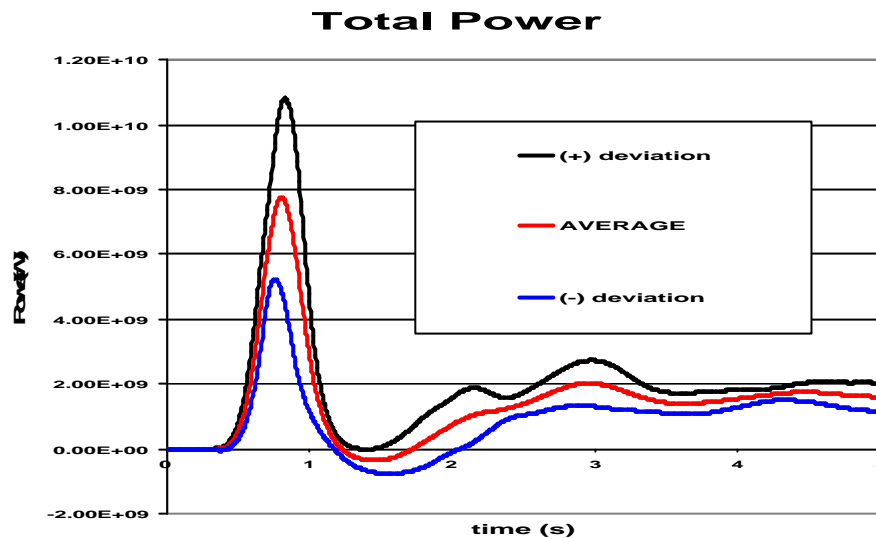


Figure 7. Exercise 3 – Extreme Scenario 2 – Average and Deviations of the Participants' Results

One of the sensitivity studies, performed in a collaboration between CEA, Saclay and PSU with the coupled code CRONOS2/FLICA-IV was on the number of thermal-hydraulic channels and spatial mapping schemes with the neutronics core model. This sensitivity study suggested that the 33 channel mapping, which has been used for the turbine trip benchmark may be adequate to provide global core behavior during the transient since it is predominantly a 1D event. However, detailed information about the local power distribution during the transient would require a large number of channels. – see Figure 8. Furthermore the use of 33 channels would not be able to provide accuracy even for global parameters for events, which are more 3D in nature, such as out-of-phase instabilities which were also performed as part of the Peach Bottom tests.

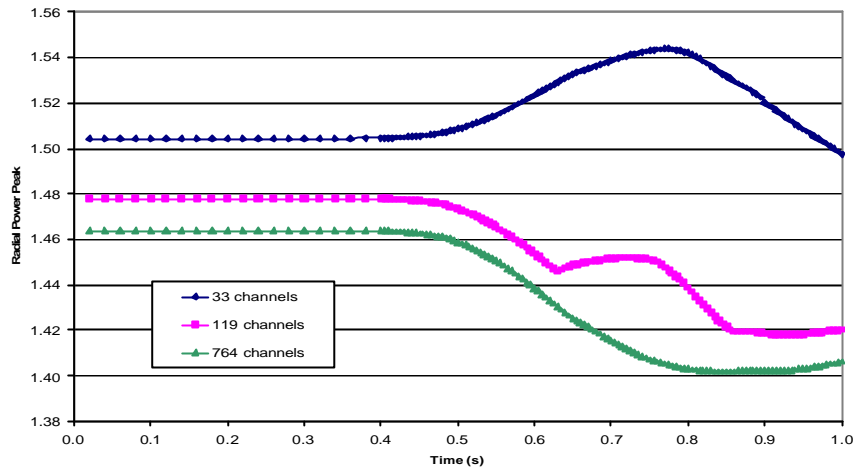


Figure 8. Radial Power Peak Evolution During Turbine Trip Transient

## 4 OECD/DOE/CEA V1000CT BENCHMARK

In the framework of a joint effort between the NEA/OECD, US DOE and CEA, France a coupled 3-D neutron kinetics/thermal hydraulics benchmark was defined for a VVER-1000 reactor. The benchmark is based on data from the Unit 6 of the Bulgarian KNPP. The benchmark consists of two phases: Phase 1: Main Coolant Pump Switching On; and Phase 2: Coolant Mixing Tests and MSLB. In addition to the measured (experiment) scenario of Phase 1, an extreme calculation scenario was defined for better testing 3D neutronics/thermal-hydraulics techniques: rod ejection simulation with control a rod being ejected in the core sector cooled by the switched on MCP. Since the previous coupled code benchmarks such as the PWR MSLB benchmark indicated that further development of the mixing computation models in the integrated codes is necessary, a coolant mixing experiment and MSLB transients are selected for simulation in Phase 2 of the benchmark. The MSLB event is characterized by a large asymmetric cooling of the core, stuck rods and a large primary coolant flow variation. Two scenarios are defined in Phase 2: the first scenario is taken from the current licensing practice and the second one is derived from the original one using aggravating assumptions to enhance the code-to-code comparisons.

### 4.1 Transient

In Phase 1 the reference problem chosen for simulation in a VVER-1000 is a main coolant pump (MCP) start-up when the other three main coolant pumps are in operation. The MCP start-up test was conducted during the plant-commissioning phase at KNPP Unit #6 (VVER-1000, model 320) in November 1991 as part of the plant start-up tests. This investigation was performed on the stage when the reactor power was at 75% of the nominal level. Before the experiment the reactor power level was reduced from 75% (2250 MW) to approximately 21% by consecutive switching off of MCP 2 and MCP 3. A few hours before the experiment MCP 2 was switched back on, and the power was stabilized at 30% following the Technical specification requirements. According to the Technical specification for safety operation of the Unit 6, a switching on one main coolant pump in operation is performed when the reactor power is at 30% of the nominal level. The MCP start-up test is characterized by rapid increase in the flow through the core resulting in a coolant temperature decrease, which is

spatially dependent. Although the reactivity perturbations in the core are not very strong the benchmark team decided to choose this transient because of the available plant data.

In Phase 2 a mixing experiment, conducted at Kozloduy-6 as part of the plant-commissioning phase, is utilized as the first exercise. The experiment includes isolation of a steam generator at 9.3% of the nominal power causing single loop heat-up, with all MCP in operation. It is characterized by temperature rise of about 14 degrees and a decrease of mass flow rate by 3.4% in the disturbed loop, affecting the neighboring loops as well. For the second and third exercises the transient to be analyzed is initiated by a main steam line break in a VVER-1000 between the steam generator (SG) and the steam isolation valve (SIV), outside the containment. A mechanical failure of the main feed water regulation valve is assumed. This event is characterized by a large asymmetric cooling of the core, stuck control rods and a large primary coolant flow variation.

## 4.2 Methodology

Following the approach for assessing coupled codes, established in PWR MSLB and BWR TT benchmarks, three separate exercises were defined in Phase 1 of the benchmark:

- V1000CT-1 Exercise 1 – Point kinetics plant simulation: The purpose of this exercise is to test the primary and secondary system model responses. The benchmark specification provides all the necessary point-kinetics data. Using this exercise the participants can verify their system input decks and can eliminate all the deviations coming from the user modeling, which later could be helpful for the best estimate comparisons.
- V1000CT-1 Exercise 2 – Coupled 3-D neutronics/core thermal-hydraulics response evaluation: The purpose of this exercise is to model the core and the vessel only. The benchmark provides inlet and outlet core transient boundary conditions. Using this exercise the participants can verify their coupling schemes and cross section library utilization.
- V1000CT-1 Exercise 3 – Best-estimate coupled code plant transient modeling: The third exercise combines elements of the first two. In this exercise the participants must analyze the transient in its entirety, and computation results will be compared against measured plant data. This phase of the benchmark contains also an extreme scenario, which involves a rod ejection in the part of the core cooled by the MCP #3, which will develop very peaked spatial power distribution and nonlinear asymmetric feedback effects. The extreme scenario was developed to test and better compare the predictions of the coupled 3-D kinetics/thermal-hydraulics codes.

Since the previous benchmarks indicate that further improvement of the vessel mixing models in the integrated codes is necessary, a coolant mixing and MSLB benchmark for VVER-1000 (V1000CT-2) was defined. Exercise 1 of Phase 2 is: computation of coolant mixing experiments: it will be used to test and validate vessel-mixing models (CFD, coarse-mesh and mixing matrix). Vessel boundary conditions and core power distribution along with pressure above the core will be part of the exercise specification. The task is to calculate the core inlet and outlet distributions. The V1000CT-2 Exercises 2 and 3 are on Main Steam-Line Break (MSLB) modeling. Two scenarios are defined: the first scenario is taken from the current licensing practice and the second is derived from the original one using aggravating assumptions to enhance the code-to-code comparison. The main objective of the study is to clarify the local 3D feedback effects depending on the vessel mixing. Special emphasis is put on testing 3D vessel thermal-hydraulics (T-H) models and the coupling of 3D neutronics/vessel thermal hydraulics. The MSLB is thus divided in two exercises (to be done for the two scenarios): Exercise 2 consists of coupled 3D neutronics/vessel thermal-

hydraulics simulations using specified vessel T-H boundary conditions and Exercise 3 consists of best estimate coupled plant simulations (plant, 3D vessel and core).

### 4.3 Results

Eight organizations from six countries have participated in Phase 1. The analyses of the results of Exercise 1 show that the participants' results for each parameter are in good agreement. The explanation for some of the discrepancies are in the utilization of the provided SG BC, MCP #3 rotor speed, and decay heat modeling as well as different vessel nodalization and/or number of channels. The discrepancies of the predictions of power change during the transient reflect the corresponding discrepancies in prediction of the total reactivity change. The total reactivity change during the transient is determined by the Doppler and moderator temperature feedback effects. Since the DTC and MTC are provided for Exercise 1, the discrepancies arise from the differences in prediction of core average fuel temperature and core average moderator temperature time evaluations. The discrepancies in predictions of the fuel temperature arise from differences in modeling of fuel rod (heat structure) components (for example gas gap conductance model, nodalization, and the relation for obtaining the effective Doppler temperature).

The code-to-plant data comparison is given for 129 seconds while the code-to-code comparison is presented for 800 seconds. Transient plots show the change of the parameter relative to the initial value of this parameter. In such a way the initial deviation is neglected which allows us to better assess the transient predictions of the codes. For the cold leg temperatures, the comparison shows good agreement between the plant data and the calculated values. The largest difference is observed in loop #3 (Figure 9) in the interval from 7 to 14 seconds during the start-up of MCP #3. The predicted temperature in this leg drops by approximately 3.5 K while such drop of the temperature cannot be observed in the plant data. This phenomenon can be explained as follows. Initially, when the pump is off, the direction of the flow in this loop is reversed. After the pump starts, the flow that once has passed through the SG is forced back and goes through the SG again, causing the temperature to decrease further. The codes predict the exact situation. However, the measurement did not register this temperature drop because the given experimental points do not correspond to instant temperature measurements but to mean temperatures between the different sampling times and also because of the time delay of the thermo-resistors. A method for accounting of the time delay of the temperature measurement system has been developed in cooperation with VTT, Finland and will be utilized in the final benchmark reports.

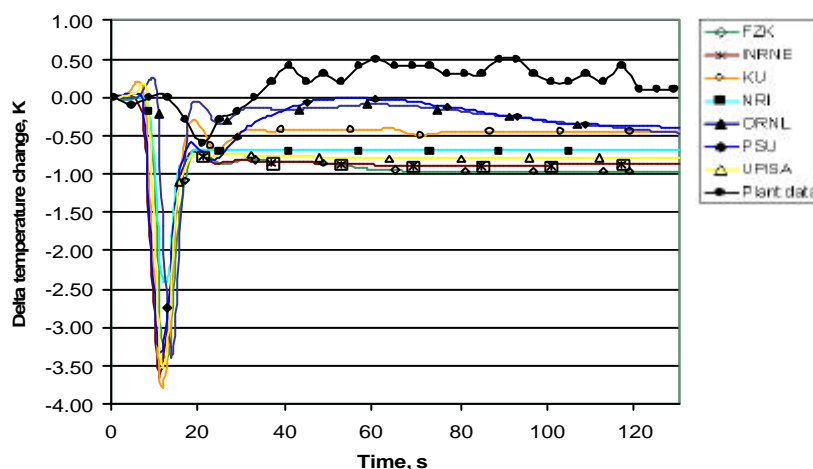


Figure 9. Cold leg #3 temperature change during the transient

When analysing the submitted results for Exercise 2 two clusters of participants' results for the normalized radial power distribution were formed. The observed difference in the results between these two clusters is in the range of  $\pm 11\%$ , while the difference within each of the clusters is in the range of  $\pm 1.5\%$ . These differences were analyzed by the benchmark team by performing sensitivity studies, which narrowed down the possible sources of the deviations to two. As it was expected the first contributor was revealed to be the differences in the methods used in the different codes for solving the diffusion equation in hexagonal geometry, which is more challenging than the one for Cartesian geometry. The second contribution was related to the VVER reflector properties (it contains much more steel than the PWR reflector) which were also found to enhance the discrepancies by increasing flux gradients at the core/reflector interface thus highlighting further the difficulties in the methods for handling high exponential flux gradients.

For Exercise 3 of Phase 1, which is a combination of the first two exercises and modeling of the transient in its entirety the most sensitive parameters were identified to be: fuel temperature differences (due to fuel modeling, gap conductance, rod nodalization); and different vessel models (3D vs 1D modeling) and BC (SG boundary conditions, MCP 3 rotor speed, and decay heat modeling) utilization. Modeling of the coolant mixing in the upper plenum is important for the initial conditions. The spatial mesh overlays are important mostly for the extreme rod ejection scenario – the results submitted by participants are compared in Figure 10.

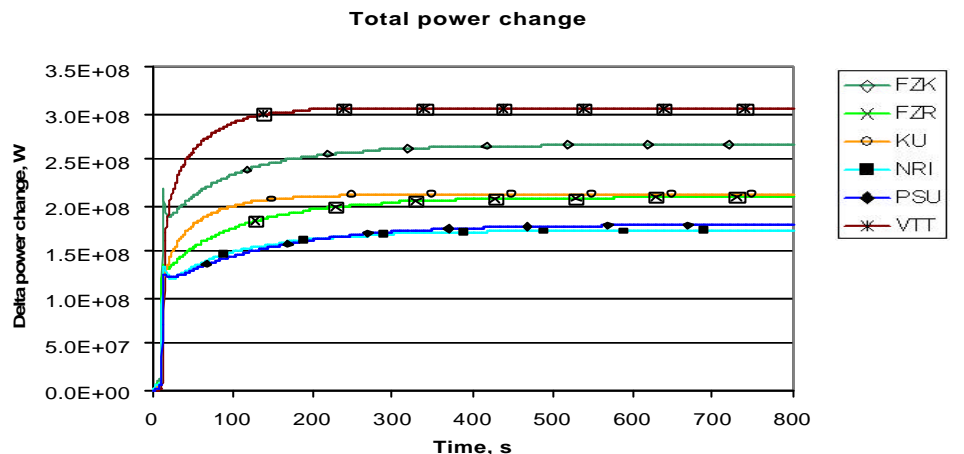


Figure 10. Reactor power change during the transient (Extreme scenario of Exercise 3, Phase 1)

The specification of V1000CT-2 Exercise 1 based on a vessel mixing experiment at the Kozloduy site was distributed by the NEA/OECD. The experimental data show a net counter clock angular shift of the main loop flows in certain VVER-1000 V320 flow patterns. This rotation towards the other loop has been observed in other VVER-1000 units too. The loop-to-loop mixing occurs both due to turbulent mixing and the angular turn of the flow.

Exercise 1 of Phase 2 provides a test of the impact of real geometry description on the simulated flow pattern. A description, based on general design data, is not sufficient to reproduce the rotation but is good for code-to-code comparison. In order to assess the code-experiment discrepancies, a second geometry description closer to the actual plant has been prepared as part of the specifications. Giving two geometries will enable the participants to identify the key parameters of the geometry description for a good flow pattern simulation.

These data are available both in spreadsheet format with tables and drawings, and as a CAD geometry file.

CFD computations with the Trio-U code have been carried out. The experimentally detected swirl can be reproduced with the Trio-U code only by using real plant geometry data. The calculated and measured temperature distribution at the core inlet is given in Figure 11. Here, the stabilized thermal hydraulic situation about 20 minutes after the isolation of SG-1 is shown. The locations of the cold legs are also added to this Figure. The calculated asymmetric temperature field and the counter clockwise rotation of the temperature maxima of 24° with respect to the axis of cold leg no.1 are in excellent agreement with the experimental data.

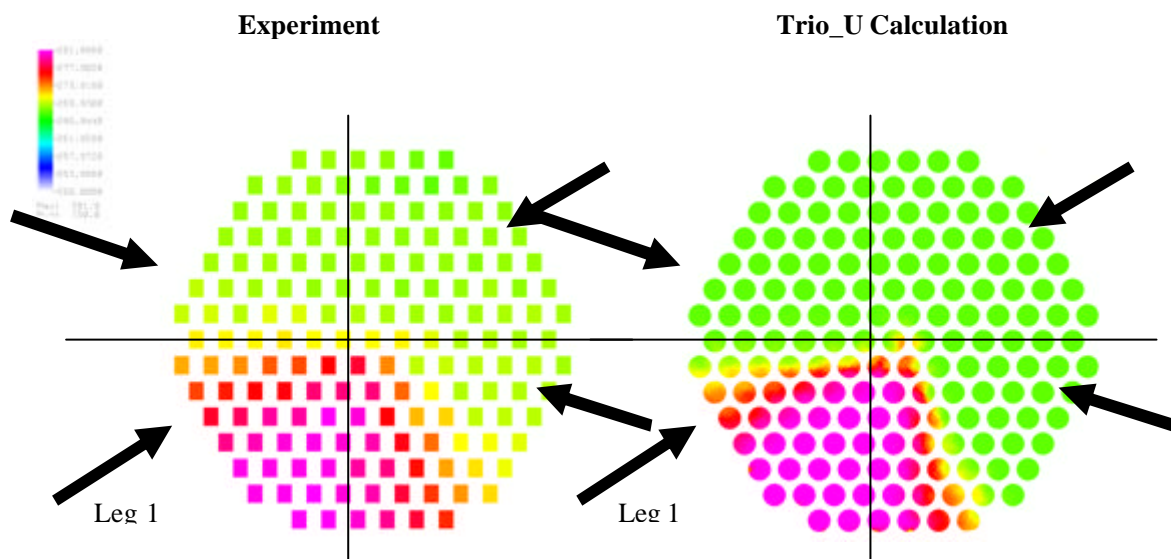


Figure 11: Temperature distribution at the core inlet at the end of the test

## 5 CONCLUSION AND OUTLOOK

The presented three benchmarks are developed in international co-operation to provide a validation basis for the new generation best estimate codes – coupled 3D kinetics system thermal-hydraulic system codes. Based on the previous experience, three benchmark exercises were defined for each benchmark, which allow for a consistent and comprehensive validation process. The introduction of the extreme scenarios contributes to the study of different numerical and computational aspects of coupled simulations. The participants use the 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. The systematic validation approach developed includes comparisons on different modeling levels – point kinetics and 3D kinetics; neutronics with and without T-H feedback; and core boundary conditions modules and core-plant coupling. In most of the current 3D analyses the cross-section functionalization for instantaneous dependencies is done either by using polynomial fitting procedures or the procedure using multilevel tables with base and partial cross-sections. In both cases the instantaneous cross-term effects (which are important for the transient analysis) are not modeled completely, which can lead

to different degrees of approximation of the thermal-hydraulic feedback phenomena depending on the procedure used. In this way the three benchmarks provided 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.

During the course of the benchmark activities a professional community of experts has been established, which allowed carrying out in-depth discussions of different aspects considered in the validation process of coupled codes. This positive output has certainly advanced the state-of-the-art in the area of coupling research. In addition to the benchmark workshops and ad-hoc meetings, special sessions for each benchmark were organized at different international conferences and meetings followed by the publication of special journal issues devoted to the specific benchmark activity. The special session on PWR MSLB benchmark was organized at the 2001 ANS Summer Meeting and a special issue was published in Nuclear Technology [11]. The special session on BWR TT benchmark took place at PHYSOR 2002 in Seoul, Korea followed by a special benchmark issue of the Nuclear Science and Engineering journal [12]. The Phase 1 of V1000CT benchmark was presented in a special session at NURETH-11 in Avignon, France, 2005 and a special issue is being prepared for Progress of Nuclear Energy.

These benchmarks have stimulated also follow up developments and benchmark activities such as the OECD/NRC BFBT benchmark [14] and OECD PBMR-400 coupled code benchmark [15]. 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. It was during the 4<sup>th</sup> OECD/NRC BWR TT Benchmark Workshop on 6 October 2002 in Seoul, Korea, that the need to refine models for best-estimate calculations based on good-quality experimental data was discussed. The needs arising in this respect should not be limited to currently available macroscopic approaches but should be extended to next-generation approaches that focus on more microscopic processes. It is suggested that this international benchmark be 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. An 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 will be that the uncertainty analysis will be added as an additional exercise as proposed by CEA, Saclay. This exercise will take into account uncertainties on input data (boundary conditions, geometry, etc. provided by the Specifications) and on models and produce results with "errors", which will be compared with measurement uncertainties

The accumulated international experience and expertise in developing coupled code benchmarks for LWRs has been recently extended to other reactor types. The PBMR is a

High-Temperature Gas-cooled Reactor (HTGR) concept, which has attracted the attention of the nuclear research and development community. The deterministic neutronics, thermal-hydraulics and transient analysis tools and methods available to design and analyse PBMRs have, in many cases, lagged behind the state of the art compared to other reactor technologies. This has motivated the testing of existing methods for HTGRs but also the development of more accurate and efficient tools to analyse the neutronics and thermal-hydraulic behavior for the design and safety evaluations of the PBMR. In addition to the development of new methods, this includes defining appropriate benchmarks to verify and validate the new methods in computer codes. Such an international OECD Coupled Neutronics/Thermal Hydraulics Transient Benchmark for the PBMR-400 Core Design has been established and is an ongoing international activity. The scope of the benchmark is to establish a well-defined problem, based on a common given set of cross sections, to compare methods and tools in core simulation and thermal hydraulics analysis with a specific focus on transient events through a set of multi-dimensional computational test problems.

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