Lessons Learned for Participation in Recent OECD-NEA Reactor Physics and Thermalhydraulic Benchmarks

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Abstract

Over the last 6 years the OECD-NEA has initiated a series of computational benchmarks in the fields of reactor physics and thermalhydraulics. Within this context McMaster university has been a key contributor and applied several state of the art tools including TSUNAMI, DRAGON, ASSERT, STAR-CCM+, RELAP and TRACE. Considering the tremendous amount of international participation in these benchmarks, there were many lessons of both technical and non-technical that should be shared. This paper presents a summary of the benchmarks, the results and contributions from McMaster, and the authors opinion on the overall conclusions gained from these extensive benchmarks. The benchmarks discussed in this paper include the Uncertainty Analysis in Modelling (UAM), the BWR fine mesh bundle test (BFBT), the PWR Subchannel Boiling Test (PSBT), the MATiS mixing experiment and the IAEA super critical water benchmarks on heat transfer and stability.

1. Introduction

With the ongoing support of NSERC and the University Network of Excellence in Nuclear Engineering (UNENE), McMaster University has participated in several ongoing OECD-NEA activities related to the uncertainty in reactor physics and Thermalhydraulic code predictions. These benchmarks include:

- Uncertainty Analysis in Modelling – The objective of this benchmark is to propagate fundamental uncertainties through all scales up to macroscopic predictions of reactor behaviour in transients. Phase 1 of this benchmark was recently completed and focused on the propagation of nuclear data uncertainties through lattice physics calculations. During UAM participation, McMaster applied the TSUNAMI-1D code, part of the SCALE code package, in addition to developing its own Monte Carlo propagation tool.
- BWR Subchannel Fine Mesh Benchmark (BFBT) – This benchmark is focused on the prediction of subchannel flows, enthalpies, void fraction and CHF in BWR assemblies. Experimental data included high fidelity x-ray computed tomography of the void fraction and flow regime at the subchannel level, gamma-densitometers for cross sectional void fraction, and thermocouples for wall temperature and CHF detection. Steady-state and transient tests were included in the benchmark.
- PWR Subchannel Boiling Test (PSBT) – This benchmark examined the void fraction, heat transfer and DNB under PWR conditions within a rod assembly. The tests also included x-ray measurements but only for the interior assembly subchannels.

- MATiS Computational Fluid Dynamics Assembly Mixing Benchmark – For this benchmark a series of experiments were conducted with a simulated PWR assembly, grid spacers and mixing vanes under various conditions and geometries and the local velocities and turbulence levels were recorded. The data was not released to the participants until after the computational submissions and hence was a blind test of CFD capabilities in this regard.
- IAEA benchmarks on flow stability in super critical water and super critical water heat transfer. These benchmarks focused on SCWR conditions and involved the application of the TRACE code as well as CATHENA. Since the focus of this paper is on the OECD-NEA benchmarks discussed above, the results of the IAEA SCWR work can be found in references [1, 2].

Details of the benchmarks and a sample of our results are described below.

2. The Uncertainty Analysis in Modelling

2.1 Evaluations of Fundamental Nuclear Data and Associated Uncertainties

The Phase I of the UAM benchmark has largely been completed and focused on the sensitivity and uncertainty in lattice physics calculations as a result of nuclear data for PWR, BWR and VVER reactor applications as well as the KRITZ-2 critical experiments. A major lesson to be transferred here is that at the outset it was clear that every participant needed a common frame of reference for comparing nuclear data and their associated uncertainties. The fundamental data in question includes: resonance parameters; microscopic cross-sections; angular and energy distributions; and other neutron interaction parameters. This data is disseminated in Evaluated Nuclear Data Libraries (ENDLs), such as ENDF/B, JEFF, JENDLE, and others. Contemporary ENDLs also include covariance matrices to quantify the uncertainty associated with many of those physics parameters. The libraries are referred to as “evaluated”, because both the physics parameters as well as their uncertainties ultimately arise from experiments, and that experimental data requires interpretation and expert judgement in order to provide useful information suitable to nuclear systems analysis. Consequently, different ENDLs, which are evaluated by different experts and draw from different experimental data, do not contain identical sets of data. Furthermore, when used for reactor lattice calculations, analysts may adopt a wide range of possible energy discretization schemes (with typical energy structures ranging from a few dozen to a few hundred energy groups).

A framework was therefore established and implemented as Exercise 1 of Phase I, whose objective was to study the impact of the selection of an ENDL, energy group structure and self-shielding treatment on the results of the uncertainty analysis. This framework involved comparing propagated uncertainties under a number of different constraints, such as weighting by a constant (problem-independent) neutron flux, and the use of a common (ENDL-independent) covariance matrix evaluated by Oak Ridge National Laboratory (ORNL). At the time the UAM benchmark began, most major ENDLs contained only partial covariances for a small number of nuclides (22 nuclides in ENDF/B-VII.0, for example). All participants therefore used, for Exercise 1, the ORNL *44GROUPV6REC* covariance file. This covariance was interpolated by each participant to their own energy structure, so that proper uncertainty propagation comparisons could be made between the participants for over 400 nuclides covered in *44GROUPV6REC.*

2.2 Sensitivity and Uncertainty Tool Development

It was clear at the initiation of the benchmark that sensitivity and uncertainty analysis tools that existed at the time were unequipped to perform multi-scale analysis involving all the parameters relevant to reactor analysis. Indeed, one objective of the benchmark as a whole was to foster the development of new tools to perform such analysis. Starting at the lattice level, most industry calculations utilize deterministic transport solvers like WIMS-AECL and DRAGON, along with multi-group data libraries processed from an ENDL using a cross-section processing code such as NJOY. NJOY performs several transformation, homogenization, and averaging calculations to create discrete-energy, temperature-dependent (Doppler-broadened), self-shielded cross-sections from the physics parameters stored in the ENDL. To correctly propagate lattice uncertainties requires the precise assessment of sensitivities of lattice outputs with respect to these inputs, as well as the sensitivities of the inputs with respect to one another.

The industry-leading tool for the assessment of lattice sensitivities and the performing of associated uncertainty propagation is the TSUNAMI-1D code developed by ORNL. TSUNAMI-1D calculates sensitivities using perturbation theory of one-dimensional nuclear geometries. At the time the benchmark began, TSUNAMI-1D (versions 5.1 and 6.0) could calculate sensitivities of *k*-infinity with respect to microscopic cross-sections, and the resulting uncertainty of *k*-infinity. An excellent tool, providing highly-reliable, and high-fidelity sensitivities, TSUNAMI-1D is generally the standard by which other tools are compared and validated. The one-dimensional nature of TSUNAMI-1D was also fairly well-suited to two-dimensional LWR fuel pin lattice problems, as it is straightforward to reduce pin geometries to a single dimension using the Wigner-Seitz model approximation.

At McMaster our initial efforts were focused on the application of the TSUNAMI-1D code and its *44GROUPV6REC* covariance file. However, despite the capabilities of TSUNAMI-1D, it became evident to us that some additional analysis capabilities would be required for realistic applications, such as the capability to assess sensitivities of additional output responses (i.e. homogenized two-group lattice properties, assembly discontinuity factors, etc.), additional uncertain input parameters (i.e. fuel pin diameter, material densities), higher spatial dimensionalities, and the capability to assess uncertainties during burnup. While some of these features have seen been added to newer versions of TSUNAMI-1D using generalized perturbation theory, we began to explore Monte Carlo uncertainty propagation methods which we felt were more well-suited to those tasks, particularly burnup calculations.

Due to our desire for flexibility we adopted the open-source lattice physics tool DRAGON as a transport solver and developed a new Monte-Carlo tool, DINOSAUR for uncertainty propagation. As we developed DINOSAUR, it became clear that classical multi-group libraries were ill-suited to facilitate uncertainty propagation. Accessing multi-group data of best-estimate lattice libraries was hindered by lack of availability of library formats – the WIMS-AECL library format was not publicly available, and the format of the WIMS-D4 library was not entirely documented. Furthermore, lattice libraries (WIMS-D4 and CASMO libraries, for example), tend to contain "lumped" cross-sections rather than individual reaction cross-sections. For example, the WIMS-D4 library contains a single lumped absorption cross-section, which is a sum of the cross-sections of fission, neutron capture, (n, 2n), (n, α), and so on. Therefore, perturbing this lumped cross-section does not provide useful sensitivity information related to individual reactions of interest, such as (n, 2n). We found that NJOY was needed to provide supplementary data for individual reaction cross-sections in order to perform sensitivity and uncertainty analysis using the WMIS-D4 library. The total effort in decoding multi-group libraries and generating supplementary data using NJOY proved to be non-trivial.

Once completed, the first version of our DINOSAUR tool was validated against TSUNAMI-1D for one-dimensional test-cases, comparing sensitivities to microscopic cross-sections as well as total uncertainty on *k*-infinity, and was then applied to the UAM benchmark. However, since DINOSAUR can work on 2-dimensional geometries and also has burnup capability, we have also applied the tool to CANDU lattices cases and examined the effects of nuclear data and other uncertainties on burnup, Coolant Void Reactivity, and other lattice output responses. Some prototypical results are shown below and further detail is provided by Ball [3].

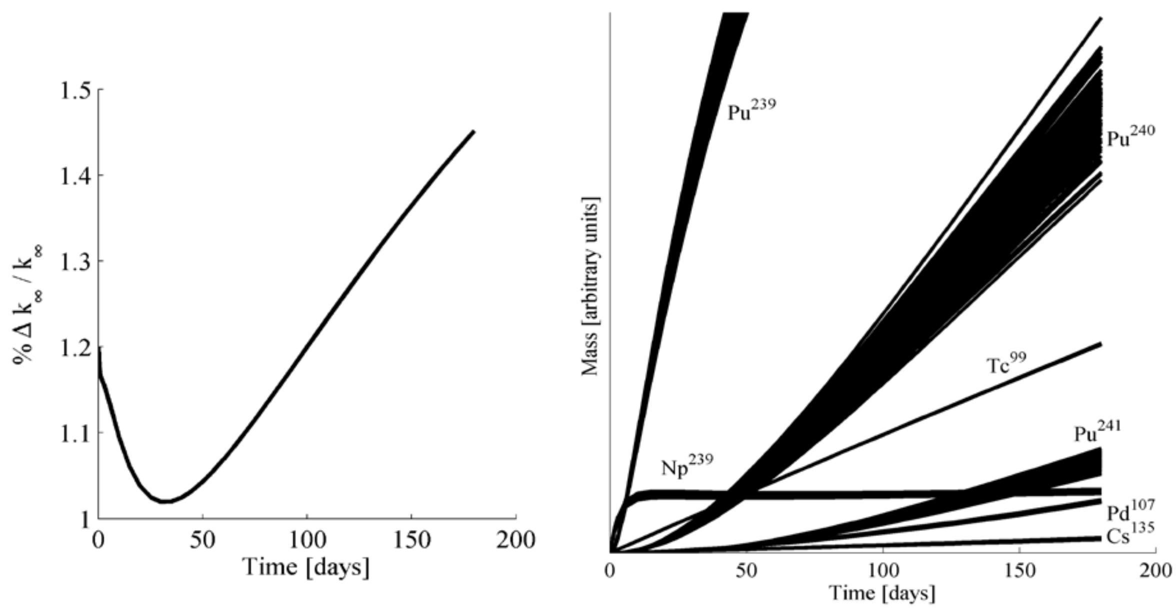

Figure 1: a) Uncertainty in Neutron Multiplication Constant as a Function of Brunup b) Uncertainty in CANDU Fuel Composition as a Function of Brunup

3. Steady-state and Transient Void Fraction, Dryout and DNB Benchmaks

The OECD/NEA BWR Full-size fine-mesh Bundle Tests (BFBT) and PWR Sub-channel Bundle Tests (PSBT) Benchmarks were a series of computational studies aimed at assessing the accuracy of modern subchannel and CFD codes. Experiments performed by the Japanese

Nuclear Power Engineering Corporation (NUPEC) using electrical heated rods cooled by water at pressures and flow rates typically found in both BWRs and PWRs served as the basis for the benchmark dataset. Participants were asked to simulate a range of bundle conditions and report the steady state void fraction at the subchannel level. The code predictions were then compared to the supplied experimental data which was obtained through gamma or x-ray densitometry and tomography. A series of high power tests were also analyzed in order to determine how accurately codes could predict the critical heat flux in the bundles.

McMaster has participated in both benchmarks using the ASSERT-PV R3V1 thermalhydraulics code as well as RELAP5-3D. ASSERT-PV is a Canadian code developed and maintained by Atomic Energy of Canada Limited (AECL) in support of activities involving fuel design and safety analysis in the Canadian nuclear industry. This code models the behavior of the coolant at the subchannel level and specializes in representing conditions found in Pressurized Heavy Water Reactors (PHWR). Results for both the BFBT [4] and PSBT [5] benchmarks were published in either conference or journal papers.

In both the BFBT and PSBT benchmarks, the overall void fraction was generally predicted well by ASSERT. However, for our initial attempts at modelling the distribution of the void within the bundle was prone to error. Subchannels at the periphery of the bundle tended to under-predict the void fraction whereas those near the middle tended to over-predict. The effect was caused by the subchannel mixing model in the code which is more suitable for representing the geometrical obstructions found in the fuel channels of CANDU type reactors rather than the complex mixing phenomena encountered in LWR spacer-mixing vanes. Both BWR and PWR reactors utilize combinations of spacer grids and mixing vanes in order to structurally support the fuel rods, to mix the subchannel enthalpies and to enhance heat transfer and the critical heat flux. The appendages on these grids are designed to introduce turbulence into the flow and homogenize both the bundle enthalpy and void distribution immediately downstream of their location. Since grids cause much more mixing in LWRs as opposed to the end-plates of CANDUs, in order to compensate for this effect in simulation, the magnitude of the mixing coefficients in the lateral momentum source term were adjusted based on a single phase study where the outlet temperatures at each subchannel were measured.

Figure 2 compares the void fraction predicted by ASSERT after the source term adjustment against the values measured experimentally at the central subchannels [4]. It is evident that most of the code predictions fall within the uncertainty of the experiment, with a slight tendency for the code to over-predict at the lower levels and under-predict at the upper elevation. Our experience with applying the RELAP codes 3-dimensional volume connections for subchannel analyses was less successful, mainly due to the lack of a lateral momentum 'mixing' term in for the 3D component [6].

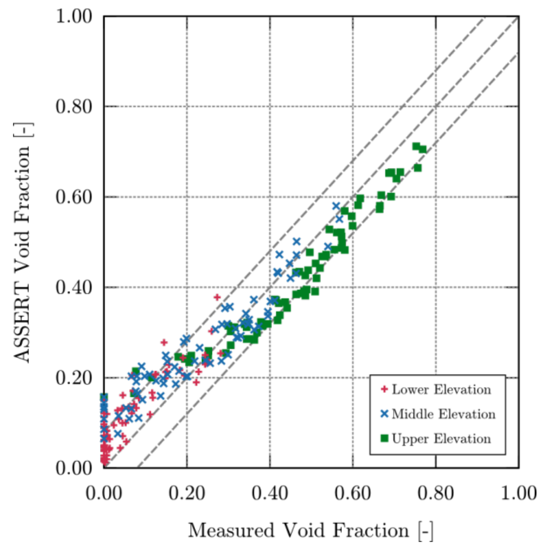

Figure 2: Accuracy of the ASSERT void fraction predictions for bundle B5 of the PSBT benchmark. Error bands represent the experimental error estimated at 2σ = 0.08.

Some of the experimental cases utilized bundle powers which were high enough to cause a departure from nucleate boiling (DNB) in one or more subchannels. The critical heat flux was predicted by the ASSERT code using the Groeneveld lookup table, and in general, consistently predicted the steady state DNB Power once the issues with the mixing were accounted for. This is illustrated in Figure 3, which plots ASSERT's predicted DNB power against the measured value [5]. In this particular set of experiments, a total of 93 cases were examined, and amongst these, the ASSERT had a mean bias of -0.079 MW representing an average error of -1.6%.

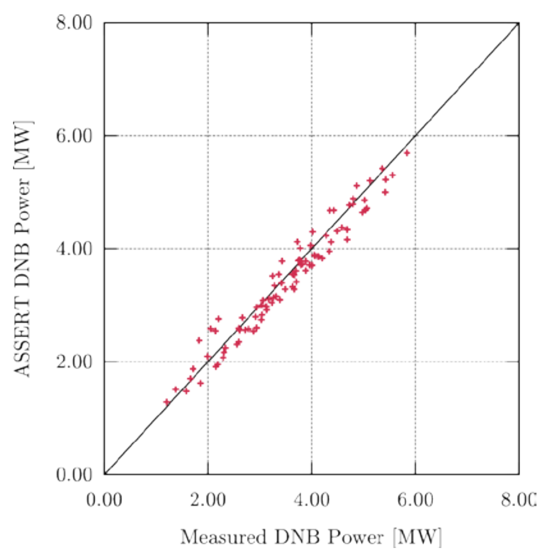

Figure 3: Accuracy of the ASSERT DNB Power predictions for test series A8 of the PSBT benchmark. Experimental uncertainty is estimated to be 2σ = 2%, and is not illustrated.

Four types of transients leading to DNB were examined in the PSBT benchmark cases: power increases, depressurization, mass flow reductions and inlet temperature increases. The initial conditions for these transients along with the maximum rate of change of each parameter are listed in Table 1. In general, ASSERT demonstrated a tendency to predict the time at which DNB occurred slightly early as demonstrated in Table 2. This effect was most significant in the coolant mass flow reduction cases where the code was predicting DNB between 4.7 and 6.2 seconds earlier than recorded in the experiment. Some of the benchmark participants have suggested that the experimental DNB times reported may be influenced by both the presence of thermowell on the fluid measuring thermocouple, and the location of the inlet temperature monitoring device being far enough upstream of the bundle inlet that a delay of several seconds appears [7]. The results presented in Table 2 are not modified to account for these possible discrepancies.

Table 1: Initial test conditions along with maximum rates of change for the transient DNB tests.

	Initial Condition	Maximum Rate
Power	2.5 MW	+15% / s
Mass Flow	3.11 Mg/m^2s	-25% / s
Pressure	15.3 MPa	-0.03 MPa/s
Inlet Temperature	291^oC	+1 ^oC / s

Table 2: Transient DNB times as recorded in the experiment and predicted by ASSERT.

Test Set	Transient	$t_{DNB,exp}$ (s)	$t_{DNB,ASSERT}$ (s)
A11	Power Increase	106.7	105.4
	Flow Reduction	52.9	48.2
	Depressurization	88.8	86.2
	Inlet Temp. Increase	140.6	139.4
A12	Power Increase	86.6	82.8
	Flow Reduction	55	48.8
	Depressurization	143.8	144.8
	Inlet Temp. Increase	128.8	126

4. Computational Fluid Dynamics Benchmark

Grid spacers within PWR and BWR nuclear fuel assemblies play a critical role in fuel performance and contribute to safety margins by enhancing the margins to the Critical Heat Flux (CHF). The OECD-NEA has organized a blind computational benchmark wherein the prediction of flows and turbulence downstream of a mixing-type grid spacer are examined. The goal at the outset of the McMaster study was to obtain a reasonably accurate solution with a minimum number of nodes and appropriate turbulence models such that the results would be relevant for engineering applications which include property variations and heat transfer. As such advanced modeling methods such as Large Eddy Simulation or Unsteady Reynolds Average Navier Stokes (URANS) were not included within the scope of the models tested at McMaster. Other participants from Canada and abroad provided contributions utilizing a wide range of CFD approaches from steady to unsteady simulations.

To support the model selection used in our final submission we first performed a comprehensive separate effects study. Several partial geometries were studied for steady and unsteady behavior as well as for mesh sensitivity, turbulence and wall modeling effects. A series of successively more complex simulations, sometimes involving unsteady modeling, was performed up to and including a study of similar 5x5 rod bundle geometry reported in literature. These sensitivity and separate effect studies alone took the better part of 1 person year to complete, prior to computations of the final test cases. These studies however generated wealth of information which helped to ensure that the final submission achieved some of the most accurate results possible for a 2-equation engineering scale CFD application.

One particularly challenging aspect of this benchmark was that some of the flow within the PWR grid spacer is extremely complex, and either required an extremely large number of meshes (making it less attractive as an engineering scale approach) or implementing a coarse mesh such that these complicated features are not numerically resolved (thereby losing some of the physics involved). The figure below illustrates the results of the CFD simulations for a single centralizing button located within a subchannel. Here the wall shear stress demonstrates clear unsteady behavior and required a full URANS approach with extremely fine computational meshes. To perform such detailed simulations for all centralizing buttons and including heat transfer computations would make the solution time less attractive for engineering scale applications. So the final solution was to implement a coarser mesh such that these unsteady features are not resolved within the grid spacer, and accept that our final simulations may tend to be biased low with respect to downstream turbulence level. Indeed this is exactly what was observed in our simulations when the blind data was released (where our results showed excellent agreement on velocities and subchannel flow distributions, but where turbulence levels were generally under predicted).

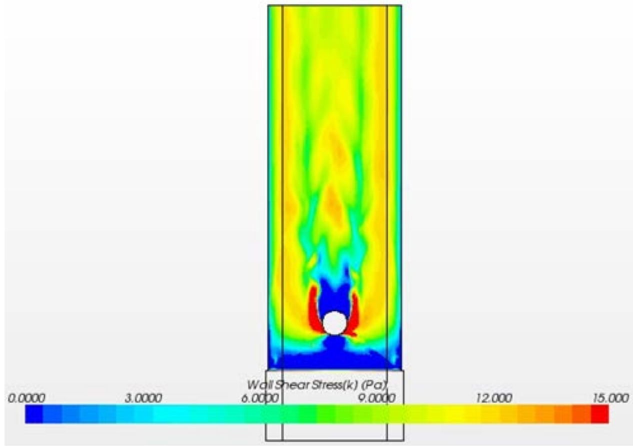

Figure 4: The unsteady flow behavior and turbulence generation around a single centralizing button within a PWR grid spacer.

Another interesting result can be observed in the determination of circulation levels downstream of the mixing vane, and in particular in the decay of circulation with respect to distance. Since circulation and turbulence lead to downstream heat transfer and CHF enhancement, it is interesting to see how well the simulations can predict the downstream decay of these properties. In general, the CFD predictions done at McMaster agreed very well with the downstream decay as shown in terms of the circulation, and absolute circulation in the figures below. Further details can be obtained from references [8] and [9].

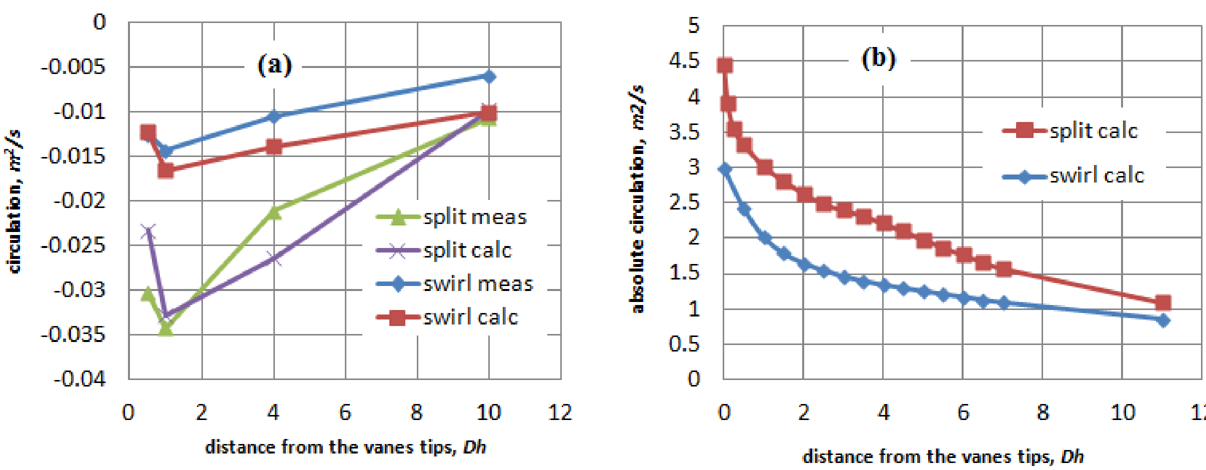

Figure 5: Decay of flow circulation downstream of mixing vanes a) circulation and b) absolute value of circulation.

5. Conclusions

The following conclusions and lessons can be drawn from our participation in these benchmarks.

UAM – While TSUNAMI-1D represents an excellent tool for sensitivity and uncertainty analysis, it is difficult to extend its capabilities beyond nuclear data alone, and this is compounded with burnup, geometrical and operational uncertainties which must be considered in a full-scale uncertainty analysis. In order to resolve these limitations, we adopted a full Monte-Carlo approach to nuclear data uncertainty propagation and sensitivity analysis, however we encountered several issues with respect to the suitability of best-estimate multi-group libraries for such analysis. The tool was validated against TSUNAMI-1D for the UAM Phase 1 benchmark and we found very good agreement.

BFBT – Here one of the largest benefits obtained was access to new and independent CHF data and high fidelity void fraction distribution data obtained by JNES for a BWR assembly under prototypical BWR conditions. We observed that the Canadian subchannel code predicted the void fraction and dryout quite successfully for conditions at the higher pressure and elevation within the database, however some predictions discrepancies were observed in other regions of the database where conditions deviated from those which for the constitutive relationships within ASSERT. These deviations were particularly evident under low-pressure and low-mass flux conditions, and difficulty obtaining accurate predictions was experienced by many benchmark participants.

PSBT – ASSERT also predicted the dryout and void fraction distribution quite well for the PWR benchmark, in particular for lower degrees of subcooling. Under conditions where subcooled nucleate boiling occurs and DNB type dryout occurs, ASSERT showed some deviations from experimental results which can be attributed to both the deviation from the conditions used to derive the constitutive relationships as well as some issues within the 1995 CHF look-up table which is used in ASSERT.

The authors would like to sincerely thank NSERC and UNENE for supporting our contributions to the OECD-NEA benchmarks. It has provided the opportunity for students to get involved in international activities and facilitated the transfer of high-value experimental data from other jurisdictions to Canadian universities.

6. References

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