SCIENCE & TECHNOLOGY

CASL

Consortium for Advanced Simulation of Light Water Reactors

Verification and Validation Supporting VERA Neutronics Code

As CASL produces its VERA software each physics capability must be tested, verified, and validated (V&V). The overarching objective of code verification is to establish that a computational model implemented in a code accurately represents the developer's conceptual representation of the physics, while validation refers to the process of determining the degree to which a computational model provides an accurate representation of the real world. Researchers on CASL's Radiation Transport Methods (RTM) team has implemented a rigorous V&V program for it's MOC capability as implemented in the MPACT code.

CASL's verification activities encompass both the source code and the code solution, providing comprehensive software testing and evaluation of the numerical error in the solution. Unit testing is used to isolate small bites of source code to determine whether they are fit for use. In contrast, regression testing seeks to uncover bugs in existing functional areas of the code after changes have been made to the source. RTM's practice is to create unit tests for all functions and methods while the code itself is being written; unit testing accelerates the process of finding and correcting bugs by allowing the location of the fault or failure to be easily traced. One of the challenges of writing the unit tests is the difficulty of setting up realistic tests with relevant initial conditions such that the part of the application being tested behaves like part of the complete system. If these initial conditions are not set correctly, the test will not be exercising the code in a realistic context, which diminishes the value and accuracy of unit test results.

Since unit testing only examines the functionality of the units themselves, it is recognized that unit testing will not catch every error in the program. Specifically, unit testing does not catch integration errors or broader system-level errors. Therefore, RTM also incorporates regression testing as a part of its verification process. Regression tests are a series of tests that are repeated as the code development progresses. The results are compared against previously recorded outputs to ensure that new features and enhancements do not alter the reproducibility of existing features. The best practice used in MPACT is that when a bug is located and fixed, a test is recorded that exposes the bug and the test is rerun regularly after subsequent changes to the program.

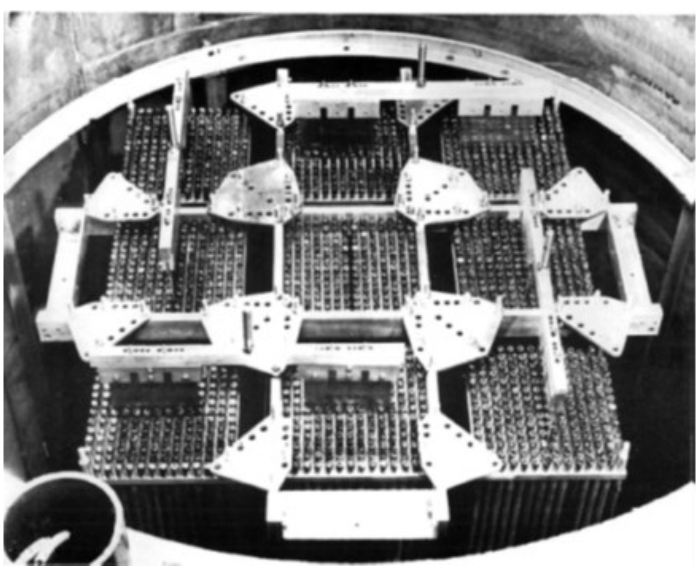

Figure 1 Babcock and Wilcox critical experiment facility. The experiments reported by the facility are used in the validation of VERA's MOC neutronics code.

A summary of some of the key capabilities tested during verification include:

- **Geometry**
  - ◊ Cylindrical, Quarter, Rectangular and Generalized cylinder pin geometries
  - ◊ Inserts
  - ◊ Control rod (+ rod movement)
  - ◊ Baffle/Reflector
  - ◊ Upper/lower nozzle, core plate, reflector
  - ◊ Multiple assemblies/modules
  - ◊ Symmetry
  - ◊ Grids
  - ◊ Detectors
- **Transport Solvers**
  - ◊ P0 and Pn 2D MOC
  - ◊ P0 and Pn 2D-1D with SP3 (and NEM)
- **Other Solvers**
  - ◊ Depletion (native and Origen)
  - ◊ Search (boron, rod)
  - ◊ Multistate
  - ◊ CMFD (Multilevel, MGNode, 1Gsweep)
  - ◊ Feedback (internal and CTF)
  - ◊ Eq Xe/Sm
  - ◊ XS Shielding (Subgroup vs ESSM)
  - ◊ Cusping treatment
- **Parallel**
  - ◊ MPI (space, angle, space+angle), explicit file
  - ◊ OpenMP (threading)

Another principal motivation of CASL's verification activities is the evaluation of the numerical error in the solutions produced by the code. Initially, this was focused on mesh convergence studies; however, a more comprehensive and thorough verification has been planned based on the Method of Manufactured Solutions (MMS). The essential concept behind MMS is, rather than solving a specified problem with prescribed boundary and initial conditions, to specify the solution (Manufactured Solution) and substitute the solution into the governing equation/neutron transport equation. This results in an extra analytical source (Manufactured Source). The boundary and initial conditions can be obtained by evaluating the manufactured solution at the boundary and at initial time. This set of boundary and initial conditions, together with the manufactured source have "manufactured" a problem from which the exact analytical solution is known. By comparing the numerical solution from the solver with the manufactured analytical solution and observing the expected rate of convergence in the successive grid refinements, the numerical solution can be verified.

Additionally, verification of VERA's code solution is being accomplished through comparisons with calculated quantities on fine scales from continuous energy (CE) Monte Carlo methods, including 3D core pin-by-pin fission rates at operating conditions, intra-pin distributions of fission and capture rates, reactivity and pin power distributions of depleted fuel, and support for other capabilities such as gamma transport and thick radial core support structure effects.

For validation, the goal is to identify those tests which will increase confidence in the quantitative predictive capability for practical reactor applications; thus, it is important to compare VERA's predictions to measured reactor data in addition to experimental data. A comprehensive validation plan was developed for VERA's core simulator capability (coupled MOC and subchannel thermal-hydraulics), with the primary validation sources identified as:

1) Measured data from experiments with small critical nuclear reactors. This includes critical conditions, fuel rod fission rate distributions, control rod or burnable poison worths, and isothermal temperature coefficients.

2) Measured data from operating commercial nuclear power plants. This includes critical soluble boron concentrations, beginning-of-cycle (BOC) physics parameters such as control rod worths and temperature coefficients, and measured fission rate responses from in-core instrumentation.

3) Measured isotopics in fuel after being irradiated in a nuclear power plant. This includes gamma scans of ^{137}Cs activity, burnup based on ^{148}Nd concentrations, and full radiochemical assays (RCA) of the major actinides and fission products.

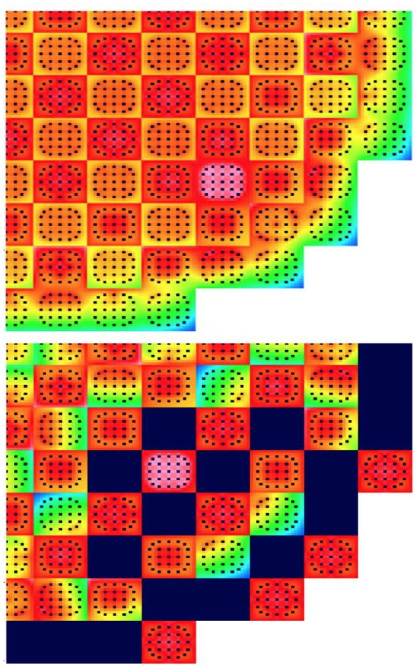

Figure 2 Pin Exposure at End of BEAVRS Cycle 1 (top) and Beginning of Cycle 2 (bottom)

During the first phase of CASL, progress has been made in each of these areas, with the exception of fuel depletion / measured isotopics in item 3. The comprehensive validation matrix developed within CASL-U-2014-0185-000 lists the required code capabilities, features, and the application range with the proposed benchmarking activities. Although it is unlikely that CASL can complete all of the validation activities listed, the matrix provides guidance towards prioritizing validation activities to ensure that sufficient effort is performed across the full range of capabilities and features for VERA's core simulator. Similar matrices for VERA's other capabilities are under development.

CASL-U-2015-0143-000 describes a series of benchmark calculations performed by University of Michigan and Oak Ridge National Lab researchers using VERA's MOC radiation transport code, MPACT, to validate its results against the B&W-1484 [1] and B&W-1810 [2] benchmark experiments (see an image of he experimental facility in Figure 1). 18 of the 44 critical configurations were examined in depth. For the B&W-1484 cases, agreement was within 200 pcm of the measured eigenvalue for cases using P_2 scattering. For the B&W-1810 cases, the root-mean-squared value was 77 pcm for and 208 pcm for P2 and TCP0 scattering, respectively, with a maximum discrepancy of 112 pcm and 261 pcm for P2 and TCP0 scattering, respectively. The fission rate comparisons, which were available for four of the 1810 cores, yielded RMS comparisons between 0.47% and 0.76% with maximum errors between 1.27% and 2.11%.

CASL-U-2015-0076-000 describes the modeling of the Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS) [4, 5, 6] using VERA. The BEAVRS benchmark provides two cycles' worth of operational history, including power levels and boron concentrations. Figure 2 illustrates VERA's shuffle feature with the pin exposures mapped from the end of cycle 1 to the beginning of cycle 2. Figure 3 provides a graph of the VERA-predicted critical boron concentration against that measured in the BEAVRS experiments. In addition, flux maps are provided at several points during each operating cycle. Comparisons with VERA predictions show reasonable agreement, with a 2D RMS error of 2.7%. BEAVRS cycle 1 critical boron concentration compared well with VERA predictions, and flux map comparisons were consistent with measured trends.

More information is available in CASL-U-2014-0185-000, CASL-U-2015-0234-000, CASL-U-2015-0143-000, and CASL-U-2015-0076-000.

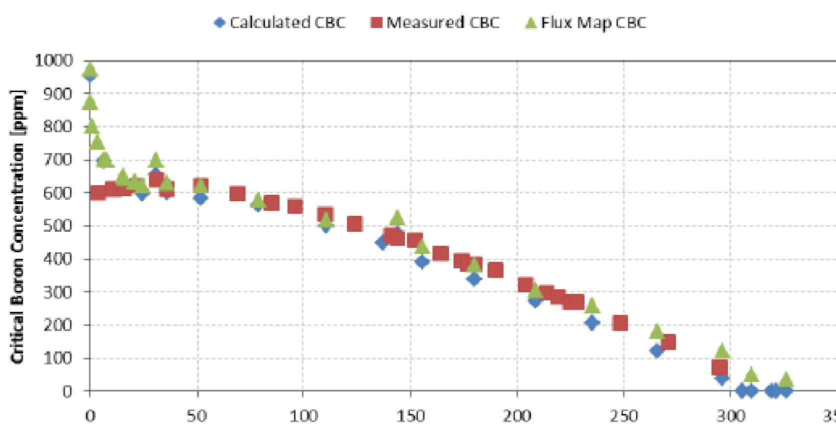

Figure 3 Calculated versus Measured Critical Boron Concentration as a function of effective full power days for BEAVRS cycle 1

References cited in this article include:

[1] M. N. Baldwin and G. S. Hoovler, "Critical Experiments Supporting Close Proximity Water Storage of Power Reactor Fuel," Tech. Rep. BAW-1484-1, The Babcock & Wilcox Company, 1978.

[2] L. W. Newman, W. A. Wittkopf, W. G. Pettus, M. N. Baldwin, H. A. Hassan, V. O. Uotinen, J. D. Connell, and P. S. Campbell, "Urania Gadolinia: Nuclear Model Development and Critical Experiment Benchmark," Tech. Rep. BAW-1810, The Babcock & Wilcox Company, 1984

[3] N. Hoerlik, B. Herman, B. Forget, and K. Smith. "Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS)," v1.0.1 *Proc. Int. Conf. Mathematics and Computational Methods Applied to Nuc. Sci. & Eng.*, Sun Valley, Idaho (2013).

For a full listing of relevant references, please see the CASL reports cited.