Overview of the OECD-NEA Expert Group on Multi-physics Experimental Data, Benchmarks and Validation

Timothy Valentine¹, Maria Avramova², Michael Fleming³, Mathieu Hursin⁴, Kostadin Ivanov², Alessandro Petruzzi⁵, Upendra Rohatgi⁶, Kiril Velkov⁷

¹Oak Ridge National Laboratory, USA
²North Carolina State University, USA
³OECD Nuclear Energy Agency, France
⁴Paul Scherrer Institut, Switzerland
⁵Nuclear and Industrial Engineering S.r.l., Italy
⁶Brookhaven National Laboratory, USA
⁷Gesellschaft feur Anlagen und Reaktorsich, Germany

ABSTRACT

The OECD Nuclear Energy Agency (NEA) Nuclear Science Committee (NSC) established the Expert Group on Multi-physics Experimental Data, Benchmarks and Validation (EGMPEBV) in 2014 to bridge the gap between advanced, multi-physics simulation capabilities and the relatively low availability of dedicated, high-fidelity experimental data and benchmarks specifically for multi-physics modelling and simulation tools. The EGM-PEBV was mandated to establish mechanisms for the certification of experimental data and benchmark models and to establish the processes and procedures for the validation of multi-physics modelling and simulation tools.

The EGMPEBV oversees three task forces, covering (1) experimental data qualification and benchmark evaluation, (2) validation guidelines and needs and (3) example application of validation experiments. These have generated numerous reports surveying the state-of-the-art in multi-physics validation, challenge areas and recommendations for the evaluation of multi-physics benchmarks, while in parallel developing the specifications for multi-physics benchmarks. Three benchmark specifications are in active development, including a reactivity compensation scenario in the Rostov Unit 2 VVER-1000, multi-cycle depletion of the TVA Watts Bar Unit 1 and study of pellet cladding mechanical interaction within ramp tests performed at the Studsvik R2 reactor.

We provide an overview of the recent progress in these areas and a summary of the future activities of the EGMPEBV in establishing international multi-physics benchmarks.

KEYWORDS: Multiphysics, International, Benchmark, Experiments, Validation

Corresponding author valentinete@ornl.gov

1. INTRODUCTION

The use and reliance on coupled multi-physics modelling and simulation (M&S) tools continues to expand to meet the demands of the researchers, designers, developers, operators and regulators. This greater reliance on M&S tools has also led to the development of high-fidelity, coupled multi-physics M&S tools that enable rigorous modelling of coupled behaviours including among other things reactor physics, thermal-hydraulics, fuel performance, structural mechanics, and materials chemistry.

Although the fidelity of the simulations and the sophistication of the coupling methodologies have increased substantially, the underpinning models and data still need to be validated against experiments. This requires a complex array of validation data because of the range of time, energy, and spatial domains of the physical phenomena that are being simulated and also to address the validation of the coupling approaches. Coupling of two or more physics models may accentuate the importance of some parameters due to feedback effects that are not modelled when boundary conditions are used to couple codes; these potential multi-physics phenomena manifest themselves from multi-physics experiments. The validation challenge is further complicated by the fact that legacy experimental data for single or coupled physical phenomena may not be adequate for validation of high-fidelity M&S tools, the fact that there are few experimental facilities available for conducting experiments, and the fact that in some instances instrumentation and experimental techniques may not exist to validate some models or approximates. Rigour in the validation processes and principles along with qualified validation data will be a prerequisite to further enhance the use and acceptance of coupled, multi-physics M&S tools.

2. OPERATION OF THE EGMPEBV TASK FORCES

Validation of multi-physics M&S tools requires that the coupled M&S tools be validated for each physical phenomenon that is simulated as well as the coupling among the physical phenomena. To address the needs of member states, the OECD Nuclear Energy Agency (NEA) launched the Expert Group on Multi-physics Experimental Data, Benchmarks and Validation (EGMPEBV) under the guidance of the Nuclear Science Committee (NSC) in 2014. The EGMPEBV was organised into three Task Forces, focusing on

- 1. the evaluation of the current status and expected needs for validation of multi-physics M&S tools, identifying the major challenges and priorities;
- 2. the needs and best practices for development of models for validation; and
- 3. the development of example application of experiments for validation.

These Task Forces were identified with several inter-related tasks, which are shown in Figure 1, that have or will summarise the current understanding of these topics within NEA publications. Task Force 3 is focused on the demonstration of recommended practices for multi-physics validation through the specification and execution of benchmarks.

Task Force 1 (TF1) is organised into seven tasks with the first two tasks shared with Task Force 2. The first task of the group was to define the scope of multi-physics applications that would be con-



Figure 1: Organisation of the EGMPEBV Tasks within Task Force 1 (blue), Task Force 2 red) and those shared between the two (purple) [1].

sidered by the group and to categorise the phenomena and simulation processes. The EGMPEBV determined that 'traditional' multi-physics tools, where separate simulations are have limited coupling between different physical phenomena, should be differentiated from novel tools that utilise more tightly and/or explicitly coupled phenomena.

The second task has focused on the expected needs for multi-physics M&S validation, which was further sub-divided into reviews of the current international multi-physics M&S development projects, uncertainty propagation methodologies and a review of available experimental data for

multi-physics validation.

Within the Task Force 1, the third task focuses on identification of major challenges for validation, which has resulted in multiple phenomena assessment and ranking chart (PARC) studies for challenges problems identified as part of the US CASL project. The objective of the fourth task is to establish recommendations and processes for the evaluation of existing experimental data including uncertainty quantification and the fifth task proposes to examine the needs, options, recommendations and mechanisms for performing specific validation experiments. A sixth task aims to identify developments in instrumentation, experimental methods, and data treatment that would be needed for validating novel M&S tools. The ultimate, and as yet unrealised goal for Task Force 1 is to draft guidance for the development of multi-physics benchmark evaluations from existing or new experiments that serve as validation experiments.

Task Force 2 (TF2) beyond the first two shared tasks include the review of current approaches to multi-physics validation for traditional tools including approaches to sensitivity and uncertainty analysis. The fourth task focuses on creating recommendations for validation processes for novel multi-physics M&S tools, including uncertainty analyses. The fifth task will develop validation matrices using phenomena importance ranking tables (PIRTs) for challenges problems that have been identified in the first task shared by both of the first task forces.

Task Force 3 (TF3) activities are focused on the demonstration of validation processes in different application domains. These include nuclear power plant benchmarks as well as scenarios in startup experiments, transient reactors and other test reactor experiments.

3. MULTI-PHYSICS BENCHMARKS

While the capabilities of multi-physics M&S tools can be demonstrated through the simulation of standard benchmark experiments, designers, operators and regulators must validate these codes for specific problems in order to quantify the limits of their applicability and the uncertainties in the predictive capabilities.

3.1. Multi-physics pellet clad mechanical interaction validation benchmark

The EGMPEBV has selected several industry challenging problems to demonstrate validation principles and practices. The first case that was developed considered both traditional and novel multiphysics M&S tools to simulate Pellet Cladding Mechanical Interaction (PCMI) experiments. This is of interest for both operators and regulators as PC(M)I fuel failures can reduce reactor performance and limit the extent of power uprates, burn-up and fuel enrichments.

The Multi-physics PCMI Validation (MPCMIV) exercise was selected based on two cold ramp tests performed at the Studsvik 50 MW_{th} tank-in-pool R2 test reactor [2,3]. The experiment itself was carried out within a test loop that is positioned in the central region of the transient reactor core and requires coupled simulation of reactor physics, thermal hydraulics, and fuel performance phenomena. The experiment was conducted in a step-wise fashion in that the rod was first held in cold conditions followed by a relatively fast transient in which the power generation in the rod increased from zero to 45 kW/m in approximately 5 seconds. Within approximately 10 to

15 seconds the heat flux and fuel temperature reached their maximum upon termination of the power ramp. In this exercise, coupling of the fuel performance and reactor physics, through fuel temperature and reactor power, is the primary focus, while the coupling of thermal hydraulics still plays a secondary role. The overall coupling scheme is shown in Figure 2 [4].



Figure 2: Coupling of phenomena in the MPCMIV exercise, including reactor core (c) and experimental rod (r) domains [4].

This exercise includes modelling of the full R2 reactor as well as the experimental in-pile loop. Two ramps were selected to include a power calibration and pre-qualification, before blind simulation with uncertainty analyses in the second. Four tiers, as described in Table 1, were identified to allow a broad range of participants with different simulation methodologies. The 'Tier 1' will include full 3D heterogeneous multi-physics modelling of both the reactor core and the test fuel rod with novel tools, while increasing levels of approximation and use of boundary conditions are used in the lower tiers.

Table 1: Tiers of the MPCMIV benchmark covering Reactor Physics (RP),Thermal-Hydraulics (TH) and Fuel Performance (FP) of the reactor core and experimental
loop.

	RP				TH			FP	
	R2 depletion	R2 criticality	Rod depletion	Transient ramp	R2 core	Loop & U-tube	Only U- tube	Rod depletion	Transient ramp
Tier-1	x	X	X	X	X	Optional	X	X	X
Tier-2	-	-	x	x	-	Optional	x	X	X
Tier-3	-	-	Optional	х	-	Optional	x	х	x
Tier-4	-	-	-	-	-	-	-	х	x

Multiple responses of interest (ROIs) have been identified for simulation within the exercise specifications [5], however the outcome of the simulations is less important than the principles, assumptions, and approaches that the participants implement in simulating the actual experiment. Participants are required to document these for both the single physics phenomena and the coupled physics phenomena. Where possible, participants are requested to perform and document their processes for uncertainty analyses, with an aim to extrapolate results beyond the validation domain to the problem of interest.

Validation requirements will be established for each of the aforementioned steps. The participants will be required to quantify the accuracy of their simulations for each phase based on the approaches and data sets that were used to validate the M&S tools that were used.

3.2. Rostov Unit 2 VVER-1000 transient benchmark

Several experiments with detailed measurements of neutron-physics and thermal-hydraulics data have been performed at the Rostov Unit 2 (Rostov-2) VVER-1000 reactor. Both integral quantities and locally recorded data have been collected and have been used in the preparation of a benchmark for the validation of traditional and novel multi-physics codes. These measurements include many of the standard parameters recorded during power plant operation, as well as through a special system of experimental control (SEC).

An international team including institutes from Germany, Russia and the US have selected a transient test of a reactivity compensation experiment with diluted boron with stepwise insertion of control rod clusters into the Rostov-2 core, with experimental data provided by the Russian ROSATOM company. The movement of the control rod cluster occurred over an approximately 2 hour period, with spatial negative reactivity insertion compensated by a decrease in the coolant boron concentration [6].

The first phase includes coupled three-dimensional neutronics and thermal-hydraulics simulation with both hot zero power and hot partial power conditions. The second phase will allow participants to simulate with one of three options to model the steady-state and full transient scenario: full core pin-by-pin simulation, hot channel pin-by-pin or simulation of an array of 7 assemblies around the control rod cluster of interest.

3.3. TVA Watts Bar Unit 1 multi-cycle benchmark

As part of the verification and validation activities within the VERA-CS of the US Consortium for Advanced Simulation of Light Water Reactors (CASL), a set of progression benchmark problems were created [7,8]. These cover a range of cases, from two-dimensional pin cells to threedimensional multi-physics reactor core modelling. The specifications of these problems were based on data provided by the Tennessee Valley Authority (TVA), which operates the Watts Bar Unit 1 (WB1), and Westinghouse.

As part of the cooperation on multi-physics between US Department of Energy (DOE) and the NEA, the TVA-WB1 data and specifications have been provided as the input for an international, collaborative, multi-cycle benchmark activity co-ordinated through the EGMPEBV. The NEA

multi-physics benchmark draft specifications are based on Cycles 1 and 2 of the WB1 operation, split into five exercises. Planned extension to these problems will include cycles 3 through 5.

The five benchmark exercises are defined based of the first two cycles of TVA WB1 data. The exercises are organized in such a way that they span: (1) start-up zero power physics tests including the 3D neutronics modelling of the hot zero power reactor; (2) the multi-physics steady state model for hot full power, including coupled neutronics, thermal-hydraulics and fuel performance; (3) the multi-physics cycle depletion for the first test cycle; (4) the continuation with fuel shuffle and decay, simulating the initial core for the hot zero power of the second cycle; and (5) multi-physics simulation of the second cycle with depletion [9].

In the development of the benchmark, the first exercise with zero power physics tests has been developed as a submission to the International Reactor Physics Evaluation (IRPhE) Project [10], following the uncertainty guidance established as part of the NEA benchmark evaluation projects [11]. Through the evaluation process of the NEA Technical Review Group these uncertainty standards will be applied to the first tests and further extended as part of the Expert Group's studies.

4. CONCLUSIONS

The NEA Expert Group on Multi-physics Experimental Data, Benchmarks and Validation (EGM-PEBV) was established to address challenges in validating multi-physics modelling and simulation tools, taking into account the lack of consensus on validation of coupled tools and the availability of data to support such validation.

Having reviewed the international activities on multi-physics validation, the EGMPEBV is moving forward with multiple experimental benchmarks and validation exercises, using data from test and nuclear power reactors in different member countries. The first example is the MPCMIV benchmark, which focuses on the simulation of experiments that demonstrate the ability of both traditional and novel multi-physics simulation methods to replicate fuels performance measurements conducted in the Studsvik R2 reactor. New benchmarks have been prepared and are being updated as part of the ongoing activities co-ordinated by the NEA, including the specification from the CASL TVA Watt's Bar Unit 1 cycles 1-2 and a reactivity compensation experiment carried out at the Rostov Unit 2 VVER-1000.

These exercises will provide the opportunity to evaluate the validation principles and approaches, to identify challenges and inadequacies in validation data sets and methodologies. These will ultimately be documented in reports by the EGMPEBV and in benchmark reports that will be distributed by the NEA to member countries for use in the verification and validation of multiphysics modelling and simulation tools.

REFERENCES

[1] P. Finck, T. Valentine, J. Dyrda, J. Gulliford, J. P. Hudelot, and U. Gohatgi. "OECD-NEA Expert Group on Multi-Physics experimental Data, benchmarks and Validation." PHYSOR 2016 Conference, Sun Valley, ID, May 1–5, 2016.

- [2] M. Carlsson and U. Engman. "Test Facility and Experimental Technique for Fuel Ramp Tests." Report No. N(R)-99/063, Studvisk Nuclear, 15 Oct. 1999.
- [3] J. Karlson. "B64, Special Cold Ramp Test of Rod 2653." Report No. N-05/174, Studsvik Nuclear, 10 May 2007.
- [4] V. Mousseau and N. Dinh. "CASL Verification and Validation Plan." CASL-U-2016-1116-000, June 30, 2016.
- [5] D. De Luca, L. Lampunio, V. Parrinello, A. Petruzzi, M. Cherubini, and J. Karlsson. "OECD-NEA Multi-physics Pellet Cladding Mechanical Interaction Validation Input and Output Specifications." Revision 1, March 16 2018.
- [6] M. Avramova, K. Ivanov, K. Velkov, I. Pasichnyk, S. Nikonov, M. Denisova, A. Denisenko, P. Gordienko, and B. Shumskiy. "OECD-NEA Benchmark on reactivity compensation with diluted boron by stepwise insertion of control rod cluster into the VVER-1000 core." Version 1.3, January 2018.
- [7] A. Godfrey. "VERA Core Physics Benchmark Progression Problem Specifications, Revision 4." CASL-U-2012-0131-004, August 24, 2014.
- [8] A. Godfrey et al. "VERA Benchmarking Results for Watts Bar Nuclear Plant Unit 1 Cycles 1-12." CASL-U-2015-0206-000, June 30, 2015.
- [9] A. Godfrey, S. Palmtag, F. Franceschini, L. Moloko, T. Albagami, P. Rouxelin, M. Avramova, and K. Ivanov. "OECD-NEA TVA Watts Bar Unit 1 Multi-Physics Multi-Cycle Benchmark Specifications." in preparation.
- [10] Nuclear Energy Agency. "International Reactor Physics Evaluation Project Handbook." OECD Nuclear Energy Agency, Paris 2019, (NEA-7496), https://doi.org/10.1787/a112bf8een.
- [11] V. F. Dean and L. G. Blackwood. "ICSBEP Guide to the Expression of Uncertainties." in: International Handbook of Evaluated Criticality Safety Benchmark Experiments [DVD], OECD Nuclear Energy Agency, Paris 2019, (NEA-7328), ISSN: 2618042, https://doi.org/10.1787/e2703cd5-en.