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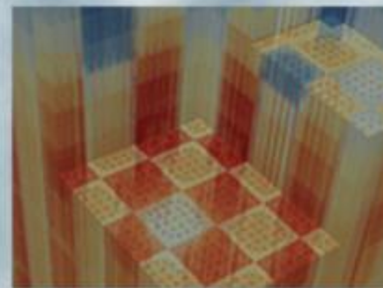

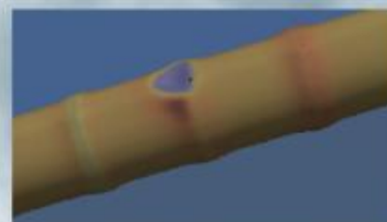

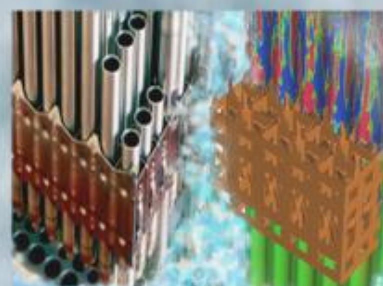

VERA-CS
Verification & Validation Plan
(rev 0)

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February 28, 2017

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

REVISION LOG

Revision	Date	Affected Pages	Revision Description
0	2/28/17	All	Initial Release

Document pages that are:

Export Controlled ____________ None

IP/Proprietary/NDA Controlled__ None

Sensitive Controlled___________ None

Requested Distribution:

To:

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EXECUTIVE SUMMARY

This report summarizes the current status of VERA-CS Verification and Validation for PWR Core Follow operation and proposes a multi-phase plan for continuing VERA-CS V&V in FY17 and FY18. The proposed plan recognizes the hierarchical nature of a multi-physics code system such as VERA-CS and the importance of first achieving an acceptable level of V&V on each of the single physics codes before focusing on the V&V of the coupled physics solution. The report summarizes the V&V of each of the single physics codes systems currently used for core follow analysis (ie MPACT, CTF, Multigroup Cross Section Generation, and BISON / Fuel Temperature Tables) and proposes specific actions to achieve a uniformly acceptable level of V&V in FY17. The report also recognizes the ongoing development of other codes important for PWR Core Follow (e.g. TIAMAT, MAMBA3D) and proposes Phase II (FY18) VERA-CS V&V activities in which those codes will also reach an acceptable level of V&V.

The report then summarizes the current status of VERA-CS multi-physics V&V for PWR Core Follow and the ongoing PWR Core Follow V&V activities for FY17. An automated procedure and output data format is proposed for standardizing the output for core follow calculations and automatically generating tables and figures for the VERA-CS Latex file. A set of acceptance metrics is also proposed for the evaluation and assessment of core follow results that would be used within the script to automatically flag any results which require further analysis or more detailed explanation prior to being added to the VERA-CS validation base. After the Automation Scripts have been completed and tested using BEAVRS, the VERA-CS plan proposes the Watts Bar cycle depletion cases should be performed with the new cross section library and be included in the first draft of the new VERA-CS manual for release at the end of PoR15. Also, within the constraints imposed by the proprietary nature of plant data, as many as possible of the FY17 AMA Plant Core Follow cases should also be included in the VERA-CS manual at the end of PoR15.

After completion of the ongoing development of TIAMAT for fully coupled, full core calculations with VERA-CS / BISON 1.5D, and after the completion of the refactoring of MAMBA3D for CIPS analysis in FY17, selected cases from the VERA-CS validation based should be performed, beginning with the "legacy" cases of Watts Bar and BEAVRS in PoR16. Finally, as potential Phase III future work some additional considerations are identified for extending the VERA-CS V&V to other reactor types such as the BWR.

CONTENTS

ACRONYMS

CASL Consortium for Advanced Simulation of Light Water Reactors
CP Challenge Problem
CRUD corrosion-related unidentified deposits or Chalk River unidentified deposits
CTF COBRA-TF subchannel thermal-hydraulics code
DOE US Department of Energy
EPRI Electric Power Research Institute
FA Focus Area
HZP Hot Zero Power
LANL Los Alamos National Laboratory
LWR light water reactor
MOC method of characteristics
OLCF Oak Ridge Leadership Computing Facility
OR operational reactor
ORNL Oak Ridge National Laboratory
PCI pellet-cladding interaction
PCM percent mille (10-5)
PHI Physics Integration
PoR plan of record
PWR pressurized water reactor
QOI quantity of interest
RSICC Radiation Safety Information Computational Center
RTM Radiation Transport Methods
SA sensitivity analysis
SNL Sandia National Laboratories
T/H thermal-hydraulics
THM Thermal Hydraulics Methods
UQ uncertainty quantification
UM University of Michigan
V&V verification and validation
VERA Virtual Environment for Reactor Applications
VMA Validation and Modeling Applications
VR virtual reactor
VUQ Validation and Uncertainty Quantification
VVUQ Verification, Validation and Uncertainty Quantification
WEC Westinghouse Electric Company

SECTION 1

INTRODUCTION

Several government and commercial institutions are now developing large-scale computational simulations for massively parallel platforms to simulate the performance of complex, coupled multi-physics phenomena similar to the CASL efforts on nuclear reactor simulation. These include research in climate and weather prediction, magnetic and inertial fusion energy, environmental systems, astrophysics, aerodynamic design, combustion, biological and biochemical systems, and other areas. A brief review of the literature describing some of the more successful efforts in these areas [Post, 2004] suggests a few V&V best practices for multi-physics that might be useful for planning the verification and validation (V&V) of VERA-CS.

Foremost among these is the importance of exploiting the hierarchical nature of the multi-physics solution and first performing thorough V&V on the single physics codes before moving to the coupled physics solutions. In fact, this has generally been the case with VERA-CS during the last few years where the principal focus of V&V effort has been on the individual codes. This has especially been the case for MPACT, CTF, and BISON. The exceptions to this have been for the codes which are not yet sufficiently mature for an extensive V&V to be appropriate such as the coupling code TIAMAT and the MAMBA code, or the suite of code modules used to prepare cross sections for MPACT.

Another best practice that is common to all successful efforts in V&V of multi-physics simulations is the importance of having a clearly identified "Quantity of Interest" (QOI) that provides the basis for quantifying the status or maturity of the code. In the case of CASL the ultimate QOI are the Challenge Problems which include CRUD, PCI, RIA, etc. In fact, the CASL Challenge problems will provide the basis for the PCMM that will be performed by VVI as part of their milestone in 2017 on the assessment of VERA-CS V&V. Therefore the focus of the V&V plan that will be performed by PHI is concerned not directly with a specific CASL challenge problem, but with the principal VERA-CS functionality of ***PWR core follow*** which is common to all challenge problems.

Finally, the essential distinction between V&V for single and multi-physics codes is the presence of an additional code or module required to do code coupling. In the case of VERA, the principal code coupling modules are MPACT, which drives the VERA-CS coupling of the transport with ORIGEN depletion, CTF thermal-hydraulics, and MAMBA clad-coolant chemistry, TIAMAT, which is used to couple VERA-CS with BISON, and Cicada, which is used to couple MAMBA with CFD (CCM+). There are notable differences in the maturity of these coupling modules, with VERA-CS being very mature and TIAMAT and Cicada developing with attention to V&V but not yet ready for delivery to AMA.

Because of the uneven maturity of both the VERA-CS codes and the code coupling capability, a multi-phase plan is proposed for VERA-CS V&V which can be accomplished over the next several PoR's. The following sections will first review the components and status of the VERA-CS codes and coupling, and then outline the details of the multi-phase VERA-CS V&V plan.

SECTION 2

OVERVIEW AND STATUS OF VERA-CS SINGLE PHYSICS V&V

A. OVERVIEW OF SINGLE PHYSICS CODES

The Virtual Environment for Reactor Analysis (VERA) is a simulation environment being developed by CASL, which is comprised of codes collectively used for nuclear reactor modeling and simulation. Figure 2.1 shows the components of VERA, and VERA-CS is considered to be the subset of VERA for core simulation, which is typically neutronics and thermal hydraulics. The primary deterministic neutron transport solver is MPACT, and CTF is the subchannel thermal hydraulics solver. However, for purposes of VERA-CS V&V for core follow calculations, the cross section generation and the fuel temperature tables derived from the BISON fuel performance code are also considered.

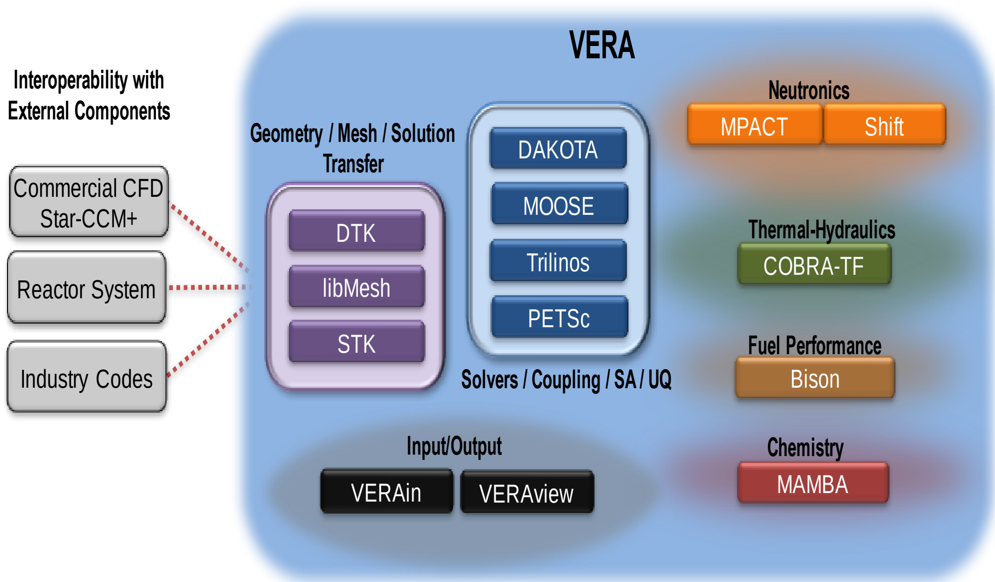

Fig. 2.1 VERA and VERA-CS

A.1 MPACT

The MPACT neutron transport solver, being developed collaboratively by Oak Ridge National Laboratory (ORNL) and the University of Michigan (UM), provides pin-resolved flux and power distributions [Larsen, 2017]. To solve three-dimensional (3D) problems, it employs the 2D/1D method, which decomposes the problem into a 1D axial stack of 2D radial planes [Collins, 2014]. Typically, 2D Method of Characteristics (2D MOC) is used to solve each radial plane, and 1D nodal methods are used to solve axially along each rod. While there are a variety of axial solvers available, the nodal expansion method (NEM)-simplified P3 (SP3) solver is the default, which wraps a one-node NEM kernel [Stimpson, 2014]. These 2D and 1D solvers are coupled together through transverse leakage terms to ensure neutron conservation, and they are accelerated using 3D coarse mesh finite difference (CMFD).

Fuel depletion in MPACT [Zhu, 2014] is performed using the point depletion calculation in ORIGEN which is coupled to MPACT using an application program interface (API) which enables the transfer of the MG scalar flux and microscopic cross sections from MPACT to ORIGEN and particle number densities from ORIGEN to MPACT. The ORIGEN [Gauld, 2011] has been well verified and validated in previous work and will not be considered in this plan. However, some issues have been identified with testing of the ORIGEN API [Wieselquist, 2015] and as discussed in section B.1 will be included in planning for future MPACT V&V.

A.2 CTF

CTF is a subchannel TH code being developed by ORNL and North Carolina State University (NCSU) specifically for light water reactor (LWR) analysis [Avramova, 2009]. CTF includes a wide range of thermal-hydraulic models important to LWR safety analysis including flow regime dependent two-phase wall heat transfer, inter-phase heat transfer and drag, droplet breakup, and quench-front tracking. CTF also includes several internal models to help facilitate the simulation of actual fuel assemblies. These models include spacer grid models, a fuel rod conduction model, and built-in material properties for both the structural materials and the coolant (i.e. steam tables). CTF uses a two-fluid, three-field representation of the two-phase flow. The equations and fields solved are:

- Continuous vapor (mass, momentum and energy)
- Continuous liquid (mass, momentum and energy)
- Entrained liquid drops (mass and momentum)
- Non-condensable gas mixture (mass)

CTF provides significantly higher resolution and physics detail than the internal thermal hydraulics solver (Simplified TH) in MPACT, and thus longer execution times. However, several improvements have been made to CTF to improve performance and parallelism and the CTF execution times have been reasonable for PWR core follow application.

A.3 MULTIGROUP XSEC LIBRARIES

Changes to the material composition in the reactor because of the temperature and nuclide density changes modifies the macroscopic cross sections used in the MPACT transport solution. The macroscopic cross section calculation in MPACT requires the Multi-group (MG) cross section library and the parameters necessary to perform the resonance self-shielding calculation. The MG library is precomputed for use by MPACT and contains microscopic cross section and resonance integral data tabulated as a function of temperature and energy. The generation of the MPACT MG library is based on the MG AMPX library and a number of supporting methodologies within the SCALE code package at the Oak Ridge National Laboratory (ORNL) [Scale, 2009]. The latest release of the MPACT MG library includes a total of 295 isotopes and 51 energy groups, of which 17 groups (1.46-9118eV) are defined as resonance groups with resonance integral data and subgroup parameters. The resonance calculation is performed for the 17 resonance groups for a subset of 49 resonance isotopes, including the important actinides and fission products. Outside this range, base cross sections from the library (only a function of temperature) are directly used to compute the macroscopic cross section of a material region. Most recently, the V4.2m5 and V5.0m0 Multigroup Cross Section Libraries for MPACT have been released for PWR and BWR as described in [Kim, 2017].

A.4 BISON / FUEL TEMPERATURE TABLES

The BISON fuel performance code is being developed by Idaho National Laboratory (INL) [Williamson, 2012] to provide fuel performance modeling capability to assess best-estimate values of design and safety criteria and the impact of plant operation and fuel rod design on thermomechanical behavior. BISON is built on INL's Multiphysics Object Oriented Simulation Environment (MOOSE) package [Gaston, 2009] which use the finite element method for geometric representation and a Jacobian Free Newton-Krylov (JFNK) scheme to solve systems of partial differential equations. Because of the computational intensity of the BISON fuel performance calculation, most practical analysis in CASL has used a "one-way" coupling of VERA-CS with BISON in which the time-dependent power shape/history and moderator temperature heat source data from MPACT-CTF is used in a 2D azimuthally symmetric (R-Z), smeared-pellet thermomechanical fuel pin model in BISON. In FY17 significant progress has been made to reduce the computational requirements for BISON by introducing a lower dimensionality "1.5 D" option and enable a full two-way coupling with VERA-CS using the coupling code TIAMAT.

However, core calculations within VERA-CS are currently performed using Fuel Temperature Tables which functionalize the fuel temperature to key variables (e.g. power, burnup) and are based on BISON single pin calculations performed at representative core conditions. The development of the Fuel Temperature tables began in MPACT early in FY15 and used a quadratic fit with respect to power, with burnup dependent coefficients [Stimpson, 2016a]:

$$\Delta T = Fuel - Tcool = aP + bP^2$$

In the above equation, P is the local linear heat rate, which is determined by the power profile in MPACT, ΔT is the difference between the average fuel temperature ($Tfuel$, which is considered to be constant radially) and the bulk coolant temperature ($Tcool$). (note: for applications with CTF this would be clad surface temperature, since this assume the user-defined clad-coolant heat transfer coefficient is equal to the CTF physics-based one that includes subcooled boiling.

Originally, nine predefined axial power shapes were input to BISON to formulate the temperature table in order to cover a range of linear heat rates by using several different rod powers along with top and bottom peaked distributions. The fuel temperature tables based on this approach were used in the simulations of WBN1, Cycles 1-12 [Godfrey, 2015]. During FY16, improvements were made to the original tables (e.g. extending the burnup range, etc) and a new table was developed [Stimpson, 2016b] and has been used in subsequent core follow analyses.

A.5 MAMBA

The MAMBA code [MPO Advanced Model for Boron Analysis] was developed to predict the evolution of CRUD buildup throughout the fuel cycle. MAMBA was designed as a first principles code capable of understanding CRUD at the microscale as well as at the engineering scale to predict crud growth, composition, boron hideout, and elevated temperature distributions due to crud buildup [Kendrick, 2011]. Version 1.0 of MAMBA was the first realization of the crud models that was first applied within CASL in 2011. The original MAMBA 1D code was later extended to 3D (MAMBA3D) [Kendrick, 2014].

MAMBA is an essential part of both the CIPS (Crud Induced Power Shift) and CILC (Crud Induced Local Corrosion) CASL Challenge problems. For purposes of PWR core follow, the application of MAMBA1D to CIPS was successfully demonstrated [Collins, 2016] in the analysis of Watts Bar I. For the CILC challenge problem a more detailed thermal-hydraulic modeling capability was necessary and MAMBA3D was successfully coupled to CFD [Manera, 2016]. However, the high computational burden for MAMBA3D required maintaining separate codes with some differences in the physics. The current focus of MAMBA development within CASL has been to refactor the MAMBA3D code and to achieve significant improvements in the performance to enable a single MAMBA code for both CIPS and CILC applications [Collins, 2017]. The expectation is for a preliminary version of the code to be ready for testing in March, 2017 and then to recover and demonstrate all MAMBA3D functionality necessary for both CIPS and CILC in PoR15. In FY18 specific milestones will be established for the refactored MAMBA3D to achieve V&V consistent with the other VERA-CS codes.

B. STATUS OF SINGLE PHYSICS V&V

The overall assessment of the V&V status of each of the codes within VERA-CS for the CASL challenge problems is the purview of VVI. However, for purposes of planning the VERA-CS V&V activities within PHI, a brief assessment of each of the single physics codes noted in Section A is provided for the specific QOI of Core Follow.

B.1 V&V Status of MPACT

The Verification and Validation of the MPACT code has matured over the past few years and the most recent V&V status is summarized in revision 2 of the MPACT V&V manual [Downar, 2016]. Several ongoing and planned FY17 activities will continue to strengthen code verification, particularly in the area of solution verification using the Method of Manufactured Solutions (MMS), and in the area of source code verification to improve the unit and regression test coverage. However, the status of MPACT V&V appears to be acceptable and provides confidence in the ability of MPACT for the QOI of core follow.

MPACT validation work has also matured with additional work on critical experiments and the use of post-irradiation examination (PIE) tests for evaluation and validation of the isotopic depletion capability in MPACT. A recent significant contribution to the MPACT validation base has been the results for the WB2 start-up tests. However, this work also identified some possible issues with certain models (i.e. fuel temperature model) that are currently being investigated [Godfrey, 2017]. But in general the results of V&V efforts this past year and the ongoing efforts in FY17 have increased the confidence level in the ability of MPACT to model an operational Pressurized Water Reactor. However, one gap in the MPACT V&V that should be addressed is the testing of the ORIGEN API. A higher priority should be given to the existing defect tickets and a plan should be developed to improvement of the overall testing of the ORIGEN API:

https://vminfo.casl.gov/trac/casl_phi_kanban/ticket/4580

It should also be noted that in previous MPACT V&V manuals, the results of core follow operation were included as MPACT validation, even though the results were multi-physics MPACT-CTF. Beginning in Rev 3, the MPACT V&V will include only single physics results (e.g. critical experiments, fresh core start up tests, etc) and all MPACT-CTF core follow data will be moved to the VERA-CS manual.

B.2 V&V Status of CTF

The most recent CTF V&V manual [Salko, 2016] provides a thorough review of the predictive capabilities of CTF for the scenarios it was designed to model—rod bundle geometries with operating conditions that are representative of prototypical Pressurized Water Reactor (PWR)s and Boiling Water Reactor (BWR)s in both normal and accident conditions. The validation was accomplished by modeling a variety of experiments that simulate these scenarios and then presenting a qualitative and quantitative analysis of the results that demonstrates the accuracy to which CTF is capable of capturing specific quantities of interest.

Several of the CTF validation tests have been incorporated as regression tests which are run on a continual basis to demonstrate code results are not changing. Many additional regression tests are included in the CTF automated test matrix that do not have experimental results or an analytical solution to compare against and simply exercise some feature or combination of features that have an effect on the output file, which is checked against a gold version. The CTF V&V document does not describe all regression tests being performed on CTF. Instead, documentation for such tests is provided in the "CMakeLists.txt" file that drives the automated test matrix or in the corresponding test input files found in COBRA-TF/cobra tf/test matrix. This is appropriate, however, in the next version of the CTF V&V manual, specific verification activities should be summarized in a separate section of the manual, which should include Source Code Verification (ie Unit Testing/Code Coverage and Regression Testing/Test Matrix) as well as Solution Verification. Overall, however, the results of CTF V&V efforts this past year have matured and increased the confidence level in the ability of CTF to perform core follow for an operational Pressurized Water Reactor.

B.3 V&V Status of MULTIGROUP XSEC LIBRARIES

Significant progress was made in FY16 to formalize the methodology for generating the multi-group cross section library for MPACT [Kim, 2016]. This past year the methodology was successfully implemented in the generation of a new 51-group library [Kim, 2017]. The CASL library has matured and testing has substantiated the ability of the library to model the range of PWR conditions necessary for core follow. The next step for the CASL multigroup cross section library would be the development a formal Verification and Validation manual. The proposed outline for the manual would include the following:

Outline

1. Introduction
2. Code Verification
    - 2.1 AMPX Library Generation Procedure
    - 2.2 MPACT Library Generation Procedure
3. Validation by Code to Code Comparisons (MCNP)
    - 3.1 VERA progression problems 1-4
    - 3.2 Reaction Rate Analysis
    - 3.3 Extensive PWR pin and assembly benchmark problems
    - 3.4 BWR pin and assembly benchmark problems
    - 3.5 Non-uniform fuel temperature problems
5. Uncertainty Analysis

6. Conclusions

Appendices

A. CASL document for each section,
B. All MPACT inputs in VERA-CS repository,
C. All reference inputs and outputs in VERA-CS repository,
D. Setup automatic calculations of MPACT as needed,

B.4 V&V Status of BISON / FUEL TEMPATURE TABLES

The V&V for the BISON code is extensive and has been well described in a separate V&V manual [INL, 2014]. The validation base for BISON is extensive and currently includes 24 validation cases that include several of the key quantities of interest for core follow such as the fuel centerline temperature at beginning of life, throughout life, and during power ramps. The planned BISON validation work will add several new cases from the FUMEX data base. In general, the status of BISON V&V is acceptable and provides confidence in the ability of BISON to provide fuel performance for the QOI of PWR core follow.

The principal interest for purposes of fuels modeling for core follow with VERA-CS then becomes the ability to verify the BISON model is being used properly to generate the fuel temperature data for VERA-CS. As noted in section A.4, the fuel temperature tables have been used successfully within VERA-CS for the past few years for core follow applications. During the development of the scripts to generate the fuel temperature tables, the developers performed selected code verification to include the development of regression tests which used to perform parametrics to assess the error of alternate data processing methods. One example noted in [Stimpson, 2016] was that " … from assessing the accuracy of a quadratic fit to the linear power, it was observed that the inaccuracies ranged from -20K to +10K, with the largest differences present at 5 kW/ft, which is close to the average linear heat rate in the core." The potential error because of this modeling could be as large as 50-60 pcm (or 5-6 ppm) which can become worth noting for core follow operations. The authors also note that one possibility for reducing these errors would be to utilize a bilinear lookup in burnup and power, which would be important to quantify in the verification report, especially if the model were considered for extension to other applications (e.g. BWR).

In general the fuel temperature tables have performed well for core follow and provide confidence in the overall fuel temperature used in PWR core follow calculations. However, a future milestone should include the expansion and documentation of unit testing and regression testing to include an uncertainty analysis of various user input options. This will be especially important since the fuel temperature tables capability will likely continue to be an important modeling option in VERA-CS, even if a two-way coupling with BISON become feasible in the future.

B.5 V&V Status of MAMBA

As noted in section A.5, the MAMBA3D code is under active development in FY17. And as part of the MAMBA3D refactoring the developers are implementing a unit and regression testing protocol that should result in robust source code verification when the code is completed at the end of PoR15. However, considerable work will remain for the V&V of MAMBA3D and specific milestones are proposed for Phase II of the VERA-CS V&V plan in FY18 for continued MAMBA3D V&V.

SECTION 3

OVERVIEW AND V&V STATUS OF VERA-CS CODE COUPLING

This section will provide an overview and discuss the V&V status of the coupling in VERA-CS. In general the in-line coupling of MPACT and CTF is well established, however the more generalized coupling code TIAMAT continues to be developed in FY17.

C.1 MPACT-CTF Coupling

The original coupling of MPACT and CTF reported in CASL-U-2013-0230-000 [Kochunas, 2013] and CASL-U-2014-0051-000 [Kochunas, 2014] utilized the LIME Multiphysics Environment and DTK to couple the two code packages.

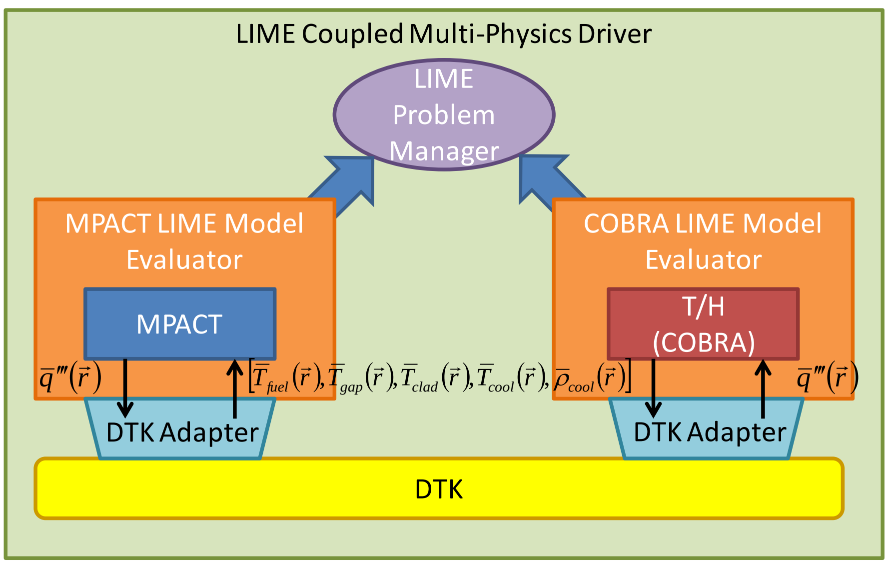

Figure 3.1 Original MPACT+CTF Coupling Based on LIME Driver [Kochunas, 2013]

While this original coupling was effective for the analysis of a single hot full power core condition, the software design was not conducive to modification for the iteration scheme required to perform reactor depletion. The decision was then made to implement a direct coupling of MPACT and Cobra-TF (CTF). This decision was motivated primarily by the simplification of the software design leading to lower costs for software maintenance and modification.

In the direct MPACT/CTF coupling [Kochunas, 2017], MPACT receives temperatures and densities computed by CTF, computes the power densities, and then passes them to CTF. Within MPACT and CTF, the spatial discretizations are different as a result of their numerical methods, and the mapping of information (e.g., power, temperature, density) between the mesh in each code was designed to preserve the respective temperature/fluid and nuclide/neutron fields. The mesh for the coupling or solution transfer between CTF and MPACT is based on the *x-y* Cartesian grid formed by the pin cell geometry and the axial mesh defined by the user. An example of the pin cell geometry in *x-y* is illustrated in Fig. 3.2. For each mesh (e.g., pin cell) in this grid, the solution variables in each code are integrated over the axial segment and transferred. Thus quantities like power and mass are conserved between the codes for each axial pin cell region when transferring solution data between the codes.

The pin cell averaged coupling for a 2 × 2 array of pin cells is illustrated in Fig. 3.2 which shows on the left an illustration of the spatial mesh used in MPACT for the 2-D MOC calculation. Each region bounded by black lines represents a discrete spatial cell in which a unique power density may be calculated. On the right of Fig. 3.2 is the subchannel mesh; again the black lines indicate the boundaries of discrete spatial cells within which the solution for the temperature or density has a discrete value. Fig. 3.2 does not show the mesh used for the conduction solve in CTF which is performed over the dark gray regions in the figure representing the solid regions in the subchannel mesh. In Fig. 3.2, the symbol T refers to the temperature, ρ is the density, and q''' is the volumetric heat generation rate. The over-bar notation indicates that the quantity has been averaged over a material region within the pin cell, and the subscript indicates the material region.

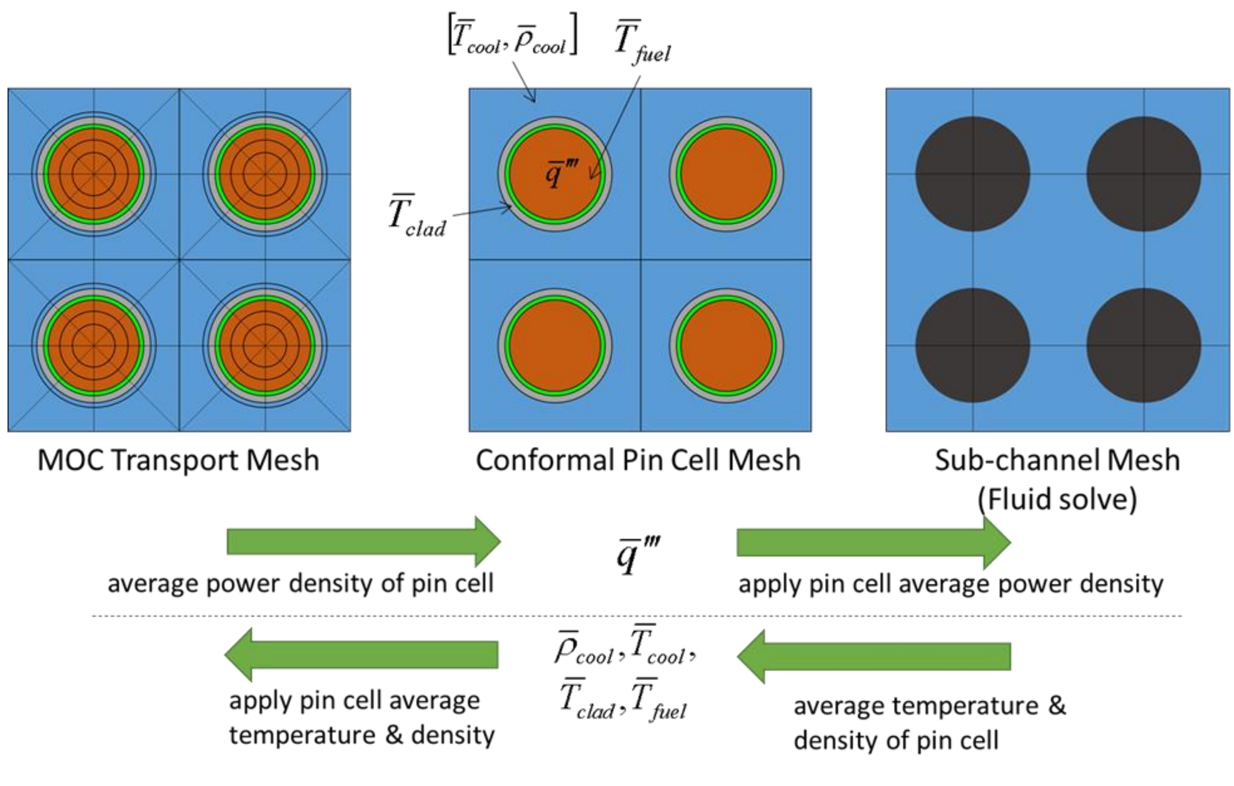

Fig. 3.2 Illustration of Direct Coupling used with MPACT and CTF in VERA-CS.

In general, the direct coupling of MPACT and CTF based on memory to memory transfer appears to have been effective for PWR core follow analysis. However, moving forward a detailed verification is recommended to address some specific issues. Additional work is merited to verify the coupling for a more general range of applications to include non-square cells, complex composition mixtures such as coolant+grid mixtures, and regions with major variation (e.g. above/below the region CTF models). Also, verification work should be performed to quantify errors introduced by mapping CTF-channel solution to pin-based density-temperatures and analysis should be performed to assess whether this is valid for BWRs or transients with large void variations? Finally, the plan should include an consideration for the impact that thermal expansion on the verification of the direct MPACT-CTF coupling.

C.2 TIAMAT

The TIAMAT code was is being developed for coupling the BISON code directly to MPACT and thereby provides an explicit coupling for fuel performance analysis and another option for providing fuel temperature data for VERA-CS core follow calculations. The TIAMAT coupling utilizes DTK to transfer data between VERA-CS codes and the PIKE module to solve the math. The original TIAMAT development created a new PIKE-based ModelEvaluator that had a direct connection to the neutronics drivers and by-passed the original CASL LIME ModelEvaluator. [Pawlowski, 2014].

In 2016 the decision was made that TIAMAT would provide the primary pathway to create a fully-coupled VERA with a fast, robust BISON for full-core analysis [Clarno, 2016]. The Tiamat and TiamatInline drivers would use the TrilinosPike communicators to manage parallel communication between MPACT, CTF, the Bison MultiApp, and each Bison fuel pin. As outlined in [Clarno, 2016] a series of FY17 milestones have been established to implement a fully-coupled Tiamat-based two-way coupling in VERA-CS. If all proceeds as planned, then FY18 will consist of scaling to full core, performance improvements, usability improvements, pre- and post-processing integration, etc., as well as a sequence of activities to continue TIAMAT V&V and achieve a status consistent with the other VERA-CS codes.

The TIAMAT code is under active development in FY17. However, TIAMAT code has a sequence of unit tests which includes both tests for MPACT and CTF to include problems with a 3x3 array of pins in a 3x3 array of assemblies. Significant work will remain for the V&V of TIAMAT and milestones are proposed for Phase II of the VERA-CS V&V plan in FY18.

SECTION 4

VERA-CS V&V

Because of the uneven maturity of both the VERA-CS codes and the code coupling capability, a multi-phase approach is proposed for VERA-CS V&V in which the most mature codes are considered in Phase I and then the other codes are considered in phase II as the codes and the coupling matures. This section will outline a plan for each phase, but is expected to be a "living document" that will be revised as the development of individual codes progresses over the next year. This section will first provide some background on previous work on CASL V&V planning and then propose metrics for the evaluation of VERA-CS for core follow analysis. Finally several V&V activities will be proposed to include a specific format for presentation and evaluation for core follow calculations.

A Background

A comprehensive validation plan was proposed for VERA-CS in 2014 [Godfrey, 2014] and this section will briefly summarize some aspects of that validation plan to include the validation matrix proposed for VERA-CS. The four principal validation components identified in the plan are shown in Figure 4.1 which was reproduced from [Godfrey, 2014].

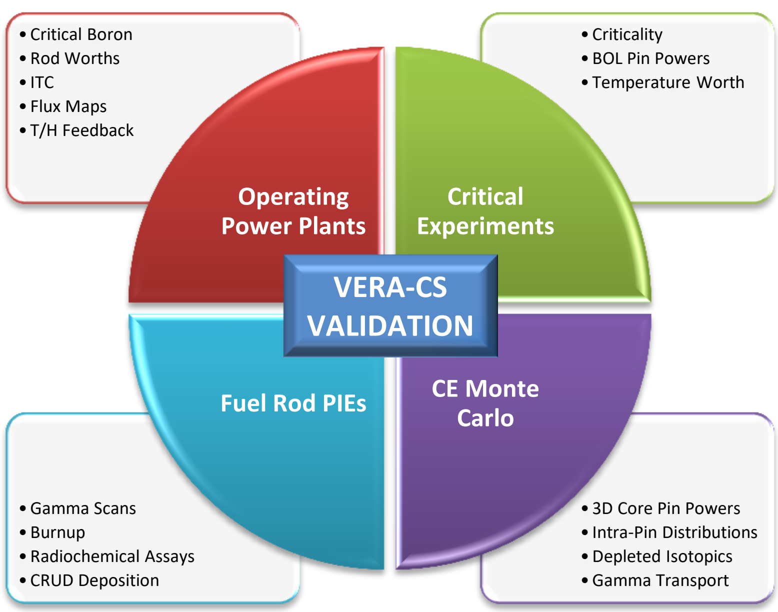

Figure 4.1 Components of VERA-CS Validation [Godfrey, 2014].

As noted in the report, each source of data is complementary and includes:

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 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.
3) Calculated quantities on fine scales from *continuous energy (CE) Monte Carlo methods*. This includes 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 which there is currently no known measurements to benchmark against.
4) Measured data from *operating 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.

As discussed in section 2, the first three of these areas are considered "single physics" neutronics and have been included in the MPACT Validation plan. During the past few years, significant progress has also been made in the area of operating plant data, and this is the area which is now considered the purview of the multi-physics VERA-CS validation for PWR core follow. Measurement data from operating nuclear power plants provides the broadest range of data for multi-physics code validation and several CASL stakeholders who own and/or operate PWR power plants have made plant data available for validation of VERA-CS. The following section will first summarize the core follow calculations completed in the past few years, and then review the specific plant calculations being performed in FY17 within AMA. The purpose of reviewing the core follow calculations previously performed is to provide context for the acceptance metrics that will be proposed in section C.

B. Current Status / Planned FY17 Core Follow Validation

The two major plant data calculations performed with VERA-CS in FY15-16 were the Watts Bar I Nuclear Plant Cycles 1-12 and the BEAVRS Cycles 1-2. This section will briefly summarize those results since they provide a basis for the metrics proposed in section C. It should be noted that the results shown here were based on the 47-group library and are being updated using the new 51-group library.

B.1 Watts Bar I Nuclear Plant

The Watts Bar Nuclear Plant is owned and operated by the Tennessee Valley Authority (TVA), a CASL core partner. Watts Bar was selected as CASL's "Physical Reactor" for initial benchmarking activities. Unit 1 was the last commercial nuclear unit to come online in the 20th century, and Unit 2 has recently come on line and is currently being analyzed with VERA-CS. Only some of the results of Unit 1 will be shown to demonstrate the types of validation data that is provided from core follow calculations.

Watts Bar Nuclear Unit 1 (WBN1) is a traditional Westinghouse 4-loop PWR is currently licensed to 3459 MWth power and is currently operating Cycle 13. WBN1 has 193 fuel assemblies of the 17x17 type, has used Pyrex, IFBA, and WABA burnable poisons, and has 57 AIC/B4C hybrid rod cluster control assemblies (RCCAs). It has a moveable in-core detector system for power distribution measurement. A schematic of the core loading is shown in Figure 4.2 and the cycle 1 operation history used to deplete cycle is shown in Table 4.1.

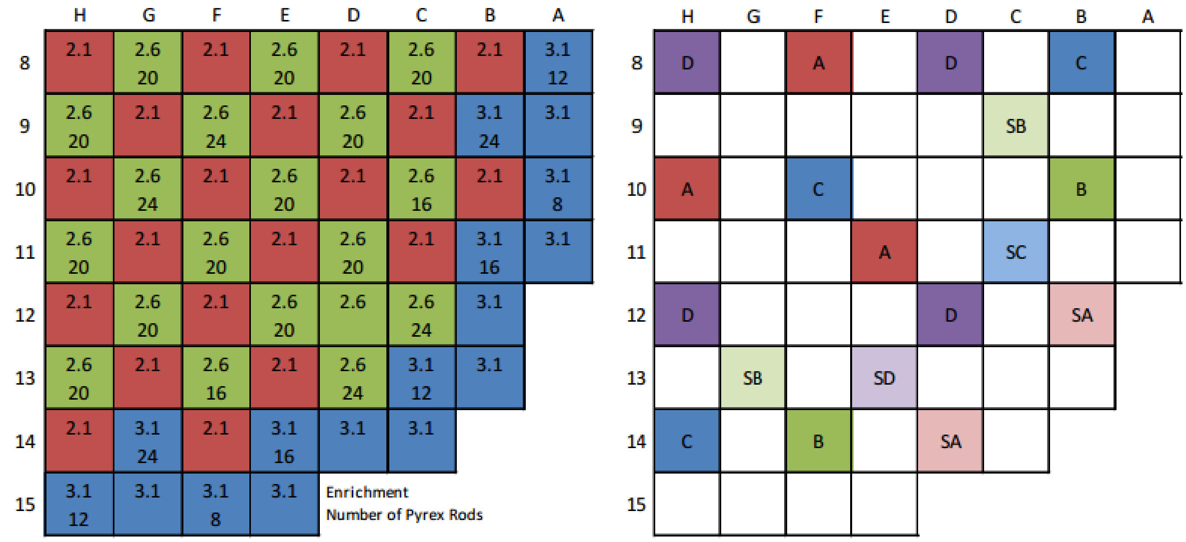

Figure 4.2 VERA Problem 5 Assembly, Poison, and Control Rod Layout in Quarter Symmetry.

Table 4.1 Cycle 1 Simulated Operating History [Godfrey, 2014]

Table P9-2: Problem 9 Cycle Depletion Specification

Case	EFPD	Cycle Exposure (GWd/MT)	Power (%)	Inlet Temp. (F)	Bank D Position (steps)
1	0.0	0.000	0.0	557.0	186
2*	9.0	0.346	65.7	557.6	192
3*	32.0	1.229	99.7	558.1	219
4	50.0	1.920	98.0	558.2	218
5	64.0	2.458	100.0	558.6	219
6	78.0	2.996	99.7	558.7	215
7	92.7	3.561	99.7	558.6	217
8	105.8	4.064	99.8	558.8	220
9	120.9	4.644	99.8	558.4	220
10	133.8	5.139	99.5	557.9	219
11	148.4	5.700	98.0	558.0	214
12	163.3	6.272	95.1	557.9	216
13	182.2	6.998	94.8	557.9	214
14	194.3	7.463	99.8	557.8	220
15	207.7	7.978	93.9	557.5	218
16	221.1	8.492	100.1	558.0	222
17	238.0	9.141	99.7	557.7	220
18	250.0	9.602	100.2	557.6	222
19	269.3	10.344	95.6	557.9	211
20	282.3	10.843	96.4	558.1	215
21	294.6	11.315	93.4	557.4	211
22	312.1	11.987	99.7	557.5	217
23	326.8	12.552	98.0	557.6	215
24	347.8	13.359	99.4	557.7	220
25	373.2	14.334	99.9	557.8	219
26	392.3	15.068	86.9	556.7	202
27	398.6	15.310	99.6	558.0	220
28*	410.7	15.775	89.9	557.1	224
29*	423.6	16.270	78.8	556.3	228
30*	441.0	16.939	64.5	554.9	230
Cycle Average			94.0	557.8	216.4

*The statepoint values are endpoints, not averages. If needed, the average values can be calculated or obtained from the author.

In June, 2015 work was completed by A. Godfrey to deplete Cycles 1-12 of Watts Bar Unit I [Godfrey, 2015]. This provided the first successful demonstration of VERA-CS ability to model the entire operating history of the Watts Bar Nuclear Unit I Plant which is currently in its 20th year and 13th fuel cycle. A rigorous benchmark was also performed using a significant amount of operating data provided by TVA, using the same rigorous analyses that are used for the validation and licensing of industrial methods. These data include criticality measurements, physics testing results, critical soluble boron concentrations, and measured in-core neutron flux distributions. This section will summarize some of the results from that report [Godfrey, 2015].

Each of the MPACT/VERA-CS calculations was performed after reloading the core and shuffling the fuel from the previous cycle (except Cycle 1). The previous fuel compositions were decayed by ORIGEN over the time span of the refueling outage, also resulting in the complete decay of 135Xe and buildup of 149Sm. The calculations were performed without T/H feedback, in quarter-core symmetry, and the MOC ray spacing was significantly decreased by 10x to improve the accuracy of neutron transport near the very thin IFBA coating. The differences between the measured critical boron concentrations and the calculated values with VERA-CS are shown in Figure 4.3.

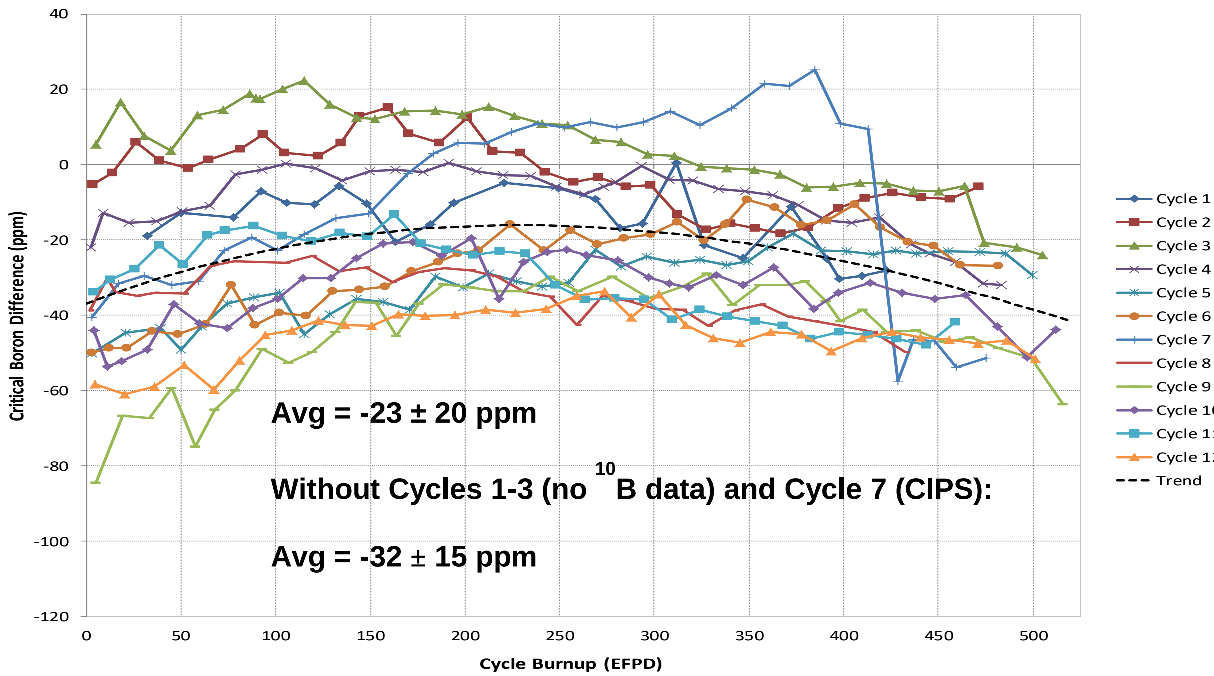

Figure 4.3 Difference Between Critical Boron and the MPACT/VERA-CS Prediction.

As indicated, the average BOC critical boron difference is about 23 ppm. As noted in [Godfrey, 2015] the prediction of Cycle 7 is particularly poor which is likely due to the occurrence of CRUD Induced Power Shift (CIPS). As also noted in [Godfrey, 2015] some other factors have been identified which account for the differences in Cycles 6-12, such as the presence of Tritium production "TPBARs" which due to the classified nature of these components their absorber loading is approximate. Results were also presented in [Godfrey, 2015] for the predicted versus measured control bank reactivity worths (CBW) at the beginning of each fuel cycle as part of the startup test procedures. The measured values from WBN1 have been provided by TVA as part of the zero power physics test results transmittals. The individual rod worths which are most useful for code validation are provided in the report. The total rod worth errors for all of the WBN1 cycles are shown here in Figure 4.4 to demonstrate what agreement could be obtained if MPACT/VERA-CS were used for startup testing predictions with the same methodologies as used for currently NRC-licensed industrial methods.

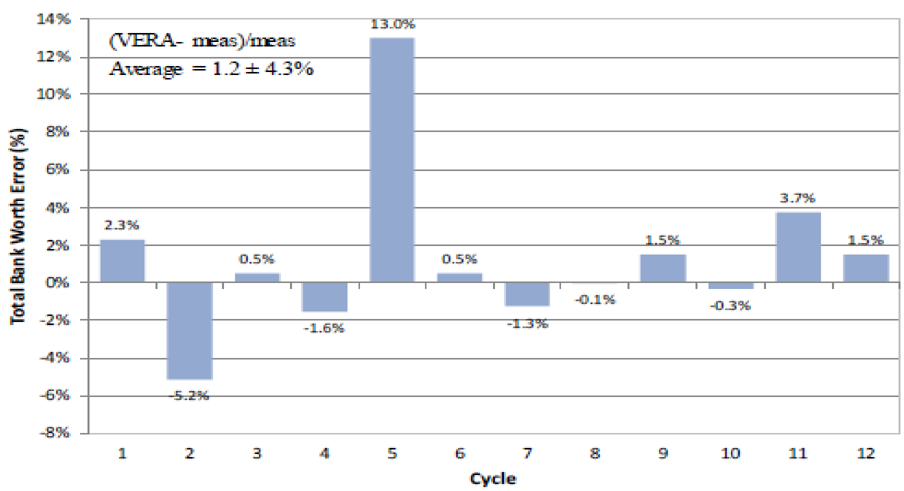

Figure 4.4 BOC HZP Total Control Bank Worth Errors.

Detailed flux map comparisons were also performed over all twelve cycles of Depletion. A total of 183 flux maps were selected for comparison to calculations from MPACT/VERA-CS and reported in [Godfrey, 2015]. A sample flux map comparison is shown in Figure 4.5 below. The image is a depiction of the SE quadrant of the reactor core, with locations containing at least one operable symmetric instrument containing data. The data is a simplified axial plot of the measured (red) and calculated (blue) signals at 61 axial locations. In the upper right of each instrumented location is the value of the 3D RMS difference of the 61 locations in that string. The lower right corner contains the difference in radial powers for that instrument (times 100). Values above 5% are highlighted in red. At the bottom right is another simplified axial plot of the 1D average axial shape of the operable instruments, with corresponding RMS. The box to the right provides the cycle, exposure, power level, and radial (2D) and total (3D) RMS values for the entire distributions. The difference in measured and calculated axial offset is also provided.

A summary of the flux map comparisons taken from [Godfrey, 2015] in Table 4.2 shows that VERA-CS can calculate the measured power distributions reasonably well, especially given the fuel temperature limitations, larger reactivity differences, and known quadrant power tilts. The radial power distribution RMS is only 1.8%, with errors tending to be ~50% higher in the first 6-8 GWd/MTU of the cycles. For the latter half of the cycles, the 2D RMS approaches 1.25% for all cycles. A plot of the 3D Total RMS during the cycle exposure is shown in Figure 4.6.

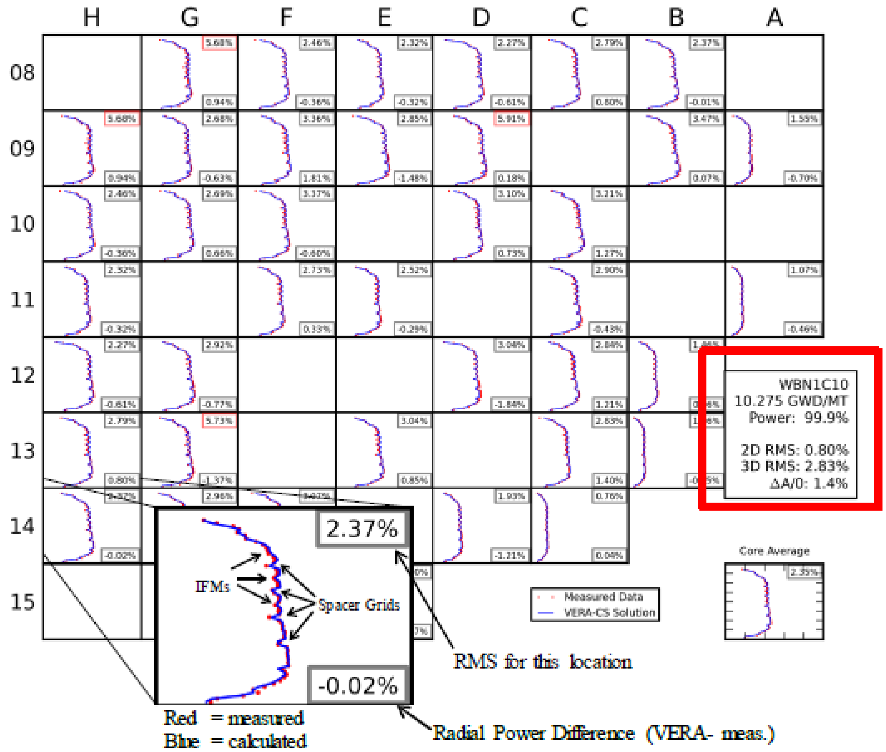

Figure 4.5 Sample HFP Flux Map – Middle of Cycle 10.

Table 4.2 Summary of Flux Map Comparisons for Cycles 1-12 of Watts Bar Unit I.

Cycle	Count	ΔAO	1D RMS	2D RMS	3D RMS	2D Max	Det Max	3D Max
1	13	-1.17	2.55	1.10	3.29	3.37	7.25	27.28
2	13	0.08	1.11	1.60	2.70	3.99	7.29	31.79
3	19	0.45	1.87	1.67	2.92	5.95	8.34	42.03
4	19	0.52	2.14	1.77	3.23	4.82	8.37	40.74
5	19	1.04	2.33	2.05	3.64	8.02	9.61	38.74
6	18	1.38	2.60	1.92	3.77	6.15	9.60	41.77
7	18	1.79	5.17	1.74	6.73	5.94	15.70	33.31
8	15	-0.35	3.03	1.77	4.00	7.67	10.27	43.63
9	19	1.32	2.41	2.35	3.94	10.03	11.88	41.72
10	16	-0.43	2.79	1.56	3.64	7.55	9.62	38.15
11	6	0.25	1.52	1.88	2.77	7.36	7.85	21.51
12	8	-0.43	2.23	2.47	3.72	11.54	12.32	37.15
Total	183	0.50	2.75	1.85	3.93	11.54	15.70	43.63
St. Dev.		0.85	0.98	0.32	1.05			

**note that the axial shapes for each detector in Cycles 4-12 are approximate*

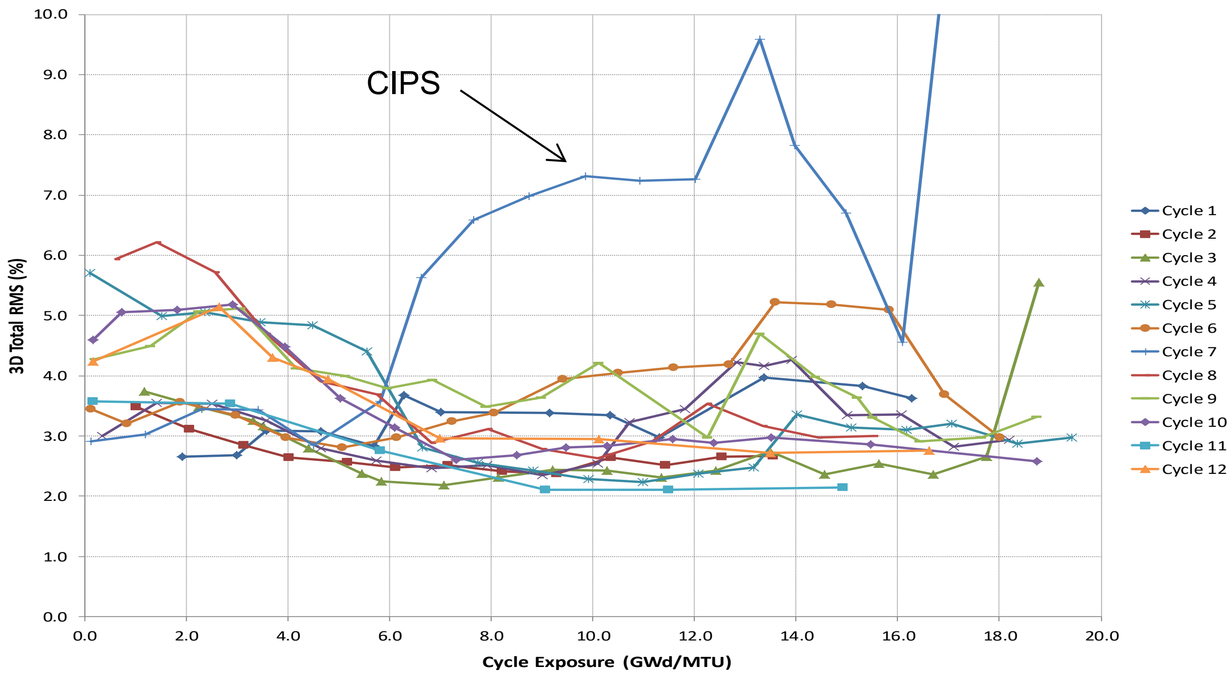

Figure 4.6 Summary of 3D Total RMS for Cycles 1-12 of Watts Bar Unit I.

An overall summary of the MPACT/VERA-CS Benchmarking results for Watts Bar Cycles 1-12 is shown in Table 4.3. Overall, these results demonstrate successful application of VERA-CS for the depletion and benchmarking of twelve fuel cycles of a commercial PWR which confirms the ability of VERA-CS to represent realistic and detailed reactor core models and perform simulations in a reasonable turn-around time and provide guidance for the performance metrics that can be expected in future VERA-CS core follow analysis.

Table 4.3 Summary of MPACT/VERA-CS Benchmarking Results for Watts Bar Cycles 1-12.

Measurement	Mean ± 1 sigma†	Runtime per Cycle‡
BOC HZP Critical Boron	-9 ± 24 ppm	1.75 hours
BOC HZP Bank Worth	1.2 ± 4.3%	3.33 hours
BOC HZP ITC	-0.8 ± 0.7 pcm/°F	0.75 hours
HFP Boron Letdown	-24 ± 19 ppm	21.9 hours
HFP Flux Maps – Radial Total	1.8 ± 0.3% RMS 3.5 ± 0.4% RMS	--

† Suspect measurements or known anomalies are excluded from this summary
‡ Typical number of compute cores is 4307 cores

B.2 BEAVRS

The Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS) is a publicly available reactor specification provided by the Massachusetts Institute of Technology (MIT) Computational Reactor Physics Group [Horelik, 2013]. The three region core loading and fuel enrichments are also similar to WBN1 however there are some differences in the lattice pattern and discrete burnable absorber types. The benchmark contains two cycles of detailed geometry and measurements from an unnamed utility's PWR, however, the BEAVRS reactor is a traditional

Westinghouse 4-loop PWR very similar to WBN1. The measured data provided for BEAVRS includes Cycles 1 and 2 ZPPT results, power escalation and HFP measured flux maps, and HFP critical boron concentration measurements for both cycles. The power history for each cycle is provided and the power history for cycle 1 is shown in Figure 4.7. Cycle 1 of BEAVRS was performed with VERA-CS previously [Collins, 2015b] and has recently been extended to cycle 2 with the updated CASL library. The following will provide a brief summary of the results from CASL-U-2015-0076-000 on the cycle 1 depletion.

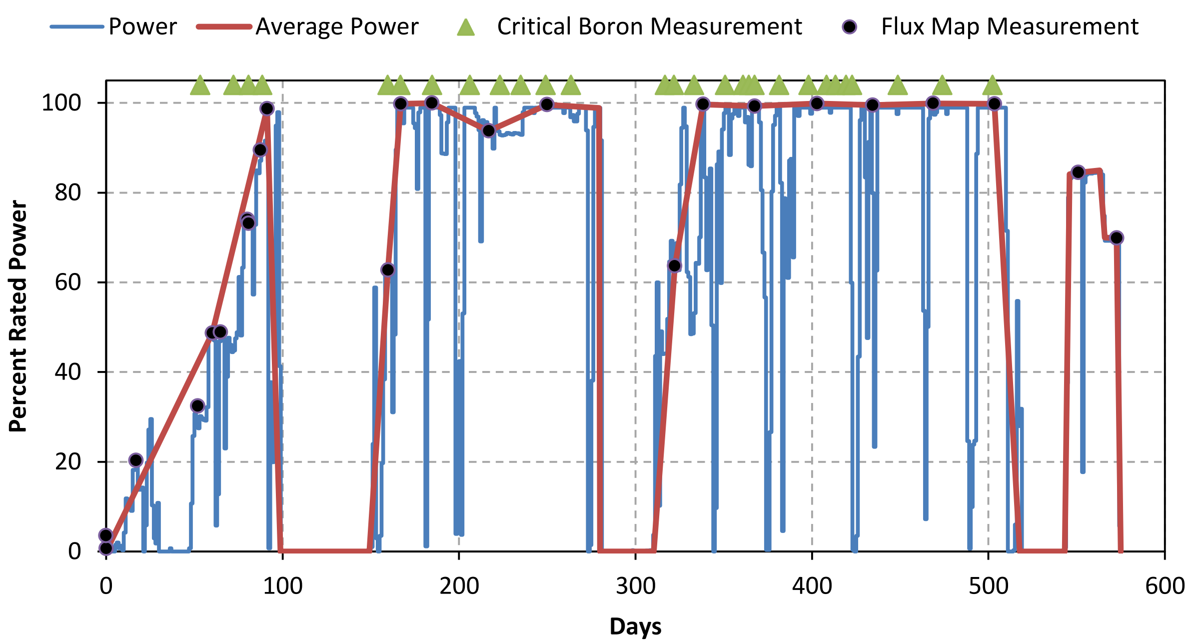

Figure 4.7 Power History used in MPACT BEAVRS Model [Collins, 2016].

A summary of some of the key results is shown in Table 4.4, and the Pin power distribution calculated by VERA-CS at three statepoints in the cycle is shown in Figure 3.8. A comparison of the Flux Measurements predicted by MPACT with the measured data is shown in Figure 4.9 for a flux map at the Middle of Cycle. The detailed data for all 16 statepoints is provided in [Collins, 2015]. In general the results for cycle 1 are in good agreement with the plant data and provide an important addition to the VERA-CS validation base. Cycle 2 of BEAVRS has been completed and similar results were observed which will be added to the future validation base of VERA-CS.

Table 4.4 Summary of Key Results for VERA-CS for BEAVRS Cycle 1.

Exposure		Power	Boron			Flux Map Comparisons		
GWD/MT	EFPD	[%]	Meas.	Calc.	Diff.	Radial RMS	3D RMS	Delta A/O
0	0	0	975	958	17	2.44%	5.14%	-2.23%
0.268	6.4	48.69	703	696	7	--	--	--
1.023	24.5	98.67	626	601	25	1.71%	4.54%	-0.46%
1.184	28.4	0	633	--	--	--	--	--

1.187	28.5	0	633	--	--	--	--	--
1.296	31.1	62.78	638	652	--	3.49%	5.46%	-2.20%
1.507	36.1	99.78	610	601	9	0.99%	3.14%	-0.52%
2.163	51.9	99.98	623	582	40	1.35%	3.02%	-0.22%
3.297	79.1	93.78	580	563	17	0.85%	3.11%	1.22%
4.614	110.6	99.6	532	503	29	0.91%	3.79%	-1.63%
5.713	137	98.9	479	452	27	--	--	--
5.734	137.5	0	478	--	--	--	--	--
5.779	138.6	0	476	--	--	--	--	--
6.013	144.2	63.65	461	--	--	1.08%	4.46%	-2.65%
6.491	155.7	99.7	444	415	30	1.28%	4.36%	1.55%
7.508	180.1	99.3	384	353	31	0.90%	3.47%	0.95%
8.701	208.7	99.86	310	284	26	1.00%	3.55%	0.98%
9.804	235.1	99.51	248	218	30	--	--	--
11.085	265.8	99.91	162	135	27	1.21%	4.01%	-0.75%
12.342	296	99.79	70	50	20	1.27%	3.73%	-1.01%
12.677	304	0	52	--	--	--	--	--
12.694	304.4	0	51	--	--	--	--	--
12.74	305.5	84.1	49	51	-2	--	--	--
12.916	309.7	84.48	39	53	-14	1.45%	4.34%	1.79%
13.31	319.2	84.94	18	17	1	--	--	--
13.411	321.6	70	13	40	-27	--	--	--
13.604	326.2	69.86	2	28	-26	1.48%	4.59%	1.00%
13.645	327.2	0	0	--	--	--	--	--

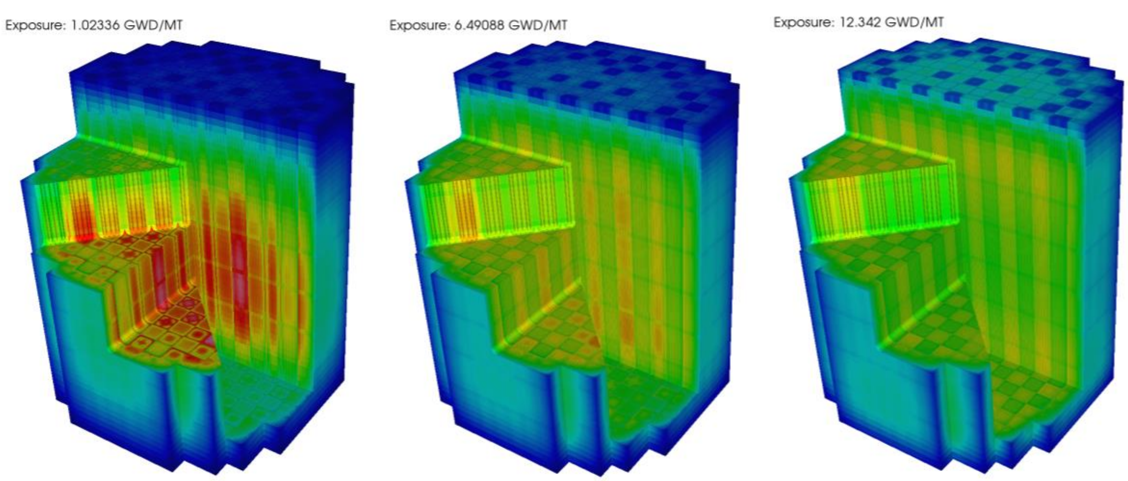

Figure 4.8 Pin Power Distribution During Cycle 1 of BEAVRS [Collins, 2015].

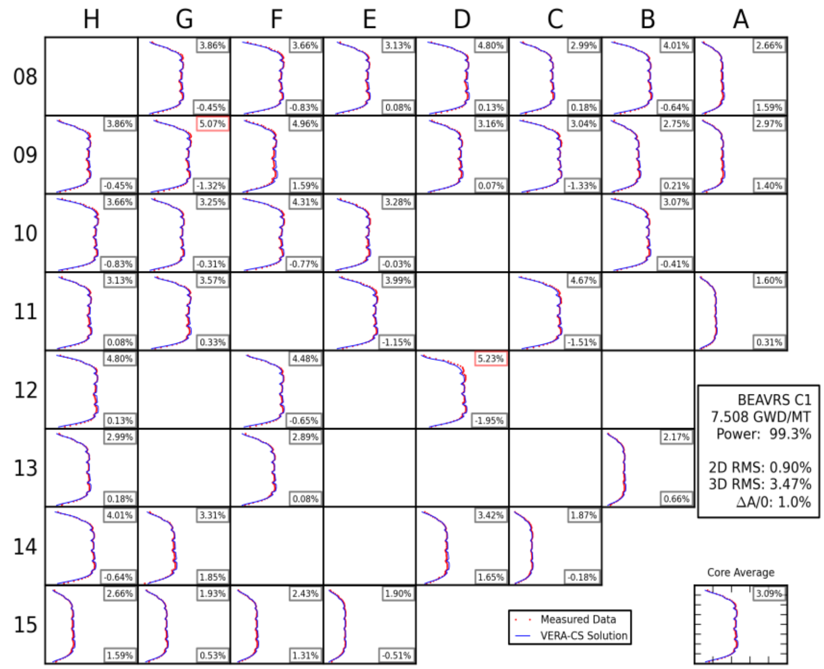

Figure 4.9 Comparison of Flux Maps to MPACT Results: MOC Cycle 1 of BEAVRS.

B.3 Planned FY17 Core Follow Validation

The Watts Bar and BEAVRS operating plant data has provided useful guidance for the initial validation of VERA-CS and for establishing the metrics for future validation calculations. As shown in the Table 4.5, five CASL milestones have been created within AMA for FY17 which will considerably expand the VERA-CS validation base of PWR core follow data.

Table 4.5 AMA FY17 Milestones for VERA-CS Core Follow Analysis

Ticket	Milestone	Lead	Plant	End Date
1924	L3:AMA.RX.P15.03	Cole Gentry	Catawba Unit 2	2017-08-01
1895	L2:AMA.P15.02	Brenden Mervin	TMI Cycles 1-10	2017-09-29
1923	L3:AMA.RX.P15.04	Ben Collins	Catawba Unit 1	2017-09-29
1925	L3:AMA.RX.P15.05	Scott Palmtag	McGuire Units 1 / 2	2017-09-29
1970	L3:AMA.RX.P15.07	Andrew Godfrey	Palo Verde	2017-09-29

Each of these plants complements the previous validation base by providing unique assembly designs and a diverse array of core loading patterns and plant operating conditions. With the expansion of the data available for validation, it becomes important to provide some consistency in the formatting and the type of data that will be used to evaluate the simulator performance, as well as to propose specific metrics that can be used to assess the adequacy of the calculation for the validation data base.

During the past month, initial work has been performed on a milestone to automate and to provide a uniform format for the results of the plant calculations. An initial plan is described in Appendix A of this report which would process the VERA-CS HDF5 output file and simplify the creation of the most relevant output for analysis and for preparation of tables and figures for a LATEX file format for the VERA-CS V&V manual. An important feature of the script would be to automatically flag and output results which fall outside the acceptance metrics which are proposed in the next section. The design of the scripts would also assist the analyst by automating as much of the calculation process as feasible in order to minimize the effort required to rerun a sequence of cycle calculations because of changes in a cross section library, modeling inputs, or any other model changes.

C. Metrics for Evaluation / Validation

The initial VERA-CS validation efforts with WB Unit 1 and BEAVRS provides sufficient basis to propose metrics that can be used to assess the adequacy of the PWR core follow calculations for addition to the VERA-CS validation base. For every new VERA-CS reactor analyzed, the following metrics are suggested as an initial proposal [Palmtag, 2016].

- At startup:
  - HZP boron: ± 20 $\boldsymbol{ppm}$
  - Rodworth: ± 7 %
  - ITC: ±1 pcm/F
- At every statepoint:
  - HFP boron: ±35$\boldsymbol{ppm}$
  - AO: ±3%
  - Pin Power Distribution and Peaking factors: ± 2 %

For the VERA-CS V&V document, all data would be included for which operational data is available. However, specific attention / analysis would be expected for any plants/cycles/measurements that fall outside of these metrics. A red-flag condition would be automatically generated on the results outside this metric and require re-evaluation and review before that data is admitted to the validation base.

D. VERA-CS V&V Plan

The following is a summary of the activities proposed in support of the VERA-CS V&V plan:

Phase I (FY17)

Single-Physics Codes:

1. **MPACT**:

A gap in the MPACT V&V has been the testing of the ORIGEN API. An explicit plan should be developed and implemented to improve the overall testing of the ORIGEN API:

(https://vminfo.casl.gov/trac/casl_phi_kanban/ticket/4580) .

The MPACT V&V should be modified to include only single physics results (e.g. critical experiments, fresh core start up tests, etc) and all MPACT-CTF core follow data should be moved to the VERA-CS manual. All results in the MPACT manual should be updated with the new 51-group library using the new automation scripts.

2. **CTF:** In addition to any planned validation activities, the CTF V&V manual should be modified with a specific section summarizing the ongoing code verification activities:

- Source Code Verification
  - Unit Testing/Code Coverage
  - Regression Testing/Test Matrix
- Solution Verification
  - Mesh Convergence Analysis
  - Manufactured Solutions (or other appropriate methods)

3. **MULTIGROUP XSEC LIBRARY**: Several of the sections for a formal XSEC Verification and Validation document appear to exist but they should be organized into a formal CASL MULTIGROUP XSEC LIBRARY manual. The proposed outline for the manual was summarized in section 2 of this report. This should be a high priority for PoR15.

4. **BISON FUEL TEMPERATURE TABLES**: As with the mutigroup library, several of the sections for a formal Fuel Temperature Tables V&V document appear to exist but they should be organized into a formal manual. The focus of this milestone would be code verification with documentation of existing tests and a modest expansion of unit testing and regression testing to include uncertainty analysis of various user input options. The validation for this document would simply point to the BISON V&V manual.

VERA-CS

1. While the direct coupling of MPACT and CTF appears to have been effective for PWR applications, additional work is merited to verify the coupling for a more general range of applications to include non-square cells, complex composition mixtures such as coolant+grid

mixtures, and regions with major variation (e.g. above/below the region CTF models). Also, verification work should be performed to quantify errors introduced by mapping CTF-channel solution to pin-based density-temperatures and analysis should be performed to assess whether this is valid for BWRs or transients with large void variations? Finally, the plan should include an consideration for the impact that thermal expansion on the verification of the direct MPACT-CTF coupling.

2. After the Automation Scripts have completed and tested using BEAVRS, the Watts Bar cases should be updated with the new cross section library to be included in the first draft of the new VERA-CS manual. This should be a high priority for completion by the end of PoR15.

3. Also, within the constraints imposed by the proprietary nature of plant data, as many as possible of the FY17 AMA Plant Core Follow cases should also be included in the VERA-CS manual at the end of PoR15.

Phase II (FY18)

Single Physics Codes

1. **TIAMAT:** The verification of TIAMAT for limited applications has already been established, however, several new capabilities to include the fully coupled BISON/VERA-CS capability will be completed and demonstrated in FY17. Verification activities for the fully coupled capability is being performed as part of the code development, however, in FY18 a specific milestone should be established to formally document all TIAMAT V&V.

2. MAMBA3D: A significant refactoring is being performed on MAMBA3D in FY17 and similar to TIAMAT, the developers are enforcing source code verification with extensive unit and regression tests during the code development. However, because extensive CASL results have been previously published with the original MAMBA3D code, the developers should also document any changes in the methods and then demonstrate the functionality of MAMBA3D is preserved by performing a series of cases which demonstrate consistency of the solution between the original and refactored MAMBA3D. This work should be performed in PoR15, and then a milestone should be established for FY18 to perform all the validation cases with the refactored MAMBA3D and to prepare a formal MAMBA3D Verification and Validation document.

VERA-CS

1. After the fully coupled, full core capability has been demonstrated with BISON 1.5D and VERA-CS using TIAMAT, all the cases in the VERA-CS validation based should be performed, beginning with the “legacy” cases of Watts Bar and BEAVRS.

2. After the testing is completed on the refactored MAMBA3D and is integrated into VERA-CS, the Watts Bar Unit I core follow cases should be performed and added to the VERA-CS V&V manual.

Phase III (FY19)

The focus of VERA-CS V&V has been on core follow for the PWR. If activities are renewed on BWR capability in VERA-CS, then it will be important to create explicit milestones in FY19 to perform BWR V&V. In preparation of this, a L3 milestone for the second PoR in FY18 would be helpful to assess the status and develop a plan, similar to what was done in this document for VERA-CS V&V for PWR Core Follow.

Section 5

SUMMARY AND CONTINUING WORK

This report summarized the current status of VERA-CS Verification and Validation for PWR Core Follow operation and proposed a multi-phase plan for continuing VERA-CS V&V. The proposed plan recognizes the hierarchical nature of a multi-physics code system such as VERA-CS and the importance of first achieving an acceptable level of V&V on each of the single physics codes before focusing on the V&V of coupled physics calculations. The report summarized the V&V of each of the single physics codes systems currently used for core follow analysis (ie MPACT, CTF, Multigroup Cross Section Generation, and BISON / Fuel Temperature Tables) and proposed specific actions in **Phase I** to achieve a uniformly acceptable level of V&V. The report also recognizes the ongoing development of other codes important for PWR Core Follow (e.g. TIAMAT, MAMBA3D) and proposed **Phase II** (FY18) VERA-CS V&V activities in which those codes will also reach an acceptable level of V&V, and then be used to perform core follow calculations as part of VERA-CS.

The report then summarized the current status of VERA-CS multi-physics V&V for PWR Core Follow and the ongoing PWR Core Follow activities in AMA for FY17. An automated procedure and format was proposed for standardizing the output for core follow calculations, as well as a set of metrics is for the evaluating core follow results and a “red flagging” procedure that requires re-evaluation before being admitted to the VERA-CS validation base. Finally, as potential **Phase III** future work some planning additional considerations would be necessary for extending the VERA-CS V&V to other reactor types such as the BWR.

Section 6

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Appendix A

Automation of VERA-CS V&V

The design of the scripting solution for the automation of the verification and validation tests will be described in this Appendix. The script will serve two general purposes. First it will provide automation to the post processing to assist the analyst and impose some uniformity to the data formatting and display in the Validation manual. The scripts will process the VERA-CS HDF5 output file and simplify the creation of the most relevant output for analysis and for preparation of tables and figures for a LATEX file format for the VERA-CS V&V manual. The second purpose is to also to assist the analyst by automating as much of the calculation process as feasible in order to minimize the effort required to rerun a sequence of cycle calculations because of changes in a cross section library, modeling inputs, or any other model changes.

In order to accomplish the second objective a script will be designed based on the pipelining concept which uses a string of “nodes” or scripts that each have defined inputs and outputs. It is possible for a single node to connect to many nodes or many nodes to connect to a single node. The general structure envisioned for the script is depicted in the Figure below. In the sample pipeline, Node 1 starts with some user inputs, spawns or calls sub-scripts for three node 2 cases, the outputs of which are given to node 3 to condense and sent for processing in node 4 which then terminates with the desired output.

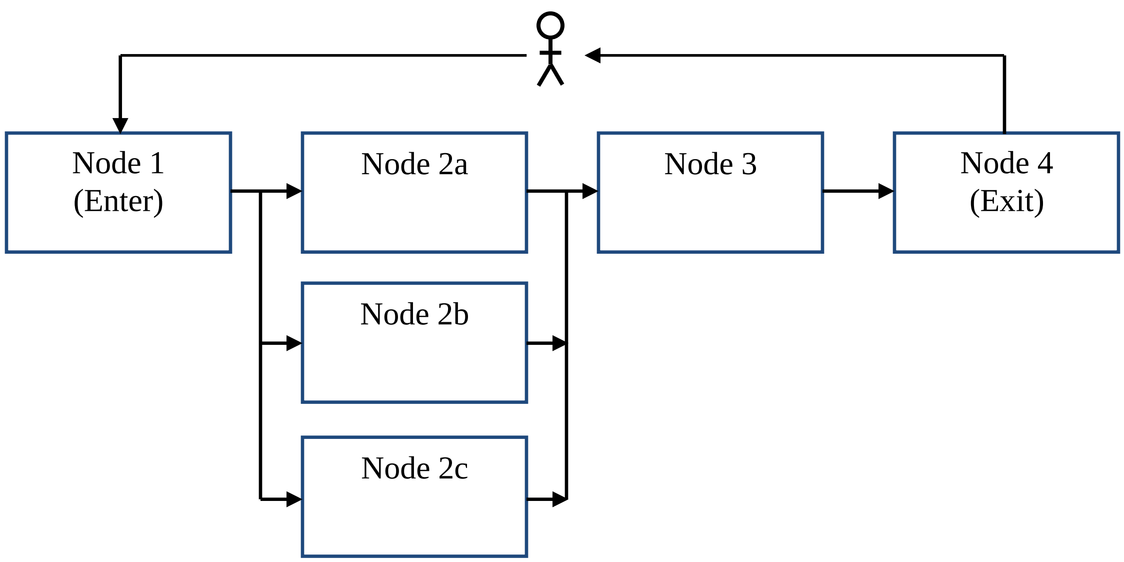

Figure A.1 Sample Pipeline

The BEAVRS core can be used to demonstrate the concept in which there are 5 inputs for cycle 1: beavrs_cy1_criticals.inp, beavrs_cy1_ fm.inp, beavrs_cy1_ITC.inp, beavrs_cy1_rod_worth.inp, and the initial case beavrs_cy1.inp. The input file names themselves can contain useful information to make automation easier to understand and implement. Based on the BEAVRS example, the full input name is beavrs_cy1_criticals.inp, which could be generalized to <core_name>_<cycle_#>_<test>.inp. This naming convention could allow the user to specify the cases to be executed with minimum additional work. The user would specify “beavrs” and any other input to perturb. For example, if the cross section library was changed to a different version the output of Node 1 would be to create all the input files that match the name search parameters with the new cross section library name and call the PBS script to submit and run the cases shown as Node 2. After all the cases have been executed, the output can be collected by Node 3 and sent to Node 4 for processing, creating tables, graph, etc. It is also possible that for certain cases, other nodes will be added, for example, if the case in question is large and is to be run on a cluster, then a node to generate a PBS script would be generated. Or if the case needs to also perturb a CTF input parameter, then xml2ctf will need to be run as a Node as well.

A description of what is expected in each node for input and output will provide information on the function to be performed by the node. Also a short description of the operations that are performed within the node will help keep the process transparent to the stake holder. The figure below describes the specific steps for the BEAVRS case.

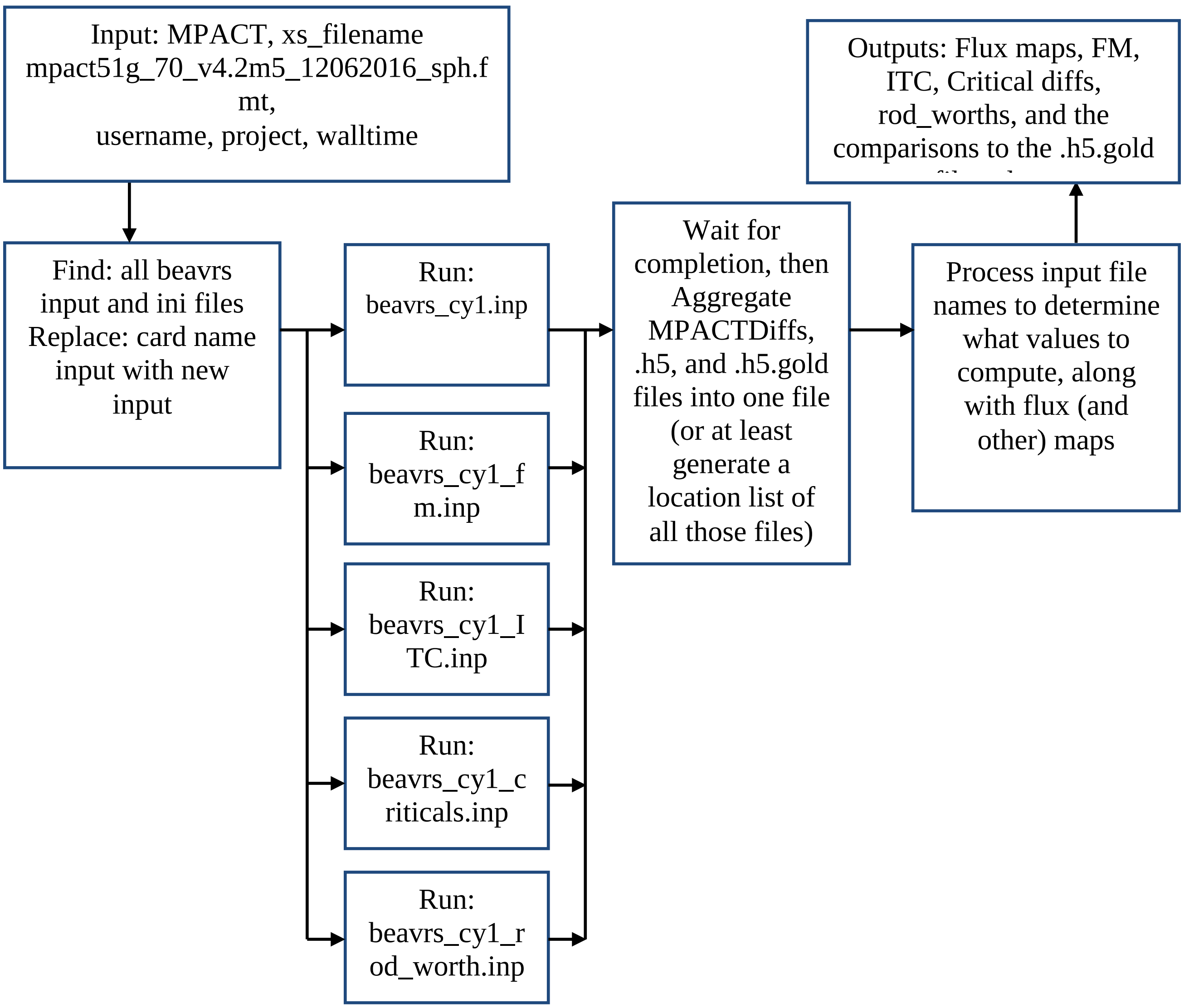

Figure 2 Prototype BEAVRS Cycle 1 Pipeline

The current prototype set of scripts processes input by the user, replaces card names specified by the user, creates xml files using the react2xml.pl script, creates case dependent PBS scripts, submits the

PBS scripts, waits until all jobs are completed, and processes the output. The primary input option is a formatted input file. This text file consists of a formatted list of MPACT input files, whether to use the "--xinit" option in the react2xml.pl script, array of other inputs this input depends on being run first, the project name on which to run the input, the wall time for the input, and whether extra memory is required. The secondary input option is the name of the post processing script. Another useful, but not necessary, input option is the VERA input card overwrite capability. This option will replace whatever is currently in all the input files with the specified value. The "--help" option for the script describes the formatting in greater detail.

The user can provide a post processing script that creates the desired output. The script would only require the MPACT HDF5 output file as an input argument and is then responsible for reading the output data, calculating required values, and displaying the desired output.

For processing the output for BEAVRS, a series of python scripts have been created to process the MPACT HDF5 output file and simplify the creation of the output required for analysis. This script set is able to process multiple state points for power, burnup, boron, control rod bank positions, rod worths, and ITC values. The script is input file specific in which values are processed. For example, only the input file with "ITC" in the filename has the ITC value computed. All of the measured reference data is hardcoded into this script for each case. The outputs include plots of the boron letdown curve, flux maps per depletion point, and tabularized data in latex format. There is also python capability to represent the tabular data graphically. A sample of this data is shown below.

The latex table data is provided for the automation of the manual. If the V&V manual is converted into latex formatting, the manual file can reference other files and import their contents. If the post-processing script creates and updates latex files, the script can be run and the manual "recompiled" to update the figures from the most recent run. This process would allow for the streamlining the process of updating the report, and thereby minimize the effort required.

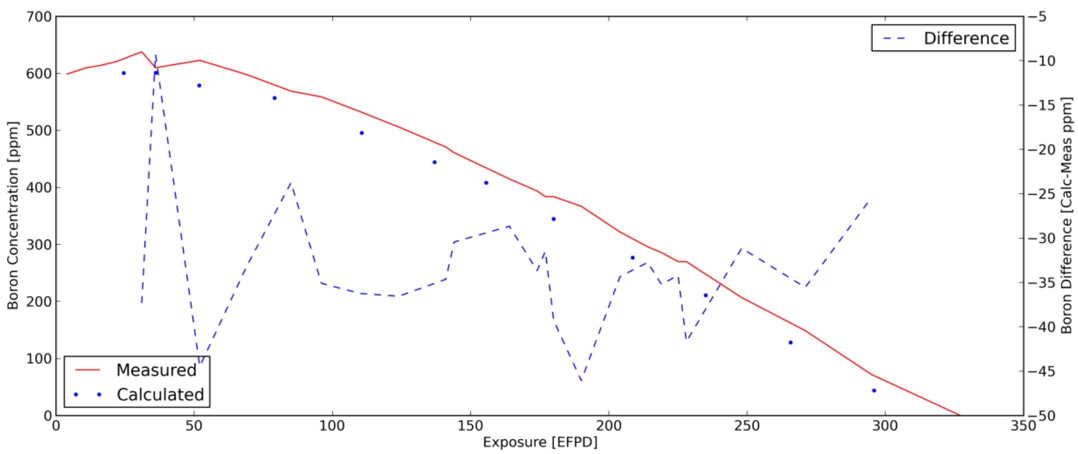

Figure A.3 BEAVRS Cycle 1 Boron Letdown

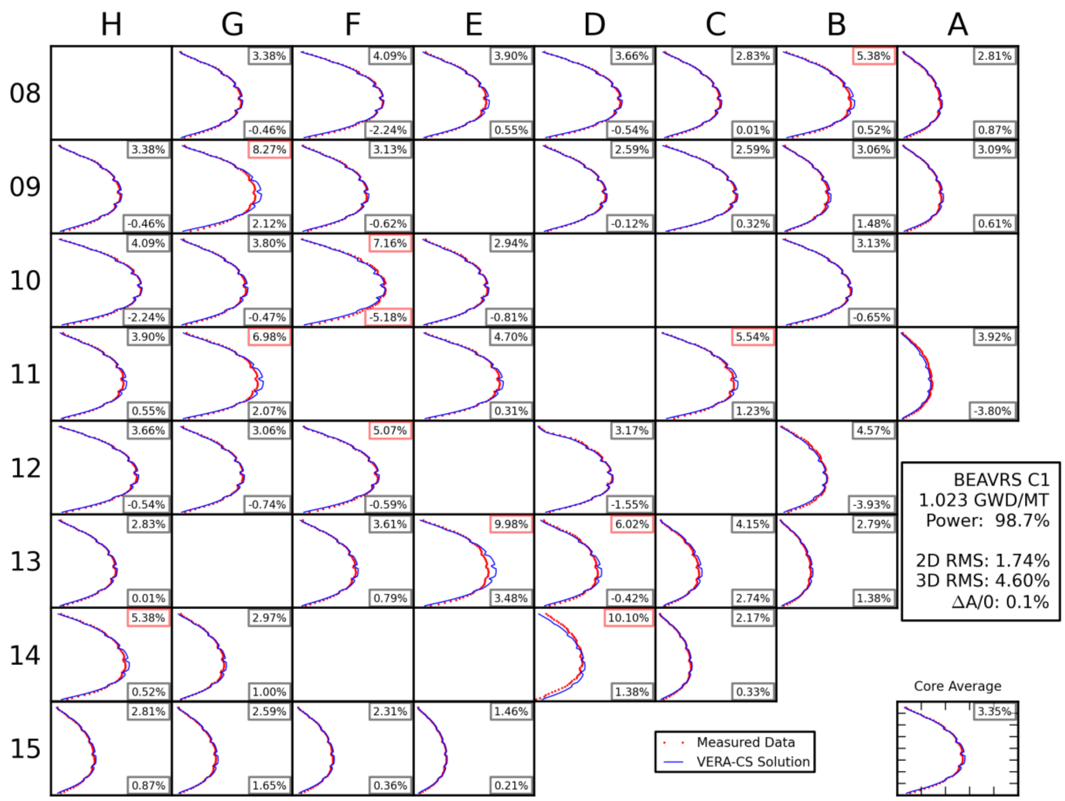

Figure A.4 BEAVRS Cycle 1 1.023 GWD/MT Flux Map

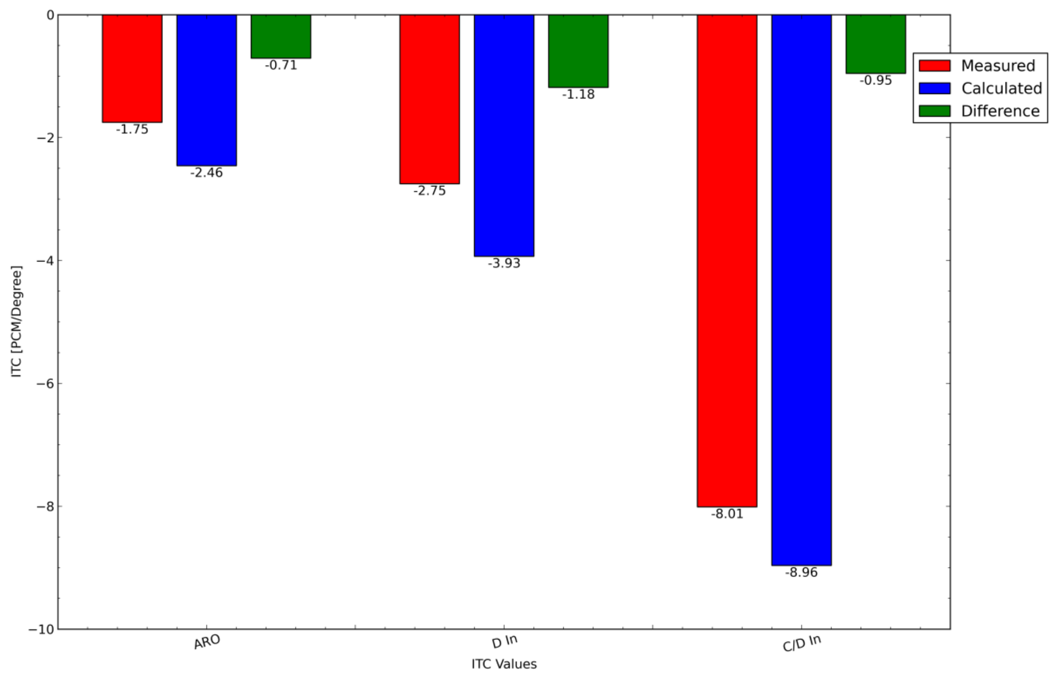

Figure A.5 BEAVRS Cycle 1 ITC Values

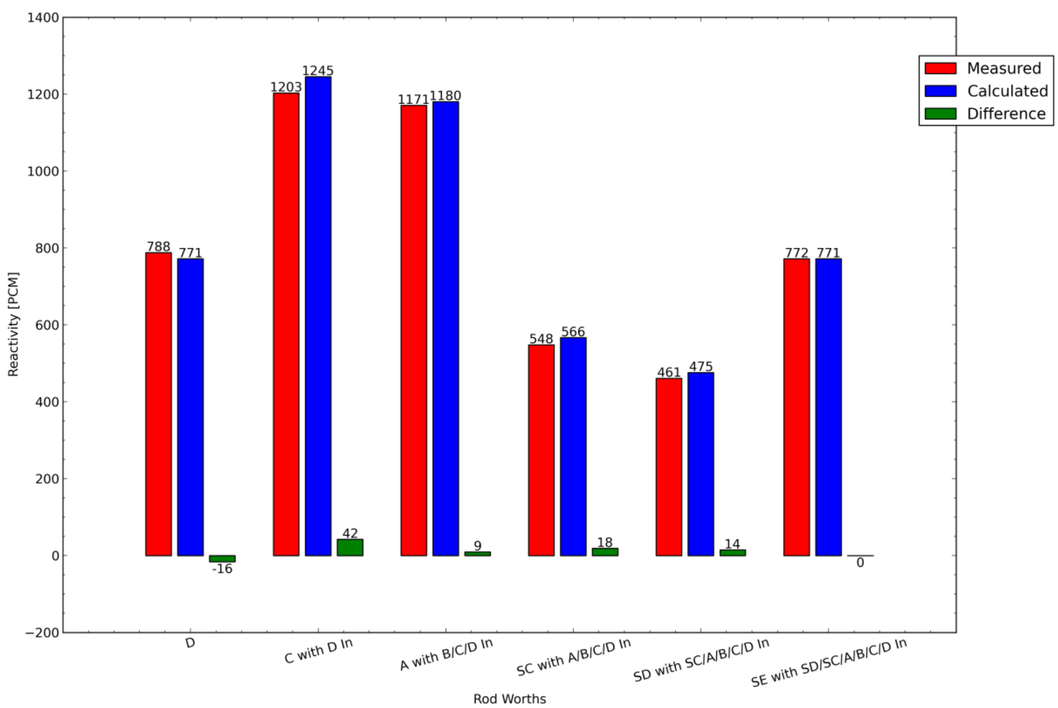

Figure A.6 BEAVRS Cycle 1 Rod Worths

```
& Measured  & Calculated & Difference  \\
\hline
&  [ppm]  &  [ppm]   &   [ppm]   \\
ARO &   975.0  &   970.7   &     -4.3   \\
D In &   902.0  &   910.3   &      8.3   \\
C/D In &   810.0  &   814.9   &      4.9   \\
A/B/C/D In &   686.0  &   681.0   &     -5.0   \\
A/B/C/D/SE/SD/SC In &   508.0  &   496.2   &    -11.8   \\

& Measured & Calculated & Difference \\
& [pcm/F]  &  [pcm/F]  &  [pcm/F]  \\
\hline
ARO &  -1.75  &   -2.46   &   -0.71   \\
D In &  -2.75  &   -3.93   &   -1.18   \\
C/D In &  -8.01  &   -8.96   &   -0.95   \\

& Measured & Calculated & Difference \\
&  [pcm]   &   [pcm]   &    [\%]   \\
\hline
D &    788.0  &    771.9    &  -2.04\% \\
C with D In &   1203.0  &   1245.2    &   3.51\% \\
A with B/C/D In &   1171.0  &   1180.3    &   0.80\% \\
SC with A/B/C/D In &    548.0  &    566.6    &   3.40\% \\
SD with SC/A/B/C/D In &    461.0  &    475.7    &   3.18\% \\
SE with SD/SC/A/B/C/D In &    772.0  &    772.0    &  -0.00\% \\
\hline
Total &  6042.0   &   6099.7    &   0.95\% \\
```

Figure A.7 Sample Script for BEAVRS Example