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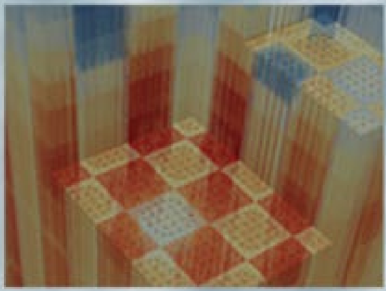

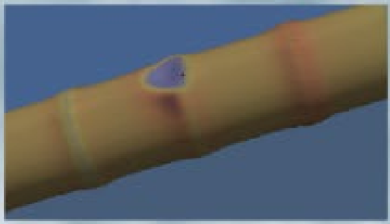

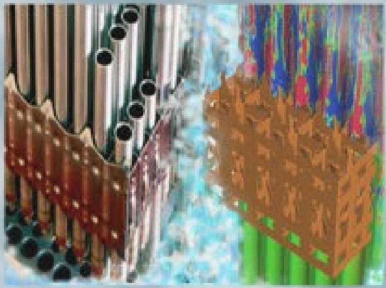

Updated Verification and Validation Assessment for VERA

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REVISION LOG

Revision	Date	Affected Pages	Revision Description
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1	2017/05/10	All	Revision to correct formatting throughout. Content Unchanged
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EXECUTIVE SUMMARY

The Virtual Environment for Reactor Applications (VERA) code suite is assessed in terms of capability and credibility against the Consortium for Advanced Simulation of Light Water Reactors (CASL) Verification and Validation Plan (presented herein) in the context of three selected challenge problems: CRUD-Induced Power Shift (CIPS), Departure from Nucleate Boiling (DNB), and Pellet-Clad Interaction (PCI). Capability refers to evidence of required functionality for capturing phenomena of interest while credibility refers to the evidence that provides confidence in the calculated results. For this assessment, each challenge problem defines a set of phenomenological requirements against which the VERA software is assessed. This approach, in turn, enables the focused assessment of only those capabilities relevant to the challenge problem. The evaluation of VERA against the challenge problem requirements represents a capability assessment. The mechanism for assessment is the Sandia-developed Predictive Capability Maturity Model (PCMM) that, for this assessment, evaluates VERA on 8 major criteria: (1) Representation and Geometric Fidelity, (2) Physics and Material Model Fidelity, (3) Software Quality Assurance and Engineering, (4) Code Verification, (5) Solution Verification, (6) Separate Effects Model Validation, (7) Integral Effects Model Validation, and (8) Uncertainty Quantification. For each attribute, a maturity score from zero to three is assigned in the context of each challenge problem. The evaluation of these eight elements constitutes the credibility assessment for VERA.

This assessment captures programmatic investment in code and solution verification, which was an identified gap in the previous assessments. Similar to the previous iteration of this assessment, this evaluation concludes that the neutronics and sub-channel thermal-hydraulics capability of VERA has good capability and credibility and this capability is used for CIPS, DNB, and PCI. The evaluation of VERA presented here culminates in the identification of various capability and credibility gaps which are intended to be used to help prioritize future CASL investment. High level conclusions can be drawn from a review of these gaps. First, capability gaps remain in all VERA codes. Next, it is observed that evidence of uncertainty quantification is lacking for all codes and challenge problems. Additionally, MAMBA is less mature than the other VERA codes and this impacts CIPS predictive maturity, though to a lesser degree than in previous assessments. The assessment presented here is fundamentally evidence based in nature and the authors propose continued efforts with the code teams and challenge problem integrators to develop capability and credibility evidence to fill gaps moving forward.

This revised V&V assessment defines a proposed structure for the V&V assessment of VERA including its component codes (MPACT, CTF, BISON, MAMBA, etc.) as well as the CASL challenge problems (CIPS, PCI, and DNB). The structure and assessment will be reviewed, refined and updated to arrive at a formal structure to provide a V&V assessment capability to track CASL's progress verification and validation and to prioritize investment for the future years.

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ACRONYMS

BFBT	BWR Full-size Fine-mesh Bundle Tests	**NRC**	Nuclear Regulatory Commission
BOA	Boron Analysis – EPRI/Westinghouse coolant chemistry code	**NSRR**	Nuclear Safety Research Reactor
CASL	Consortium for the Advanced Simulation of Light-Water Reactors	**OECD**	Organization for Economic Cooperation and Development
CASL	Consortium for the Advanced Simulation of LWRs	**ORNL**	Oak Ridge National Laboratory
CFD	Computational Fluid Dynamics	**PCI**	Pellet-Clad Interaction
CHF	Critical Heat Flux	**PCMM**	Predictive Capability Maturity Model
CILC	CRUD Induced Localized Corrosion	**PIRT**	Phenomena Identification and Ranking Table
CIPS	CRUD Induced Power Shift	**PNNL**	Pacific Northwest National Laboratory
CIPS	CRUD Induced Power Offset	**PSBT**	PWR Sub-channel and Bundle Test
CP	Challenge Problem	**PWR**	Pressurized Water Reactor
CRUD	Chalk River Unidentified Deposits	**RIA**	Reactivity Insertion Accident
CSAU	Code Scaling, Applicability, and Uncertainty	**SLB**	Steam Line Break
CTF	Modernized and improved version of the legacy sub-channel thermal-hydraulics code, COBRA-TF	**SNL**	Sandia National Laboratories
DNB	Departure from Nucleate Boiling	**SQA**	Software Quality Assurance
DOE	Department of Energy	**TH**	Thermal-Hydraulics
DOE-NE	Department of Energy Office of Nuclear Energy	**THM**	Thermal-Hydraulics Methods
EPRI	Electric Power Research Institute	**TK**	Takahama
FMC	Fuel Materials and Chemistry (CASL Focus Area)	**UQ**	Uncertainty Quantification
IFPE	International Fuel Performance Experiments	**V&V**	Verification and Validation
JFNK	Jacobian-Free Newton Krylov	**VERA**	Virtual Environment for Reactor Applications
LANL	Los Alamos National Laboratory	**VMA**	Validation and Modeling Applications
LWR	Light Water Reactor	**VUQ**	Validation and Uncertainty Quantification
MET	Multiple Effect Test	**VVUQ**	Verification, Validation and Uncertainty Quantification
MPACT	Michigan Parallel Characteristics Transport (computer code)	**WALT**	Westinghouse Advanced Loop Tester
		WEC	Westinghouse

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1 INTRODUCTION

The Consortium for the Advanced Simulation of Light Water Reactors (CASL) is developing computational modeling and simulation capabilities that target operational and safety challenges for the current fleet of operating reactors. This Verification and Validation (V&V) Assessment provides a basis to support that goal. This purpose of this document is to document the phenomena, code capabilities, and V&V/Uncertianty Quantificaiton (UQ) approach for each of the codes used for the CASL CPs. We use the Phenomena Identification and Ranking Table (PIRT) and the Predictive Capability Maturity Model as frameworks on which our approach is based. We aim to provide useful information for improving predictive code capability and quality. The present assessment reflects and documents programmatic investment in code and solution verificaiton in response to identified gaps in these areas in prior assessments.

The CASL, a U.S. Department of Energy (DOE) Energy Innovation Hub, is charged with developing computational modeling and simulation capability for light water moderated, commercial nuclear power reactors. The Virtual Environment for Reactor Applications (VERA) [1] includes a collection of tools for the simulation of neutronics, thermal-hydraulics, chemistry, and fuel performance (solid mechanics and heat transfer) in an integrated and coupled computational environment. These tools are generally designed to be employed in a high performance computing environment and are highly parallelized. Computational fluid dynamics also plays an important role, though not within VERA. The current, main CASL toolset includes the following software modules:

- VERA:
  - MPACT- Neutron and Gamma Transport [29-35]
  - CTF-Thermal-Hydraulics [37-47]
  - MAMBA-Chemistry [55, 56, 59]
  - BISON-Fuel Performance [49-51]
- Star CCM+-Computational Fluid Dynamics [61]

In addition to the main software tools, several other software utilities are used to pass data between the main codes and to solve multi-physics equations. These are principally capability within CTF to couple with MPACT and with MAMBA, TIAMAT which couples MPACT and BISON and CICADA which couples Star CCM+ with MAMBA. TIAMAT combines functionality from the Data Transfer Toolkit (DTK) and Physics Integration Kernels (PIKE) to couple MPACT, CTF, MAMBA, and BISON. CICADA also uses DTK to pass data between Star CCM+ and MAMBA and includes functionality to aggregate high resolution CFD data to lower resolution meshes. It is worth noting that while the main software modules receive the greatest attention, the coupling utilities TIAMAT and CICADA are critical for the solution of most CASL challenge problems.

Much of the work in the second phase of CASL has been organized around a handful of challenge problems (CPs) [2, 3]. These challenge problems have been identified by the nuclear industry as important to the safe and reliable operation of the current nuclear reactors. Each CP has unique set of phenomena that may span multiple traditional disciplines. Currently, there are seven active challenge problems:

- CRUD Induced Power Shift (CIPS)
- CRUD Induced Localized Corrosion (CILC)
- Pellet-Cladding Interactions (PCI)
- Grid to Rod Fretting (GTRF)
- Departure from Nucleate Boiling (DNB)
- Loss of Coolant Accident (LOCA)
- Reactivity Insertion Accident (RIA)

A subset of the physics modules is used to provide simulation results for each challenge problem. For the purposes of this V&V assessment three CPs: CIPS, PCI, and DNB will serve as the primary application, and a brief, introductory description of these three is presented here. For more information, the reader is referred to the various CP charters and implementation plans [3, 17, 21, 22, 26, 27].

The Chalk River unidentified deposits related (CRUD-related) CPs (CIPS and CILC) [17-19] involve the deposition of certain corrosion products from the reactor coolant system upon the cladding of the fuel assemblies within the reactor core and the subsequent adsorption of boron from the reactor coolant within the CRUD. The primary challenge for CRUD simulation lies in the prediction of CRUD chemical mass and deposition characteristics. MPACT, CTF, and MAMBA are the primary software modules utilized for the CRUD challenge problems. An important aspect of the CRUD-related challenge problems relates to the "source term" for nickel and iron.

The PCI CP [26, 27] involves predicting mechanical cladding deformation associated with fuel pin pressurization associated with fission gas production and the physical contact between swelling fuel pellets and the cladding. Fission energy is primarily deposited as heat in the fuel pellets. The heat is then conducted radially outward from the center of the fuel pellets, through the gap between the fuel pellet and the clad inner surface, and through the clad itself. The heat is then transferred by convection to the coolant and then away to the rest of the reactor system using CTF. While conceptually simple, the complexity for this CP arises from the numerous feedback mechanisms that influence all phases of the phenomenology. For example, as the temperature of the fuel rises, the reactivity is reduced (via Doppler broadening), thus reducing the neutron flux, and, as the temperature rises and as the fuel ages, the pellets swell thus reducing the gap distance and increasing the thermal conductivity between the fuel and cladding. Furthermore, fuel often experiences material inelasticity either through plastic flow or through discrete cracking. The engineering-scale code for computing PCI effects is BISON; however, MPACT and CTF do provide input to BISON relating to the power generation and the heat transfer at the outer clad surface.

The DNB CP [21-25, 48] is fundamentally safety-related and involves the prediction of increased boiling, leading to fuel dryout, during hypothetical accident conditions. For pressurized water reactor (PWR) operating conditions with increasing clad temperature, boiling begins as nucleate or subcooled boiling where very localized liquid-to-gas transitions occur on the surface of the clad. This continues up to the point of critical heat flux between the clad surface and the coolant. Once the critical heat flux is exceeded, the heat transfer efficiency from the clad surface to the coolant drastically decreases and fuel temperatures begin to rise. This rise in fuel and cladding temperature has implications for fuel integrity during an accident. Within CASL, MPACT, CTF, and Star CCM+ are the primary codes utilized for making predictions. CTF is particularly well-suited for this CP owing to its history as a design basis accident code for loss of coolant accidents [37, 38].

1.1 Document Organization

The rest of this document includes five sections and a conclusion. The first section describes the CASL V&V Strategy. The next three sections evaluate each of the challenge problems (CIPS, DNB and PCI) against the V&V strategy. There is a certain intentional repetition for these three sections such that each could be taken as a stand-alone document for each CP.

Following the evaluation of the three selected CPs, a section is devoted to discussion and overall gap identification. Since there is significant overlap in the codes utilized for the three CPs, it is likely areas for improvement for one CP will also be identified for another. Finally, conclusions will be provided.

An appendix describing the evidence used for this evaluation is provided for more depth and context for the CP assessments.

2 VERIFICATION AND VALIDATION PLAN FOR VERA

The CASL V&V strategy has evolved since the early phases of the program [1] [4], yet several fundamental aspects have remained unchanged. This V&V approach for CASL includes an assessment of required functionality and predictive capability and a mapping of these requirements to various codes, as well as an assessment of predictive capability maturity for the codes. **A new approach in the present assessment is the logical separation of capability and credibility assessment**. Capability captures the code's ability to represent the required physical phenomena for predicting a given quantity of interest (QoI) while credibility involves the body of evidence that supports the believability of the predicted QoI. As mentioned previously, CASL [2] has incorporated many CPs, and these, along with a series of progression problems in Phase I, have driven the requirements. Credibility captures the suitable evidence that simulation predictions are trustworthy for an intended application and is subjective in nature. Credibility assessment involves the aggregation of evidence and the evaluation thereof. The next subsections will develop and describe the CASL V&V strategy for the remainder of the second phase of CASL. We use PIRTs and gap assessments to assess capability, and we use the Predictive Capability Maturity Model to assess credibility.

2.1 Overview of the CASL V&V Process

Due to the multiphysics and multi-code nature of the challenge problems in CASL, V&V of component codes alone is not sufficient; it must extend to coupled codes. This form of V&V for coupled codes is relatively new and is continuing to increase in interest. The "correct" way to verify and validate coupled software is still a research topic, however an approach will be presented here that is based on current best practices and understanding of CASL researchers.

2.1.1 Verification Background

Each of the code teams has provided V&V plans. The verification of the capability for the individual codes are documented in these reports, along with the coupling to other codes that is provided within that software base. Verification of the coupling of MPACT's native neutronics capability with the ORIGEN-S isotopic depletion and CTF thermal-fluid dynamics is also documented in the MPACT V&V report, but the validation is provided in the VERA V&V report.

Validation Background

A comprehensive validation plan, focused on nominal core simulation, was proposed for VERA in 2014 [62], and this section will briefly summarize some aspects of that validation plan to include the validation matrix proposed for VERA. The four principal validation components identified in the plan are shown in Figure 1, which was reproduced from [62].

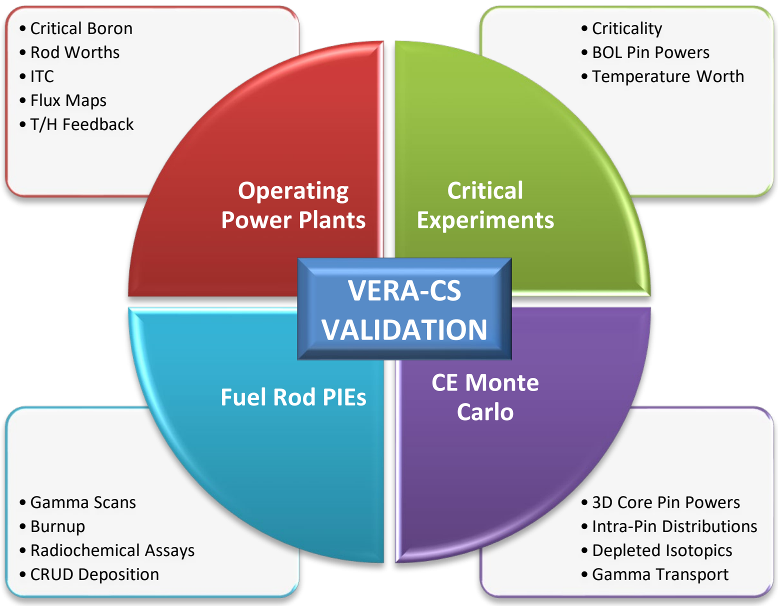

Figure 1. Components of VERA Neutronics Validation [62]

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

- 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.

- *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.

- 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.

- 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.

The first three of these areas are considered "single physics" neutronics and have been included in the MPACT Validation plan [30]. During the past few years, significant progress has also been made acquiring operating plant data, and this is the area that is now considered the purview of the multi-physics VERA validation for PWR core follow. Measurement data from operating nuclear power plants provides valuable 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.

2.2 Challenge Problem Driven Phenomenology Based Assessment

A novel approach for coupled multi-physics V&V has been developed and will be applied for this assessment as described here. Since the CASL CPs have driven the capability development for the second phase of CASL, and accordingly, this V&V assessment will be organized around the CPs. Figure 2 summarizes the five step V&V strategy that will be utilized for the remainder of the second phase of CASL. The five steps of this V&V approach include:

1. CP Phenomenon Identification and Ranking Table (PIRT),
2. Define V&V Requirements,
3. Map Requirements to Codes,
4. Assemble V&V Evidence, and
5. Perform Predictive Capability Maturity Model (PCMM) assessment.

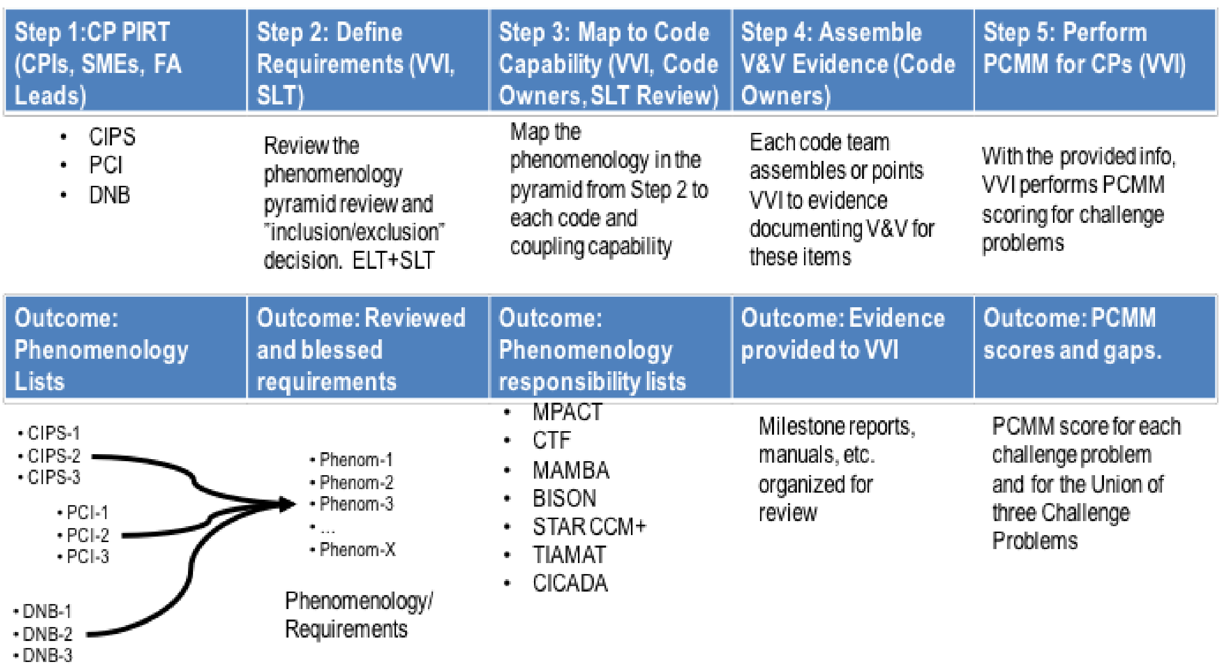

Figure 2. Challenge Problem Driven Phenomenology Based Assessment Strategy for CASL Code Maturity

The novelty of this approach involves the assessment of maturity of a collection of codes in the context of an application. If a code is developed for a single application the link between required capability and functionality is straightforward. For CASL CPs and codes, this is not the case (individual codes are used for multiple CPs) so there is significant utility in evaluating only the code capability that is used for the CP application and not the entire capability set which may be present. **The outcome of this approach is an assessment of the predictive capability maturity for an application that has significant practical value.** The predictive capability maturity very likely varies among the CASL CPs, and this approach permits flexible evaluation of each, even though many of the same codes are used.

The first step in the proposed methodology, the CP PIRT step, leverages the classical PIRT methodology [5, 6] for the identification of important phenomena associated with the problem of interest. The identified phenomena are ranked based on importance, knowledge, and code adequacy, which gives insight into the significance for each. Importance of a phenomenon is defined as how much this phenomenon influences the accuracy of the prediction. An example of this, would be understanding how much fuel cracking affects heat transfer. Knowledge level of a phenomenon assesses how well current models of the phenomenon agree with the observed phenomenon. Code adequacy assesses if the current code capability reflects the current model. For example, the appropriate phenomenological model may be too computationally expensive to practically use in a code; so, additional approximations are made (e.g., using neutron diffusion approximation instead of CE Monte Carlo transport). As suggested by Figure 2, multiple CPs will be considered in this strategy and the union of phenomena from these challenge problems will be considered in the assessment. This ranking, along with an assessment of cost of implementation, can be used to set funding and development priorities. The PIRT assessment directly informs the evaluation of capability since it is this step that links the required phenomenology with the code components designed to represent the phenomenology.

The second step in the V&V strategy involves mapping the phenomena identified and ranked in the first step into code requirements. This step can be considered analogous to a transition from qualitative to quantitative. For example, if the effect of CRUD deposition on cladding temperature is identified as an important phenomenon, then the associated requirement would be that the code must be able to compute CRUD deposition with a specified accuracy, precision, and range of validity. A backlog of code requirements is established by examining the cost of implementation and importance pay-off for each of the phenomena.

The third step involves mapping the code requirements from the second step to specific codes in the VERA suite. This step involves assigning responsibility for each phenomenon to the appropriate code. Each code development team examines their resources (i.e., developer time, computing hardware, etc.) and decides how much of the code requirement backlog they can address.

The fourth step involves accumulating V&V evidence to support the PCMM assessment in the fifth step. Evidence includes user and theory manuals for the various codes as well as documentation of V&V activities such as verification test problems (e.g., observing the correct order of convergence for the numerical discretization schemes used in the codes) or comparison to validation data and uncertainty or sensitivity studies. The sole basis that assessments about the predictive credibility rely upon is this evidence. There is some subjectivity in assessing this evidence, and the authors acknowledge that there may be some disagreement about the numerical scores.

The fifth step in the V&V strategy simply involves the assessment of the available evidence to the PCMM [7] categories. Given the relative importance of the PCMM framework to this strategy, the following subsection describes maturity based software assessment and the modified PCMM approach utilized for CASL. The PCMM evaluation is tightly linked to credibility assessment and his will be developed in the next subsection.

2.3 Predictive Capability Maturity Model

Assessing the quality of predictions made using scientific computer codes is a complex and multifaceted topic that is also relatively new compared to the technical fields for which the codes are written. This problem has become more challenging as scientific software has become more capable and includes more physical phenomena. Within CASL, prediction capability has been assessed using the Predicative Capability Maturity Model (PCMM) [7], and this model will be used for the present assessment, with a few modifications to the original framework. These modifications include the separation of software quality assurance (SQA) and software quality engineering (SQE) from the code verification category and the separation of separate effects testing (SET) validation from integral effects testing (IET) validation. The purpose of separate effect and integral effects testing validation is analogous to performing unit test and integration tests during code verification. Both strategies involve understanding the hierarchy involved in both areas.

Within CASL, there has been a relatively high level of effort and rigor expended on SQA/SQE practices while less effort has been expended on the more mathematical code verification activities such as demonstrating the expected order of convergence. Separating SQA/SQE from code verification will permit a more precise assessment and communication of expectations and achievements for each aspect. Furthermore [8] recognizes SQA/SQE and numerical algorithm verification as separate types of activities, yet they are both intended to minimize or eliminate unexpected bugs, errors, blunders, and mistakes from corrupting predictions. Similarly, for validation, the separation of IET validation from SET validation permits more resolution in the assessment and a clearer identification of expectation and accomplishments. Figure 3 shows the modified PCMM matrix that will be used in this assessment.

	Maturity Level 0	Maturity Level 1	Maturity Level 2	Maturity Level 3
	Low Consequence and Impact; Scoping or R&D Studies	Moderate Consequence and Impact; Design Support	High Consequence and Impact; Qualification Support	Highest Consequence and Impact; Decision Making, Certificaiton, or Licensing
Representation and Geometric Fidelity What geometric features are neglected or stylized?	• Judgement only • Little or no representation or geometric fidelity for the system or boundary conditions	• Significant simplification or stylization of the system and boundary conditions • Geometry or representation of major components is defined	• Limited simplification or stylization of major components and boundary conditions • Geometry or representation is well defined for major components and some minor components • Some peer review conducted	• Essentially no simplification or stylization of components in the system and boundary conditions • Geometry or representation of all components is at the detail of "as-built" • Independent peer review conducted
Physics and Material Model Fidelity Are the included physical models adequate and are they appropriately calibrated?	• Judgment only • Model forms are either unknown or fully empirical • Few, if any, physics informed models • No coupling of models	• Some models are physics based and are calibrated using data from related systems • Minimal or ad hoccoupling of models	• Physics-based models for all important processes • Significant calibration needed using separate effects tests (SETs) and integral effects tests (IETs) • One-way coupling of models • Some peer review conducted	• All models are physics based • Minimal need for calibration using SETsand IETs • Sound physical basis for extrapolation and coupling of models • Full, two-way coupling of models • Independent peer review conducted
Software Quality Assurance and Engineering Are adequate protocols in place to minimize the introduction of errors?	• No SQA/SQE formality • Codes and or scripts not tested beyond the task or application for which the software is used • No version control in place	• Some SQA/SQE formality • Some unit and or regression testing evidence • Some system of version control	• Demonstrable SQA/SQE plan in place • A significant majority of the code is unit and regression tested • Rigorous version control • Testing on multiple hardware platforms	• Rigorous SQE/SQA program in place with strong evidence of adherence • Unit and regression testing evidence for all lines of code • Rigorous version control • Testing for all anticipated hardware platforms
Code Verification Are algorithms and their implementation introducing errors?	• Judgment only • Minimal testing of any software elements	• Some comparison of major algorithms made with benchmarks • Little or no peer review	• Some algorithms are tested to determine the observed order of numerical convergence • Some features & capabilities (F&C) are tested with benchmark solutions • Some peer review conducted	• All important algorithms are tested to determine the observed order of numerical convergence • All important F&Cs are tested with rigorous benchmark solutions • Independent peer review conducted
Solution Verification Are numerical solution errors corrupting predictions?	• Judgment only • Numerical errors have an unknown or large effect on simulation results	• Numerical effects on relevant SRQs are qualitatively estimated • Input/output (I/O) verified only by the analysts	• Numerical effects are quantitatively estimated to be small on some SRQs • I/O independently verified • Some peer review conducted	• Numerical effects are determined to be small on all important SRQs • Important simulations are independently reproduced • Independent peer review conducted
Separate Effects Model Validation Are individual physical models validated with carefully generated laboratory data?	• Judgment only • Few, if any, comparisons with relevant laboratory measurements	• Quantitative assessment of accuracy of SRQs not directly relevant to the application of interest • Large or unknown experimental uncertainties	• Quantitative assessment of predictive accuracy for some key SRQs from SETs • Experimental uncertainties are well characterized for most SETs • Some peer review conducted	• Quantitative assessment of predictive accuracy for all important SRQs from SETs at conditions/geometries directly relevant to the application • Experimental uncertainties are well characterized for all SETs • Independent peer review conducted
Integral Effects Model Validation Has the integrated code been assessed in the context of system data?	• Judgment only • Few, if any, comparisons with measurements from similar systems	• Quantitative assessment of accuracy of SRQs not directly relevant to the application of interest • Large or unknown experimental uncertainties	• Quantitative assessment of predictive accuracy for some key SRQs from IETs • Experimental uncertainties are poorly known for IETs • Some peer review conducted	• Quantitative assessment of predictive accuracy for all important SRQs from IETs conditions/geometries directly relevant to the application • Experimental uncertainties are well characterized for all IETs • Independent peer review conducted
Uncertainty Quantification and Sensitivity Analysis How thoroughly are uncertainties and sensitivities assessed, characterized, and propagated?	• Judgment only • Only deterministic analyses are conducted • Uncertainties and sensitivities are not addressed	• Aleatory and epistemic (A&E) uncertainties propagated, but without distinction • Informal sensitivity studies conducted • Many strong UQ/SA assumptions made	• A&E uncertainties segregated, propagated and identified in SRQs • Quantitative sensitivity analyses conducted for most parameters • Numerical propagation errors are estimated and their effect known	• A&E uncertainties comprehensively treated and properly interpreted • Comprehensive sensitivity analyses conducted for parameters and models • Numerical propagation errors are demonstrated to be small • No significant UQ/SA assumptions made

Figure 3. PCMM Matrix to be used in the current V&V assessment

The following subsections will provide a brief description of each code quality attribute and will be based largely on the original PCMM description [7]. For more complete descriptions of the code maturity aspects, the reader is referred to [7-9].

2.3.1 Representation and Geometric Fidelity

The representation and geometric fidelity aspect of code maturity considers the ability of the code to capture and characterize physical information from the real system being modeled. The ability to resolve important geometric features is required for the application of detailed boundary conditions. Conversely, many codes make use of simplified geometry to facilitate improved computational speed. It is believed that full geometric fidelity improves predictive capability by eliminating simplifications based on developer or analyst judgement. It is understood that full geometric representation (i.e. atomistic simulation) is not possible for the length scale of interest. This element of predictive maturity addresses the question: “Is the geometric fidelity of the model sufficient for the intended purpose of the simulation, or are geometric simplifications introducing error?”

The four tiers of maturity for Representation and Geometric Fidelity are:

(1). Geometric fidelity based on analyst judgement only; Many geometric simplifications; Little or no geometric fidelity to the system; Limited application of boundary conditions

(2). Significant simplification of geometric features of the system being analyzed; Most of the major geometric features are specifically represented

(3). Limited simplification of geometric features and boundary conditions; Well defined geometric representation for all major system features; Some representation of minor system features; Some peer review of geometric fidelity conducted

(4). Essentially no simplification of geometry or boundary conditions within the system; Geometric representation can be considered “as-built” for the system being analyzed; Independent peer review of geometric fidelity to the system conducted

2.3.2 Physics and Material Model Fidelity

Physics and material model fidelity refers to the degree to which mathematical models within the code are physics-based as opposed to empirical and applicable the physics and material models are to the intended application (i.e., CP). In addition to the level of model physicality, this attribute of code maturity also incorporates the level of calibration required for mathematical models within the code. It is worth noting that calibrated, empirical models can be very powerful engineering tools, but the predictive capability of these models is limited to the state space of the calibration data. Predictions within the calibrated space are useful, while predictions made outside this space are highly questionable. For this reason, high predictive maturity requires physics-based models that rely less on calibration of model parameters.

The four tiers of maturity for Physics and Material Model Fidelity are:

(5). Physics and material mode fidelity based on analyst judgement only; Model forms are unknown or fully empirical; Few, if any, physics informed models; No coupling of models

(6). Some models are physics-based and are calibrated using data from related systems; Minimal or ad hoc coupling of models

(7). Physics-based models for all important processes; Significant calibration needed using separate effects tests (SETs) and integral effects tests (IETs); One-way coupling of models; Some peer review conducted

(8). All models are physics based; Minimal need for calibration using SETs and IETs; Sound physical basis for extrapolation and coupling of models; Full, two-way coupling of models; Independent peer review conducted

2.3.3 Software Quality Engineering and Assurance

As mentioned previously, the original PCMM presentation in [7] included activities related to SQA/SQE under the category of Code Verification since the objective of both SQA/SQE and mathematical techniques such as demonstrating the order of convergence are intended to minimize code corruption due to bugs, and other mistakes. Other research has suggested that these are two different types of activities [8, 9]. The authors believe that this is a key distinction. Specifically, for scientific simulation codes, unit and regression testing is necessary but not sufficient to identify all potential errors where other more rigorous techniques can. Furthermore, based on the findings of previous assessments and through informal interactions among CASL researchers, there is presently a relatively strong SQA/SQE culture and conversely, there is very little investment in convergence, etc.). For these reasons SQA/SQE will be assessed separately from other code verification.

The four tiers of maturity for Software Quality Assurance are:

(9). No SQA/SQE formality; Codes and or scripts not tested beyond the task or application for which the software is used; No version control in place

(10). Some SQA/SQE formality; Some unit and or regression testing evidence; Some system of version control

(11). Demonstrable SQA/SQE plan in place; A significant majority of the code is unit and regression tested; Rigorous version control; Testing on multiple hardware platforms

(12). Rigorous SQE/SQA program in place with strong evidence of adherence; Unit and regression testing evidence for all lines of code; Rigorous version control; Testing for all anticipated hardware platforms

2.3.4 Code Verification

Following from the discussion in Section 2.3.3, Code Verification involves the mathematically rigorous techniques used to identify code bugs and errors and to identify “correct” but deficient numerical algorithms. The most powerful and comprehensive technique in this area is determining the theoretical order of convergence. By demonstrating that the code converges to a highly accurate solution at the expected rate (order of convergence), the physics models, the numerical solution schemes are tested. The authors of this document direct the interested reader to the following reference [10]. Code Verification is fundamentally empirical in that the code must be shown demonstrate performance and evidence is accumulated for this purpose. It is worth noting that there can be significant challenges to obtaining analytic solutions, but the method of manufactured solutions (MMS), described in the reference, provides a straight forward approach to developing analytic solutions. For multiphysics phenomena with disparate discretization schemes, obtaining these highly accurate solutions is a more challenging exercise and could be considered a research effort.

The four tiers of maturity for Code Verification are:

(13). Judgment only; Minimal testing of any software elements

(14). Some comparison of major algorithms made with benchmarks; Little or no peer review

(15). Some algorithms are tested to determine the observed order of numerical convergence; Some features & capabilities (F&C) are tested with benchmark solutions; Some peer review conducted

(16). All important algorithms are tested to determine the observed order of numerical convergence; All important F&Cs are tested with rigorous benchmark solutions; Independent peer review conducted

2.3.5 Solution Verification

Solution verification involves estimating the magnitude error in the numerical solution for the intended application (i.e., CP) for the computed responses of interest. The primary sources of solution error are spatial discretization error (i.e., not having enough mesh), time integration error (i.e., taking too big of a time step), and numerical solver tolerances (i.e., not having a small enough tolerance for the linear solver). The purpose of code verification is to provide confidence that the physics equations were correctly encoded into software. The purpose of solution verification is to ensure that there is sufficient resolution (spatial, temporal, and numerical) in the problem of interest to provide accurate solutions for system response quantities (SRQs). Another simple way to look at this is that code verification is an activity done by developers writing the code, and solution verification is an activity performed by analysts using the code. Richardson extrapolation is the most well-known method for solution verification of the spatial discretization and involves performing identical calculations on multiple domains each with differing levels of mesh refinement. Once the calculations are performed, the error from spatial discretization can be assessed and a suitable level of refinement chosen. However, the use of goal-oriented mesh adaptivity with accurate error estimators is another potential method of determining spatial discretization error. Solution Verification is important and independent from Code Verification since error-free models and numerical solution approaches can produce unsuitable results if sufficient refinement is not provided to resolve physical phenomena of interest. The authors direct the interested read to the following reference [9].

The four tiers of maturity for Solution Verification are:

(17). Judgment only; Numerical errors have an unknown or large effect on simulation results

(18). Numerical effects on relevant SRQs are qualitatively estimated; Input/output (I/O) verified only by the analysts

(19). Numerical effects are quantitatively estimated to be small on some SRQs; I/O independently verified; Some peer review conducted

(20). Numerical effects are determined to be small on all important SRQs; Important simulations are independently reproduced; Independent peer review conducted

2.3.6 Separate Effects Validation

Separate effects validation involves comparing computed responses to analogous experimentally measured responses in tightly-controlled and carefully-constructed experiments that minimize confounding factors. Separate effects validation tests are generally conducted in a laboratory setting and are instrumented with computational model inputs in mind such that clear exposure to model response is ensured. The objective of this type of validation is to test the individual physics models that make up a larger simulation code over a range of model state space that is relevant and encompasses the expected predictive range. An important aspect of all validation is the numerical quantification of the model response to the measured response, yet defining appropriate thresholds for acceptability can be challenging. Similarly, assessing the uncertainty or variability in the experimental data is also important. Separate effects validation differs from integral effects validation in that the former purposefully excludes phenomena to eliminate confusing feedback arising from multiple, interacting physical phenomena while the latter purposefully includes more phenomena to evaluate these interactions.

The four tiers of maturity for Separate Effects Validation are:

(21). Judgment only; Few, if any, comparisons with relevant laboratory measurements

(22). Quantitative assessment of accuracy of SRQs not directly relevant to the application of interest; Large or unknown experimental uncertainties

(23). Quantitative assessment of predictive accuracy for some key SRQs from SETs; Experimental uncertainties are well characterized for most SETs; Some peer review conducted

(24). Quantitative assessment of predictive accuracy for all important SRQs from SETs at conditions/geometries directly relevant to the application; Experimental uncertainties are well characterized for all SETs; Independent peer review conducted

2.3.7 Integral Effects Validation

Integral effects validation involves the comparison of code generated system response to analogous measured system experimental response. The system can be an entire engineered system or a subsystem thereof. The goal of integral effects validation is to evaluate the ability of the code to predict system responses that include interaction between multiple separate effects. As a practical matter it can be difficult to obtain well instrumented integral effects validation tests for large or very complex systems such as commercial nuclear power reactors. As with separate effects validation, numerical quantification of code response accuracy is important for validation as is characterization of experimental uncertainty for the integral effects experimental data.

The four tiers of maturity for Integral Effects Validation are:

(25). Judgment only; Few, if any, comparisons with relevant laboratory measurements

(26). Quantitative assessment of accuracy of SRQs not directly relevant to the application of interest; Large or unknown experimental uncertainties

(27). Quantitative assessment of predictive accuracy for some key SRQs from IETs; Experimental uncertainties are well characterized for most IETs; Some peer review conducted

(28). Quantitative assessment of predictive accuracy for all important SRQs from IETs at conditions/geometries directly relevant to the application; Experimental uncertainties are well characterized for all IETs; Independent peer review conducted

2.3.8 Uncertainty Quantification

Uncertainty quantification for predictive software involves the estimation and propagation of uncertainties in the various inputs, models, and solution approaches to help bound and provide context to the otherwise deterministic predictions generated from simulation codes. Practically, this concept is incredibly important for decision making since the code prediction can be accompanied with a confidence interval. This is particularly important for the nuclear industry and the US Nuclear Regulatory Commission as described in [11]. There exists a useful separation of uncertainty types: aleatory or randomness based uncertainty and epistemic or lack-of-knowledge uncertainty. For a given physical system, there will always be some level of aleatory uncertainty associated with randomness of material properties or chaotic physical phenomena. On the other hand, epistemic uncertainty can be reduced though improved physical modeling. Thus, if a UQ study is performed with an accompanying sensitivity analysis, then one may decide whether to devote resources to reducing the uncertainty for the epistemic uncertainties. Uncertainty quantification for large models and systems can be extremely challenging owing to the large volume of data, the propagation the uncertainty through the system, and the adequate sampling of the input space (sometimes referred to as “the curse of dimensionality”). Sensitivity studies, where various model parameters are perturbed and the overall code response is observed, are a less rigorous if done alone, but often useful approach to augment UQ. Two references that the authors would point the interested reader to are [12, 13].

The four tiers of maturity for Uncertainty Quantification are:

(29). Judgment only; Only deterministic analyses are conducted; Uncertainties and sensitivities are not addressed

(30). Aleatory and epistemic (A&E) uncertainties propagated, but without distinction; Informal sensitivity studies conducted; Many strong UQ/SA assumptions made

(31). A&E uncertainties segregated, propagated and identified in SRQs; Quantitative sensitivity analyses conducted for most parameters; Numerical propagation errors are estimated and their effect known; Some strong assumptions made;

(32). A&E uncertainties comprehensively treated and properly interpreted; Comprehensive sensitivity analyses conducted for parameters and models; Numerical propagation errors are demonstrated to be small; No significant UQ/SA assumptions made.

2.4 PCMM Scoring Methodology

For each PCMM attribute, relevant evidence for each challenge problem and code are collected and evaluated against the descriptions for each maturity level shown in Figure 3. Close inspection of the PCMM maturity level descriptions reveals semi-quantitative descriptions for most PCMM attributes and this can lead to confusion on how a particular attribute receives a maturity score. This is not surprising given only 4 levels of granularity for distinguishing maturity in the PCMM framework. This subsection describes the process for making scoring decisions in the current assessment. For all PCMM attributes, the decision process is supported by the identified phenomenology from the PIRT for each challenge problem.

For Representation and Geometric Fidelity, Physics and Material Model Fidelity, the maturity scoring was based on the ability of the code(s) to address the dependent phenomenology identified for each challenge problem. For example, CRUD formation involves porosity and chimneys that promote boiling and current modeling does not resolve these features. For Software Quality Assurance and Engineering, the concept of regression test line coverage was used to help support the decision making between maturity scores. For Code Verification, the particular PDEs relevant to simulating the phenomena of interest were paid particular attention. The Code Verification evidence was considered in light of which PDEs and associated solvers are tested for convergence behavior. For Solution Verification, the descriptions in Figure 3 are sufficient to resolve between maturity levels. For both Separate and Integral Effects Validation, the phenomena of interest were closely compared to the available validation data and associated comparisons to modeled results. For every challenge problem, there is insufficient validation data to support the validation of every phenomena identified. To distinguish between maturity levels a simple “majority rule” of validated phenomena was utilized. For Uncertainty Quantification, only simulation of quantities of interest relating to the particular challenge problem were considered. As in previous assessments of VERA-CS, only published evidence was considered for evaluation.

3 EVIDENCE IDENTIFICAITON AND ORGANIZATION

V&V evidence is collected through review of V&V manuals, code development and application reports, and presentations. Often, V&V evidence for a particular maturity category is not located in a single document; rather relevant evidence may be found in a variety of sources and thus there is a need to organize this evidence into a framework that facilitates efficient location and updating. Furthermore, the evidence for VERA-CS is tied to individual codes while the current assessment is challenge problem driven.

An identifying number has been developed to refer to each piece of evidence as it relates to each software tool (e.g. MPACT, CTF, etc.) that provides information about the piece of evidence itself. The identifying numbers are of the form:

$$AB.x.y.\ z$$

where AB identifies the code to which the evidence refers, x corresponds to the PCMM attribute or set of attributes for which the evidence were identified in descending order as shown in Figure 3, z is a counter that differentiates between multiple pieces of evidence, and y is a level identifier differentiating high, medium, and low level evidence as:

(1). High level evidence (HLE): Global statement or activity related to V & V of code

(2). Medium level evidence (MLE): Specific task to support the high-level evidence

(3). Low level evidence (LLE): Reference to performance or test details.

The evidence was first collected on a code basis, since this is often how the documents are created, and tables documenting the evidence organized by code are presented in the appendix to this document. Additionally Table 13, Table 25, and Table 34 present the same evidence organized by challenge problem. For reader convenience, each evidence identifier is also hyperlinked to the source information.

4 CRUD-INDUCED POWER SHIFT

As mentioned previously, the CIPS challenge problem seeks to significantly increase the industry predicative capability for the deposition of CRUD within the reactor core and the associated top to bottom shift in power distribution. Within CASL, the CIPS challenge problem involves MPACT, CTF, BISON and MAMBA. The conceptual, physics-based understanding of computational modeling for CIPS can be described in a series of steps. First, the simulation must compute a neutron flux that produces energy from fission (deposited in the fuel and the coolant). Boron in CRUD, fuel temperature, moderator density, and moderator temperature are all feedback mechanisms. Next, the computation must conduct the energy in the fuel radially out from the center, across the gap, through the clad, and finally through the CRUD into the coolant. The fuel is changing with burn-up and the gap is shrinking. Subsequently, the code must remove the heat from the clad to the coolant and advect it out of the core. Finally, the simulation must predict how CRUD is exchanged between the fuel pin surface and the coolant (boiling and non-boiling) and how Boron deposited in and on the CRUD.

4.1 CIPS PIRT

Expert elicitation via the PIRT process has been utilized to identify important phenomena for modeling CIPS. There are three primary quantities of interest (QoIs) for the CIPS Challenge Problem:

- Total Boron Mass (Scalar)
- Boron Mass Distribution (Vector)
- Axial Offset (Scalar)

It is worth noting that the first QoI can be computed trivially from the second and that the Axial Offset implicitly depends on the second QoI as well.

4.1.1 Phenomena Considered

The phenomena considered for the CIPS Challenge Problem are presented in Table 1 through Table 4 below. Along with each phenomenon, a short description is included to facilitate understanding. Additionally, the phenomena are grouped, for convenience, into four physics areas: Thermal-Hydraulics, Fuel Behavior, Neutronics, and Chemistry.

Table 1. Phenomenology considered for the CIPS Challenge Problem related to Thermal-Hydraulics

Phenomenon	Description
Steaming Rate	The rate at which steam is being produced through boiling on the clad surface. The overall rate of crud growth depends significantly on the boiling (and hence steaming) rate.
Subcooled Boiling on a clean metal surface	Also known as "Nucleate Boiling." Boiling that occurs when the rod surface is temperature exceeds the saturation temperature when the bulk coolant is in subcooled conditions and when the heat flux from the rod is lower than the critical heat flux
Subcooled Boiling In CRUD	Subcooled boiling occurring in and on the CRUD layer on the surface of the rod
Bulk Coolant Temperature	Interpreted as the channel center temperature and generally cooler than the coolant temperature at the surface of the rod
Heat Flux	The rate of heat energy transfer through the surface of the clad into the coolant.
Wall Roughness	The surface texture of the cladding which influences nucleation sites for boiling and pressure loss along the length of the channel. This roughness changes as CRUD deposits. As CRUD deposits, the roughness changes.
Single Phase Heat Transfer	Single phase heat transfer is the transfer of heat from the fuel cladding to the coolant which is in single phase conditions (e.g., no boiling).
Nickel and Iron Mass Balance	The overall primary system balance, in terms of mass, of iron and nickel being released by corrosion of the steam generators and piping and taken up primarily on the fuel rods. The mass balance of these compounds, which are key to crud formation is used to provide their overall concentration in the coolant system.
Boron Mass Balance	The overall primary system balance, in terms of mass, of boron being injected and removed from the system to control reactivity and being taken up and released by CRUD. The mass balance of boron is needed to calculate the overall concentration of boron in the coolant system.
CRUD Erosion	The removal of CRUD buildup due to the shear forces associated with moving fluid. This is distinct from the removal of CRUD due to differential thermal expansion entering shutdown
Initial CRUD Thickness (Mass)	The initial amount of CRUD on the fuel rods at the beginning of the simulation, typically the CRUD that is retained on the fuel after a reactor shutdown for refueling.
Initial Coolant Nickel and Boron Concentration	Dissolved and particulate Iron and Nickel species in the coolant at the beginning of the simulation, typically at the startup of the reactor after a shutdown for refueling.
CRUD Source Term from Steam Generators and other Surfaces	The rate of Iron and Nickel being released through dissolution and particulates from the steam generator tube surfaces and other metal surfaces in the primary coolant loop.
CRUD Induced Change in Boiling Efficiency	The physical changes that impact boiling on the surface of the fuel pin including change in nucleation sites and change in heat transfer from the clad to the coolant
CRUD Induced Change in Flow Area	The reduction in the coolant flow area that results as crud builds up, the channel.

Table 1 (continued). Phenomenology considered in the for the CIPS Challenge Problem related to Thermal-Hydraulics

Phenomenon	Description
CRUD Induced Change in Friction Pressure Drop	The increase in pressure drop resulting from an increase in surface roughness resulting from crud deposition on fuel rods.
Change in Thermal Hydraulic Equation of State due to Change in Chemical Concentrations	The equation of state for the coolant is affected by dissolved species, particularly in the liquid to gas transition regime. This phenomenon is believed to be most pronounced near the surface of the clad and within the pores and chimneys of the CRUD.
Change in Local Heat Flux to the Coolant from the Fuel due to CRUD Buildup	The CRUD buildup changes the heat flux to the coolant because of different heat transfer efficiency
Heat Flux Distribution in CRUD	For thicker CRUD deposits, the heat flux must be distributed between convection, forced convection, and evaporation.

Table 2. Phenomenology considered for the CIPS Challenge Problem related to Fuel Modeling

Phenomenon	Description
Local Changes in Rod Power due to Burn-Up	As the operating cycle progresses, fuel is burned non-uniformly and a distribution of power in the rods is observed
Fuel Thermal Conductivity Changes as a Function of Burn-Up	As the operating cycle progresses, fuel burn-up results in differing isotopes and species in the fuel as well as cracking that results in changes in the fuel thermal conductivity
Changes in Effective CRUD Conductivity due to Internal Fluid Flow and Boiling	As the CRUD deposits fluid moves through the solidifying CRUD and boiling is likely to occur. This results in porosity and reduced heat transfer through the CRUD.
CRUD Removal due to Transient Power Changes. Mechanical Effects of Rod Contraction when Rod is Cooler	Differential thermal expansion between the clad and CRUD result in mechanical stresses when the system temperature changes. With sufficient change in temperature, the CRUD can fracture and dislodge from the clad surface
Fission Product Gas	As the operating cycle progresses, certain gaseous fission products are produced or form gasses that build up and pressurize the fuel rod
Pellet Swelling	During the operating cycle, the fuel pellets tend to swell from the accumulation of fission gas at grain boundaries in the fuel pellets
Contact Between the pellet and the clad	The fuel pellets can contact the clad material either through eccentricity in the pellet position or thorough swelling of the pellet or both

Table 3. Phenomenology considered for the CIPS Challenge Problem related to Neutronics

Phenomenon	Description
Local Boron Density Increases Absorption	As Boron accumulates in the CRUD, the neutron absorption tends to locally increase
Moderator Displaced by CRUD and Replaced with an Absorber	As the CRUD deposits and builds up on the surface of the clad, a volume of coolant is displaced. Since the coolant serves as a moderator and the CRUD products tend to absorb neutrons there is a reinforcing effect in reducing local reactivity
Xenon impact on Steady State and Transients	The fission product gasses include Xe-135, which has a very large neutron cross section that has a large impact on reactivity. Its 9.2-hour half-life results in potential impacts during slow transients when it can buildup and decay.
Geometry Changes due to Swelling, Cracks, Redistribution, Sintering, and Gaps	As the operating cycle progresses, the fuel pellets certainly change geometrically through movement, cracking, and swelling. These geometric changes may directly impact the reactivity or impact fuel temperatures, which indirectly impact reactivity.
Cross section changes	Cross sections used in the neutrons simulations are dependent upon the local temperatures, which change during operation. The changes in nuclide compositions, must also be considered
Fission product production	Fission products associated with fuel burn-up impact the neutronics calculations
Fission product decay constants	As fission products decay, the various daughter products impact the reactivity differently. These decay reactions are generally approximated with mathematical decay relationships and the accuracy of the decay constants may impact the accuracy of the neutronics calculation.
Simplified decay chains	Fission product decay chains are often simplified to exclude less important daughter products to reduce computation resource requirements. This may introduce some level of inaccuracy.
Boron Induced shift in Neutron Spectrum	Boron, as an absorber, preferentially absorbs thermal neutrons thereby removing them from the overall neutron population and thus impacting the overall energy spectrum of the neutron population
Boron Depletion due to Exposure to Neutron Flux in the coolant	As boron-10 in the coolant absorbs neutrons it become unstable and decays into helium and lithium. As a result, the overall isotopic fraction of boron-10 in the coolant is reduced resulting in lower neutron absorption for a given boron concentration.
Boron Depletion due to Exposure to Neutron Flux in the CRUD	As boron-10 in the CRUD absorbs neutrons it become unstable and decays into helium and lithium. This reduces the available boron-10 for neutron absorption.
Fuel Depletion Calculations being done at a Different Resolution than Neutron Flux Calculation	Fuel depletion calculations are done independently of the neutronics calculations and this may introduce inaccuracy.
Boron concentration in the bulk coolant is computed from a Boron search in neutronics not a conservation of boron mass equation in the thermal-hydraulics	For neutronics calculations, Boron concentration is typically calculated independent of any CRUD chemistry or thermal-hydraulics considerations. This may introduce error for the CRUD problem since significant Boron is adsorbed in the CRUD.
Iron and Nickel Neutron Absorption	While the neutron cross section for Iron and Nickel are much lower than Boron, the relative amount of Iron and Nickel are much greater than Boron.

Table 4. Phenomenology considered for the CIPS Challenge Problem related to Chemistry

Phenomenon	Description
Local changes (near the rod) in the equation of state due to higher concentrations of Nickel, Iron, and Boron	In the presumably ion-rich coolant near the clad, the equation of state for the coolant should be different for the bulk coolant with lower ion concentration. This will naturally have a large effect on predictions of phase transition.
Most of the chemical reaction rates are based on lower temperature and pressures	Much of the laboratory data available to calibrate chemical reaction kinetics models is obtained at temperature and pressure much lower than for PWR conditions. This may introduce error in chemistry predictions.
Defining the list of elements and reactions assumes that other reactions not include have a small impact	CRUD chemistry is complex and not well understood and there may be error associated with excluding certain species or reactions from the modeling of CRUD chemistry.
CRUD Porosity	The CRUD is known to contain some porosity and the simulation should be able to capture this.
CRUD Permeability	The CRUD porosity has certain interconnectivity and the permeability of the CRUD affects the transport of coolant and ions in and out of the CRUD.
CRUD Chimney Density	CRUD is assumed to form with “chimneys” that penetrate through the CRUD layer to the cladding. The spatial density of these chimneys will influence transport in and out of the CRUD.
Water pH effect on Steam Generator Corrosion	The pH of the reactor coolant will impact the electrochemistry of the metallic components in the reactor thus impacting the ion concentration in the coolant.
Water pH effect on CRUD Deposition	The coolant pH will influence the precipitation of the various ions into solid phases and thus the initiation of CRUD.
Boron Exchange in and out of the CRUD	Boron ions in the CRUD may exchange with Boron ions in the coolant

4.1.2 CIPS PIRT Results

The CIPS PIRT results presented represent two specific PIRT exercises: a preliminary or Mini-PIRT conducted in 2014 and a Mini-PIRT update conducted in 2017. Neither the preliminary PIRT nor the update should be considered exhaustive and this acknowledged as a current shortcoming of the V&V assessment. Given increased priority and resources in the future or for any new CPs undertaken, a more comprehensive PIRT should be conducted.

The PIRT update conducted for the CIPS CP was executed in two phases. First, the phenomena identified from the previous Mini-PIRT for CIPS were organized into a survey and this survey was made available electronically to CIPS experts within CASL. It is worth noting that the survey included the ability to suggest additional phenomena for consideration. The electronic survey was completed by several CASL researchers and this is documented below in Table 5. Once the PIRT survey results were obtained, an approximately two-hour phone call was arranged to discuss the results of the survey and to work through items that had significant disagreement among the survey responses. This proved relatively efficient since items where participants were already well converged could be passed by quickly and most of time spent on items with greater disagreement.

Table 5. CIPS PIRT Survey Participants

Date Completed	CASL Researcher	Institution
3/16/2017	Kenny Epperson	Epperson Engineering
3/20/2017	Bob Salko	ORNL
3/20/2017	Jeff Secker	Westinghouse
3/20/2017	Dave Kropaczek	NCSU
3/20/2017	Jack Galloway	LANL
3/21/2017	Annalisa Manera	University of Michigan

The CIPS PIRT update phone call was conducted on March 21, 2017 and included the following CASL researchers:

- Christopher Jones
- Jeff Secker
- Tom Downar
- Analisa Manera
- Jim Wolf
- Jess Gehin
- Dave Kropaczeck
- Ben Collins
- Bob Salko

A graphical example of the PIRT Update Results can for the CIPS CP is shown in Figure 4. The responses for each participant are plotted in Cartesian space with importance and knowledge values quantified numerically from zero to three with a higher number corresponding to a higher ranking for either importance or knowledge thus creating an ordered pair. For example, the ordered pair for a phenomenon with high importance and high knowledge would be (3.0, 3.0). The average value for importance and knowledge from all survey responses is also presented. The results from the Mini-PIRT and the update are presented below in Table 6 through Table 9.

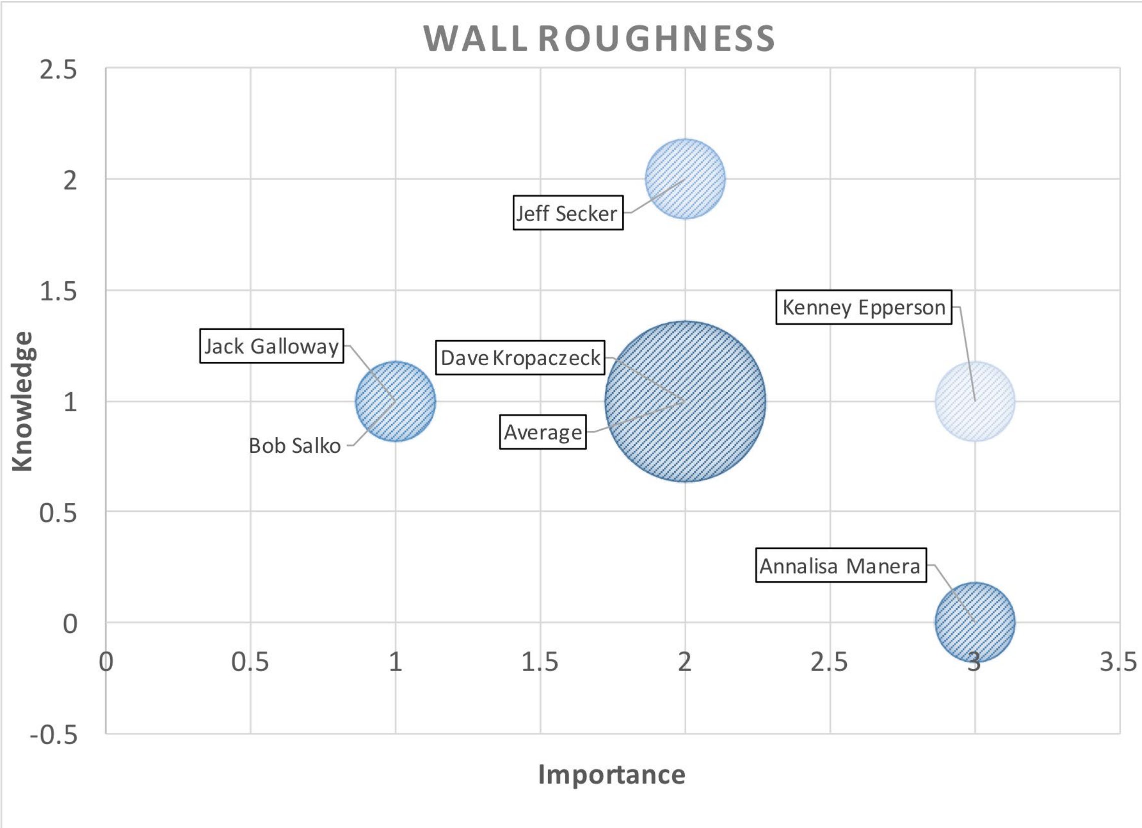

Figure 4. Graphical presentation of CIPS PIRT update results for the phenomenon 'Wall Roughness'

Table 6 documents the CIPS PIRT Survey results for importance and knowledge and reproduces the importance levels obtained from the 2014 mini-PIRT.

Table 6. PIRT results (Averaged Responses for all participants) for phenomena related to thermal-hydraulics

Phenomenon	Importance	Knowledge	Importance	Knowledge
	PIRT Update (2017)		Mini-PIRT (2014)	
Steaming Rate	3.0	2.0	3.0	2.0
Subcooled Boiling on a clean metal surface	3.0	3.0	3.0	3.0
Subcooled Boiling In CRUD	3.0	1.0	3.0	1.0
Bulk Coolant Temperature	3.0	3.0	2.0	2.0
Heat Flux	3.0	2.2	3.0	3.0
Wall Roughness	2.0	1.0	1.0	1.0
Single Phase Heat Transfer	2.0	2.5	1.0	2.0
Mass Balance of Nickel and Iron	3.0	1.8	3.0	1.0
Boron Mass Balance	2.5	2.6	1.0	3.0
CRUD Erosion	2.2	1.3	3.0	1.0
Initial CRUD Thickness (Mass)	2.5	2.0	3.0	1.0
Initial Coolant Nickel and Boron Concentration	2.7	2.3	3.0	1.0
CRUD Source Term from Steam Generators and other Surfaces	3.0	1.7	3.0	1.0
CRUD Induced Change in Boiling Efficiency:	2.7	1.3	1.0	2.0
CRUD Induced Change in Flow Area	0.7	1.4	1.0	2.0
CRUD Induced Change in Friction Pressure Drop	1.0	1.6	1.0	1.0
Change in Thermal Hydraulic Equation of State due to Chemistry	1.8	1.3	1.0	1.0
Change in Local Heat Flux to the Coolant from the Fuel due to CRUD Buildup	1.7	1.5	3.0	1.0
Heat Flux Distribution (new phenomenon)	3.0	1.0	-	-

Table 7. PIRT results (Averaged Responses for all participants) for phenomena related to fuels modeling

Phenomenon	Importance	Knowledge	Importance	Knowledge
	PIRT Update (2017)		Mini-PIRT (2014)	
Local Changes in Rod Power due to Burn-Up	2.0	2.2	3.0	2.0
Fuel Thermal Conductivity Changes as a Function of Burn-Up	1.5	1.8	3.0	2.0
Changes in Effective CRUD Conductivity due to Internal Fluid Flow and Boiling	2.0	1.0	3.0	2.0
CRUD Removal due to Transient Power Changes.	2.0	1.0	3.0	2.0
Fission Product Gas	1.0	1.3	1.0	2.0
Pellet Swelling	1.0	1.3	3.0	2.0
Contact Between the pellet and the clad	1.0	1.3	3.0	2.0

Table 8. PIRT results (Averaged Responses for all participants) for phenomena related to neutronics

Phenomenon	Importance	Knowledge	Importance	Knowledge
	PIRT Update (2017)		Mini-PIRT (2014)	
Local Boron Density Increases Absorption	2.5	2.8	3.0	3.0
Moderator Displaced by CRUD and Replaced with an Absorber	1.6	2.0	1.0	3.0
Xenon impact on Steady State Transients	1.0	1.8	3.0	3.0
Geometry Changes in the Pellet	0.5	1.3	1.0	2.0
Cross section changes	2.7	2.7	3.0	2.0
Fission product production	1.3	1.7	2.0	2.0
Fission product decay constants	1.3	1.7	3.0	3.0
Simplified decay chains	1.0	1.0	2.0	2.0
Boron Induced shift in Neutron Spectrum	1.5	2.0	2.0	2.0
Boron Depletion due to Exposure to Neutron Flux in the coolant	2.0	2.2	1.0	1.0
Boron Depletion due to Exposure to Neutron Flux in the CRUD	3.0	2.0	1.0	1.0
Fuel Depletion and Neutron Flux Calculation Resolution Disparity	1.0	1.8	1.0	1.0
Boron concentration Computation method	0.8	1.6	1.0	1.0
Iron and Nickel Neutron Absorption (New Phenomena)	2.0	3.0	-	-

Table 9. PIRT Results (Averaged Responses for all participants) for phenomena related to chemistry

Phenomenon	Importance	Knowledge	Importance	Knowledge
	PIRT Update (2017)		Mini-PIRT (2014)	
Local changes (near the rod) in the equation of state	2.4	1.3	3.0	3.0
Chemical reaction rates are based on lower temperature and pressures	2.0	1.3	2.0	2.0
Overlooked Chemical Reactions/Species	1.8	1.0	3.0	2.0
CRUD Porosity	2.8	1.8	2.0	2.0
CRUD Permeability	2.0	1.5	2.0	2.0
CRUD Chimney Density	2.6	1.6	2.0	1.0
Water pH effect on Steam Generator Corrosion	2.8	1.3	2.0	2.0
Water pH effect on CRUD Deposition	2.3	1.5	2.0	2.0
Boron exchange in and out of the CRUD (New Phenomenon)	3.0	1.0	-	-

4.2 Mapping physical phenomena requirements to code capability

Capability of VERA code to provide adequate treatment of key phenomena identified in CIPS PIRT is summarized in the Table 10. The level H-M-L is provided to reflect a tentative evaluation of the capability. Specifically, H refers to capability that has high maturity for accurate predicting the phenomenon while L corresponds to maturity for prediction. For a few items capability exists both in BISON and CTF. Depending on the nature of a particular CIPS analysis, it may be appropriate to use one code or another (e.g., balancing speed with fidelity).

Table 10. Mapping CIPS challenge problem requirements to VERA codes

Physics	Phenomena	MPACT	BISON	CTF	MAMBA
Sub channel thermal hydraulics	Steaming Rate			H	
	Subcooled Boiling on a clean metal surface			H	
	Subcooled Boiling In CRUD			L	
	Bulk Coolant Temperature			H	
	Heat Flux			H	
	Wall Roughness			L	
	Single Phase Heat Transfer			H	
	Mass Balance of Nickel and Iron			L	
	CRUD Erosion			M	M
	Initial CRUD Thickness (Mass)	L			L
	Initial Coolant Boron Concentration	H			
	Initial Coolant Nickel Concentration			L	L
	CRUD Source Term from Steam Generators and other Surfaces				M
	CRUD Induced Change in Boiling Efficiency:			L	
	Heat Flux Distribution (new phenomenon) CRUD-fluid heat transfer model			M	M
Fuel modeling	Local Changes in Rod Power due to Burn-Up	H	H		
	Fuel Thermal Conductivity Changes as a Function of Burn-Up		H		
	Changes in Effective CRUD Conductivity due to Internal Fluid Flow and Boiling				H
	CRUD Removal due to Transient Power Changes.		L		
Neutronics	Local Boron Density Increases Absorption	H			
	Moderator Displaced by CRUD and Replaced with an Absorber	H			
	Cross section changes	M			
	Boron Induced shift in Neutron Spectrum	H			
	Boron Depletion due to Exposure to Neutron Flux in the coolant	M			
	Boron Depletion due to Exposure to Neutron Flux in the CRUD				L
	Iron and Nickel Neutron Absorption (New Phenomena)	M			

Table 10 (Continued). Mapping CIPS challenge problem requirements to VERA codes

Physics	Phenomena	MPACT	BISON	CTF	MAMBA
Coolant chemistry	Local changes (near the rod) in the equation of state				M
	Temperature dependent chemical reaction rates				M
	CRUD Porosity				M
	CRUD Permeability				M
	CRUD Chimney Density				L
	Water pH effect on Steam Generator Corrosion				L
	Water pH effect on CRUD Deposition				M

Table 11 summarizes PIRT-identified phenomena and material properties of importance for CIPS prediction by eliminating unimportant items (e.g., those with PIRT importance scores < 2.0). The column "VERA Capability" shows a simplified evaluation of VERA code capability to address the respective phenomena based on the authors understanding of the PIRT discussions and the authors' perception of the VERA capability. This assessment is necessarily subjective and is representative of the authors' views and perception but should be discussed with other CASL researchers. The "gap" column describes the gap between the phenomenological importance for CIPS and the perceived VERA capability. This gap is "quantified" as the scalar difference between the importance and the capability with results greater than zero indicating a gap and larger numbers indicating a larger gap. Finally, the Gap "Description" column provides specificity on the nature of the perceived shortcoming. Note that this evaluation is tentative and open to review and update by subject matter experts, particularly VERA application engineers and challenge problem integrators.

Table 11. Phenomena of importance for CIPS challenge problem

Physics	Phenomena	Importance for CIPS	VERA capability	Gap	Gap Description
Sub channel thermal hydraulics	Steaming Rate	3.0	3.0		
	Subcooled Boiling on a clean metal surface	3.0	3.0		
	Subcooled Boiling In CRUD	3.0	1.0	2.0	Lack of SET data under reactor prototypic CRUD
	Bulk Coolant Temperature	3.0	3.0		
	Heat Flux	3.0	3.0		
	Wall Roughness	2.0	1.0	1.0	Lack of SET data under reactor prototypic CRUD
	Single Phase Heat Transfer	2.0	3.0		
	Mass Balance of Nickel and Iron	3.0	1.0	2.0	Uncertainty in using this input from other analysis
	Boron Mass Balance	2.5	1.0	1.5	
	CRUD Erosion	2.2	1.0	1.2	Lack of SET data under reactor prototypic conditions to assess the effect
	Initial CRUD Thickness (Mass)	2.5	1.0	1.5	Uncertainty in using this input from other analysis
	Initial Coolant Nickel and Boron Concentration	2.7	1.0	1.7	Uncertainty in using this input from other analysis
	CRUD Source Term from Steam Generators and other Surfaces	3.0	0.0	3.0	Lack of this capability in subchannel code
	CRUD Induced Change in Boiling Efficiency:	2.7	1.0	1.7	Lack of SET data under reactor prototypic conditions to assess the effect
	Heat Flux Distribution (new phenomenon)	3.0	2.0	1.0	Lack of SET data to assess the effect of geometry (spacer grids, mixing vanes)
Fuel modeling	Local Changes in Rod Power due to Burn-Up	2.0	3.0		
	Fuel Thermal Conductivity Changes as a Function of Burn-Up	1.5	3.0		
	Changes in Effective CRUD Conductivity due to Internal Fluid Flow and Boiling	2.0	1.0	1.0	Limited to conditions of WALT experiments

Table 11 (continued). Phenomena of importance for CIPS challenge problem

Physics	Phenomena	Importance for CIPS	VERA capability	Gap	Gap Description
Neutronics	Local Boron Density Increases Absorption	2.5	3.0		
	Moderator Displaced by CRUD and Replaced with an Absorber	1.6	2.0		
	Cross section changes	2.7	3.0		
	Boron Induced shift in Neutron Spectrum	1.5	2.0		
	Boron Depletion due to Exposure to Neutron Flux in the coolant	2.0	2.0		
	Boron Depletion due to Exposure to Neutron Flux in the CRUD	3.0	2.0		
	Iron and Nickel Neutron Absorption (New Phenomena)	2.0	2.0		
Coolant chemistry	Local changes (near the rod) in the equation of state	2.4	1.0	1.4	Need to include equation of state and properties for metastable state
	Chemical reaction rates are based on lower temperature and pressures	2.0	1.0	1.0	Uncertainty in using data in extrapolation regime
	CRUD Porosity	2.8	1.0	1.8	Lack of SET data under reactor prototypic conditions to assess the effect
	CRUD Permeability	2.0	1.0	1.0	Lack of SET data under reactor prototypic conditions to assess the effect
	CRUD Chimney Density	2.6	1.0	1.6	Lack of SET data to assess the effect

4.3 Discussion and Gap Identification

Certain phenomenology gaps are identified in Table 12 and for reader convenience are repeated below in Table 13. Qualitatively, the phenomenological gaps for the CIPS problem lie in the thermal-hydraulics and CRUD modeling areas.

Table 12.VERA Gaps for CIPS predictions

Physics	Phenomena	Importance for CIPS	VERA capability	Gap	Gap Description
Sub channel thermal hydraulics	Subcooled Boiling In CRUD	3.0	1.0	2.0	Lack of SET data under reactor prototypic CRUD
	Wall Roughness	2.0	1.0	1.0	Lack of SET data under reactor prototypic CRUD
	Mass Balance of Nickel and Iron	3.0	1.0	2.0	Uncertainty in using this input from other analysis
	CRUD Erosion	2.2	1.0	1.2	Lack of SET data under reactor prototypic conditions to assess the effect
	Initial CRUD Thickness (Mass)	2.5	1.0	1.5	Uncertainty in using this input from other analysis
	Initial Coolant Nickel and Boron Concentration	2.7	1.0	1.7	Uncertainty in using this input from other analysis
	CRUD Source Term from Steam Generators and other Surfaces	3.0	0.0	3.0	Lack of this capability in subchannel code
	CRUD Induced Change in Boiling Efficiency:	2.7	1.0	1.7	Lack of SET data under reactor prototypic conditions to assess the effect
	Heat Flux Distribution (new phenomenon)	3.0	2.0	1.0	Lack of SET data to assess the effect of geometry (spacer grids, mixing vanes)
	Changes in Effective CRUD Conductivity due to Internal Fluid Flow and Boiling	2.0	1.0	1.0	Limited to conditions of WALT experiments
	Local changes (near the rod) in the equation of state	2.4	1.0	1.4	Need to include equation of state and properties for metastable state
Coolant chemistry	Chemical reaction rates are based on lower temperature and pressures	2.0	1.0	1.0	Uncertainty in using data in extrapolation regime
	CRUD Porosity	2.8	1.0	1.8	Lack of SET data under reactor prototypic conditions to assess the effect
	CRUD Permeability	2.0	1.0	1.0	Lack of SET data under reactor prototypic conditions to assess the effect
	CRUD Chimney Density	2.6	1.0	1.6	Lack of SET data to assess the effect

4.4 V&V Requirements

The code requirements for CIPS are defined as the union of the aggregated PIRT phenomena (above,) and the CIPS Implementation Plan [17, 19] requirements. In other words**,** the requirements for CIPS are the ability to model the physical phenomena in Table 6 through Table 9 and the additional requirements from [17, 19]. A summary of the requirements in [17, 19] is provided below. It is worth noting that these requirements do not include many important practical requirements such as operating system, hardware configuration, memory constraints, communication interfaces, etc. Currently this is beyond the scope of this more physics-based assessment, but a more complete list of software requirements should include these practical aspects in addition to the more capability driven ones presented here.

CIPS: CRUD-Induced Power Shift V&V Plan (from the CIPS implementation plan)

(1). Capability assessment

- a) Benchmarking MAMBA against Westinghouse Advanced Loop Testing (WALT) loop data (updated dataset).
- b) A quarter core calculation with coupled MPACT/CTF/MAMBA for a Cycle 1 or Cycle 2 core (none of those cores would have had CIPS)
- c) VERA CIPS analysis to reload cores that had CIPS
  - Callaway Cycle 4 or Seabrook Cycle 5 (requires VERA models starting in Cycle 1)

(2). Code-to-code comparison

- a) Compare results to plant behavior, BOA 3.1 standalone

(3). Improvements/developments needed to reduce (major) uncertainty

- a) Develop corrosion product mass balance model.
  - Ongoing corrosion rates and corrosion release rates for Inconel Steam Generators and stainless steel piping, internals
  - Function of material, age, temperature, coolant pH, zinc addition history
  - Non-boiling deposition on core, ex-core surfaces
- b) Requires CRUD restart file capabilities and CRUD shuffling capability

4.5 V&V activities and evidence collection and evaluation

V&V evidence is distilled from various CASL documents and organized according to the index system as in the Appendix where low level evidence (LLE) corresponds to detailed, narrow statements or activities while high level evidence (HLE) refers to global or top-down activities or statements. These various pieces of evidence have varying degrees of significance to the PCMM level descriptors in Figure 3. Evidence is thus classified by their relevance to PCMM attributes and level of significance (L-Low, M- Medium, H-High). Note that this evidence classification is different than the evidence levels discussed in Section 3. Table 13 summarizes this evidence. Finally, the overall evaluation of the PCMM score is based on how well the evidence matches the descriptors in Figure 3. Since the original V&V activity was not portrayed in a system that would lend itself in PCMM attributes, the classification necessarily involves subjective approach, but the process is traceable and open for review, dispute, and update.

Table 13. V&V evidence for CIPS challenge problem

PCMM attribute	Significance H	Significance M	Significance L	Gap/ Overall Evaluation
RGF: Representation and Geometric Fidelity	MP.1.3. 2 MP.2.3. 1 MP.2.3. 2 MP.3.2. 2 MA.1.3. 8 MA.1.3. 9 CT.2.3. 2 CT.2.3. 3 VE.1.3. 10 VE.1.3. 11	MP.3.3. 1 MP.3.3. 3 MP.3.3. 4 MP.3.3. 5 MP.3.3. 6 MP.3.3. 7 MP.3.3. 9 MP.3.3. 10 CT.2.2. 2 VE.1.3. 1 VE.1.3. 2 VE.1.3. 3		Marginal [1.5]

Table 13 (continued). V&V evidence for CIPS challenge problem

PCMM attribute	Significance H	Significance M		Significance L	Gap/ Overall Evaluation
PMMF: Physics and Material Model Fidelity	MA.1.3. 2 MP.2.3. 3 MP.2.3. 4 VE.1.3. 1 VE.1.3. 2 VE.1.3. 3	MP.3.3. 1 MP.3.3. 3 MP.3.3. 4 MP.3.3. 5	MP.3.3. 6 MP.3.3. 7 MP.3.3. 9 MP.3.3. 10		Marginal [1.5]
SQA: Software Quality Assurance (including documentation)	MA.1.3. 2 MP.1.1. 3 CT.1.1. 1 MA.1.3. 1	MP.1.1. 2 MP.1.1. 4 CT.1.2. 1 CT.1.2. 2 CT.1.3. 1	CT.1.3. 2 CT.1.3. 5 CT.1.3. 6 CT.1.3. 7	MP.1.1. 1 MP.1.2. 1 MP.1.2. 2 MP.1.3. 1 MP.1.3. 2	CT.1.1. 2 MA.1.1. 1 MA.1.1. 2 Marginal [1.5] (MAMBA)
CVER: Code Verification	MP.1.2. 2 MP.2.3. 4 MP.1.3. 3 MP.1.3. 4 MP.1.2. 3 CT.1.2. 3 CT.1.3. 8 CT.1.3. 10 CT.1.3. 12	MP.1.3. 1 MP.1.3. 2 CT.1.3. 3			MP.2.2. 2 CT.1.1. 3 CT.1.2. 3 MA.1.1. 3 VE.1.3. 4 Need improvement [1]

	MA.1.3. 2 MA.1.3. 4 MA.1.3. 5			
SVER: Solution Verification	MP.2.1. 1 MP.2.1. 4 MP.2.3. 5 CT.1.1. 4 CT.1.2. 4 CT.1.3. 9 CT.1.3. 11 MA.1.3. 3 MA.1.3. 5	MP.2.1. 2 MP.2.1. 3 MP.2.3. 3 MP.2.3. 4 CT.1.3. 4	MP.2.2. 1 MP.2.3. 1 MP.2.3. 2 MP.3.2. 4	MP.2.2. 2 CT.1.2. 4 MA.1.1. 4 MA.1.2. 1 VE.1.3. 4 Need improvement [1]
SVAL: Separate Effects Validation	MP.3.1. 1 BI.2.3. 5	MP.2.3. 1 MP.3.1. 3 CT.2.2. 1	MP.3.2. 1 MP.3.2. 4 MP.3.3. 1 MP.3.3. 7 MP.3.3. 8 MP.3.3. 9 MP.3.3. 10	MP.3.1. 4 CT.2.1. 1 MA.1.1. 5 Need improvement [1] (MAMBA)
IVAL: Integral Effects Validation	MP.3.1. 1 MA.1.2. 2 MA.1.2. 3 MA.1.2. 4 VE.1.1. 2 VE.1.2. 1 VE.1.2. 2 BI.2.3. 5	MP.3.1. 2 MP.3.1. 3 CT.2.1. 2	MP.3.2. 2 MP.3.2. 3 MP.3.3. 3 MP.3.3. 4 MP.3.3. 5 MP.3.3. 6 CT.2.2. 2 MA.1.3. 6 MA.1.3. 7	MP.3.1. 4 MA.1.1. 5 CT.2.3. 1 Marginal [1.5]
UQSA: Uncertainty Quantification & Sensitivity Analysis			VE.1.3. 5 VE.1.3. 6 VE.1.3. 7 VE.1.3. 8 VE.1.3. 9	None [0]

4.6 CIPS PCMM Assessment

The PCMM assessment for CIPS challenge problem is given in Table 14 below. It is noted that

- MPACT offers capability to perform reactor core neutronic analysis. MPACT software quality is high. The MPACT V&V plan is a 70-page document. It includes about 10 pages of discussion software quality, code verification with the method of manufactured solutions, and solution verification. The validation covers separate effects testing with criticality experiments and integral effects testing that include matching calculations with from operating nuclear power plants. Much of the CASL V&V plan for this code has already been implemented.

- CTF is a "legacy" sub-channel thermal-hydraulics code, based on two-fluid model and hence inherited both software development practice of the 1980s, and limitations of the ill-posed two-phase flow models. Significant efforts were made by the CTF users community and by CASL PHI focus area researcher to improve software quality of CTF, and its theory and V&V manuals. Nonetheless, code verification and solution verification remain limited. On the other hand, there is a significant validation database available including separate and integral effects testing from a variety of experimental facilities.

- MAMBA is a CRUD chemistry code, which has been under development and currently under restructuring. While the code offers unique capability for modeling of complex processes in CRUD chemistry, the original software development was not performed under the same SQA standards as other CASL codes. The restructuring is bringing MAMBA into alignment with other CASL software development practices.

- VERA as an integrated code for code coupling has been introduced recently. The documentation of VERA and its testing is available only in a very high level, making it difficult to evaluate. This is an area that needs attention in the future work.

Table 14. PCMM scoring for CIPS challenge problem

PCMM attribute	MPACT	CTF	MAMBA
Representation and Geometric Fidelity	3	2	2
Physics and Material Model Fidelity	3	2	1.5
Software Quality Assurance	2	2	1
Code Verification	2	2	1
Solution Verification	2	2	1.5
Separate Effects Validation	2	1	0
Integral Effects Validation	2	2	1
Uncertainty Quantification	0	0	0

Verification for CIPS is a challenge. Certain geometry is fixed at a single control volume like a channel for CTF. However, for solution verification only sensitivity information from the temporal discretization and spatial discretization are needed. Therefore, by perturbing input quantities and measuring the impact on the CIPS quantities of interest (QoIs) and thus generate insight into the sensitivity and subsequently the error associated with discretization. This study also needs to consider convergence criteria.

A major challenge in V&V of VERA for CIPS lies in deficiency of validation data, both in quantity and quality required for assessing complex models in thermal-hydraulics (subcooled boiling), CRUD chemistry and their interactions. It is understood that obtaining the separate effects validation data at reactor prototypic conditions may be impossible.

MAMBA has restructured on a modern platform (used to support development and assessment of MPACT) that is expected to address weaknesses in software engineering and software quality assurance identified in the previous PCMM assessment. SQA aside, attention should be paid on code verification, solution verification and validation of MAMBA. Documentation for MAMBA, both theory manual and V&V manual are needed. The lack of credibility for MAMBA represents the single largest deficiency for VERA-CS overall.

The code coupling between MPACT, CTF, and MAMBA needs to be documented in detail, including the variables that are passed, with what units, and how are they used on either side. It is very important to document the assumptions in the code coupling, like steady-state or incompressible fluid. The coupled code documentation needs to address the iterations and the convergence criteria.

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5 PELLET-CLAD INTERACTION

As mentioned previously, the PCI CP seeks seek to model the thermomechanical interaction of fuel pellets with cladding that occurs during reactor operation. The end goal of the PCI CP is an evaluation of cladding integrity in response to mechanical and thermal loading. While logically straightforward, this problem has several non-linear feedback mechanisms that make prediction challenging. Principally these challenges lie in the nonlinear constitutive behavior of the ceramic fuel itself inclusive of swelling, viscoelasticity / plasticity, fracture and chemical interactions with the cladding.

5.1 PCI PIRT

The stepwise conceptual description for the PCI CP begins with the computation of a neutron flux that produces energy from fission (deposited in the fuel). This heat energy is then conducted radially out from the center of the fuel, across the gap and through the clad. The fuel swells with burn-up and the gap shrinks as fission products accumulate in the crystal structure of the ceramic fuel. As the fuel decays, fission gasses are released and the pressure within the fuel rod rise, thus stressing the clad. Additionally, the contact of the pellet and the clad induces a local contact force. The heat is removed at the surface of the clad by the coolant and is advected to the Balance-of-Plant. After the heat transfer from the fuel to the coolant, there is as safety-related interest in describing the mechanical behavior of the clad to give insight into possible clad failure.

There are two primary quantities of interest for characterizing potential clad failure:

- Spatially varying maximum cladding stress
- Spatially varying material capacity (failure threshold)

These two QoIs can be thought of as probability distributions in space. If the two QoIs can accurately be computed, then predicted failure will be defined as the intersection of the two distributions. Stated differently, for predictions where the maximum cladding stress exceeds the predicted minimum available material capacity, then the cladding will fail.

5.1.1 Phenomena Considered

The phenomena considered for the PCI CP are presented in Table 15 through Table 19 below. Along with each phenomenon, a short description is included to facilitate understanding. Additionally, the phenomena are grouped, for convenience, into four physics areas: Thermal-Hydraulics, Fuel Behavior, Neutronics, and Chemistry.

Table 15. Phenomenology considered in the for the PCI Challenge Problem related to Thermal-Hydraulics

Phenomenon	Description
Heat Transfer Boundary Condition	How the code handles transferring heat from the clad surface to the coolant
Coolant Temperature	The temperature of the bulk coolant. Note that there is non-negligible distribution of the coolant temperature from the surface of the clad to the center of the sub-channel.
Boiling	Though not typically present in PWRs, as the heat flux from the clad increases boiling can occur in some instances
Clad Temperature	Interpreted as the temperature of the surface of the clad in contact with the coolant
Flow Induced Vibration	As the coolant passes over spacer grids and mixing vanes, turbulent flow causes vibration in the fuel rods
Azimuthal Variation in Temperature	Spatial variation in temperature is most pronounced circumferentially around the fuel rod, particularly just downstream of the spacer grids / mixing vanes

Table 16. Phenomenology considered in the for the PCI Challenge Problem related to Fuel Modeling

Phenomenon	Description
Prior Irradiation Time	Since the isotopic composition of the fuel changes with irradiation, the previous irradiation may impact constitutive behavior
Power Maneuvers	Ramping power usually for load following
Cladding Creep	Time dependent deformation of the cladding in response to a constant applied load
Pellet Cracking	Fracture of the Urania fuel usually due to fission gas buildup in the crystal structure of the Urania
Pellet Swelling	Positive volume change in the Urania fuel resulting from fission gas buildup in the crystal structure
Pellet Densification	As the Urania pellets are formed from Urania powder, there is a reduction in void fraction and a corresponding increase in bulk density
Operating History (Power Profile)	The time varying power level experienced by the fuel rods. This includes power maneuvers and normal startup and shutdown.
Fission Gas Release (Internal Pressure in the Fuel Rod)	Fission gas produced by the fuel propagates to the surface of the pellet and is captured in the clad. There is an associated pressure rise associated with this gas buildup.

Table 17. Phenomenology considered in the for the PCI Challenge Problem related to Fuel Modeling (Continued)

Phenomenon	Description
Gap Model	The multiple phenomena associated with modeling heat transfer, closure, and mechanical contact across and between the fuel pellet and the clad
Pellet Thermal Expansion Caused by Power Increase	Thermal expansion of the fuel pellet associated with increased temperature caused by increased power
Thermal Creep in the Pellet and Clad	Time dependent deformation of the fuel or clad in response to a constant applied load at elevated temperature
Friction Between Pellet and Clad	Resistance to translation between the pellet and clad when the two are in contact
Chemical Interactions in the Clad	Certain fission products interact with the cladding material. These interactions may result in secondary phenomena such as stress-corrosion cracking.
Microstructure Impacts on Stress Driven Cracking	The cladding crystal texture may be relatively more susceptible to cracking owing to synergistic chemical effects
Corrosion	Zirconium is generally very corrosion resistant, however in certain situations such as the presence of fission gases, clad corrosion may be non-negligible
Hydrides	Zirconium and hydrogen can combine to form Zirconium Hydride
Material Properties for Time Varying Heterogeneous Fuel Pellet	The constitutive properties of the fuel vary with irradiation time and the subsequent decay of daughter products
Thermal Expansion	Simple thermal expansion of the fuel and clad
Thermal Conductivity	Heat conduction of the fuel components including fuel, gap, and cladding

Table 18. Phenomenology considered in the for the PCI Challenge Problem related to Neutronics

Phenomenon	Description
Energy Deposition (Fission Rate as a Function of Space and Time)	The spatially and temporally varying rate of energy deposition which directly relates to heat in the fuel
Fast Flux (As a Function of Space and Time)	The spatially and temporally varying distribution of fast flux neutrons from fission
Gamma Heating	Temperature rise in the reactor associate with gamma interaction Typically most significant in the non-fueled areas
Isotopics Impact on Fuel Performance Model	Fission products from the reaction of Urania influence the overall core behavior through secondary reactions and additional neutrons
Xenon Impact on Local Power Transients Impacts Stress	Xenon plays a unique role in absorbing neutrons thus slowing the reaction rate but is also associated with stress corrosion cracking
Change in Pellet and Clad Geometry	Fuel pellets can relocate during operation and fuel rods are known to “bow” slightly in response to thermal expansion. This geometric rearrangement effects reactivity.

Table 19. Phenomenology considered in the for the PCI Challenge Problem related to Chemistry

Phenomenon	Description
Water Clad Corrosion Rate	The rate of corrosion in the cladding in the aqueous coolant environment. This is affected by pH and general chemistry
Fuel Pellet Chemistry	Certain chemical species interact with the Zircaloy cladding in a deleterious fashion. The fuel chemistry can therefore impact clad performance.

5.1.2 PCI PIRT Results

The PCI PIRT results presented represent two specific PIRT exercises: a preliminary or Mini-PIRT conducted in 2014 and a Mini-PIRT update conducted in 2017. Neither the preliminary PIRT nor the update should be considered exhaustive and this acknowledged as a current shortcoming of the V&V assessment. Given increased priority and resources in the future or for any new CPs undertaken, a more comprehensive PIRT should be conducted.

The PIRT update conducted for the PCI CP was executed in two phases. First, the phenomena identified from the previous Mini-PIRT for PCI were organized into a survey and this survey was made available electronically to CIPS experts within CASL. It is worth noting that the survey included the ability to suggest additional phenomena for consideration. The electronic survey was completed by several CASL researchers and this is documented below in Table 20. Once the PIRT survey results were obtained, an approximately two-hour phone call was arranged to discuss the results of the survey and to work through items that had significant disagreement among the survey responses. This proved relatively efficient since items where participants were already well converged could be passed by quickly and most of time spent on items with greater disagreement.

Table 20. PCI PIRT Survey Participants

Date Completed	CASL Researcher	Institution
3/16/2017	Jason Hales	Idaho National Laboratory
3/21/2017	Tom Downar	University of Michigan
3/21/2017	Shane Stimpson	ORNL
3/21/2017	Dave Kropaczek	NCSU
3/21/2017	Joe Rashid	ANATECH-SI
3/22/2017	Kevin Clarno	ORNL

The CIPS PIRT update phone call was conducted on March 22, 2017 and included the following CASL researchers:

- Christopher Jones
- Paul Kersting
- Shane Stimpson

- Jim Wolf
- Kevin Clarno
- Joe Rashid
- Eric Mader
- Bob Salko
- Tom Downar
- Dave Kropaczeck

A graphical example of the PIRT Update Results can for the PCI CP is shown in Figure 5. The responses for each participant are plotted in Cartesian space with importance and knowledge values quantified numerically from zero to three with a higher number corresponding to a higher ranking for either importance or knowledge thus creating an ordered pair. For example, the ordered pair for a phenomenon with high importance and high knowledge would be (3.0, 3.0). The average value for importance and knowledge from all survey responses is also presented.

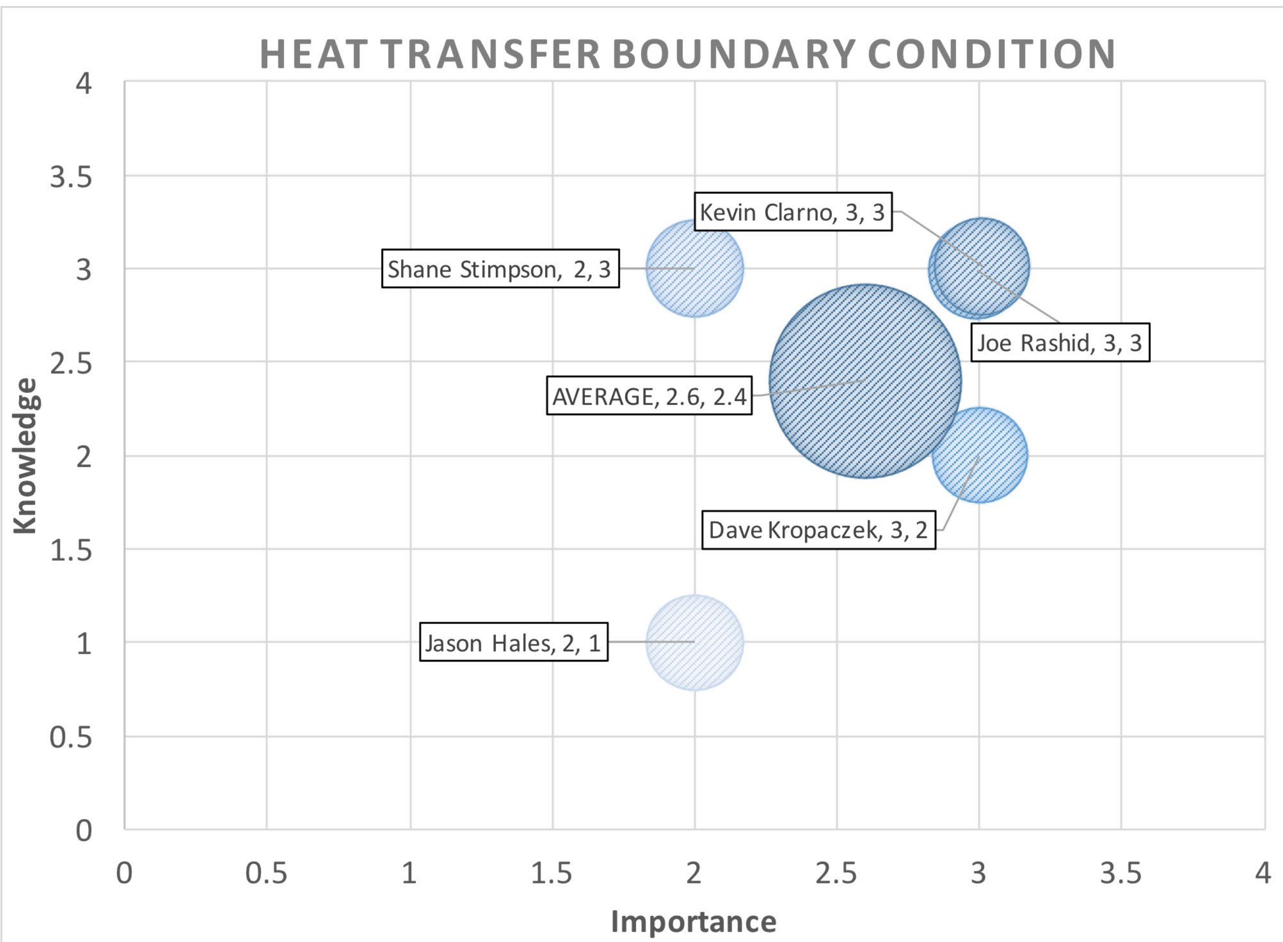

Figure 5. Graphical presentation of PCI PIRT update results for the phenomenon Heat Transfer Boundary Condition'

Table 21 below documents the PCI PIRT Survey results for importance and knowledge and reproduces the importance levels obtained from the 2014 mini-PIRT.

Table 21. PCI PIRT results (Averaged Responses for all participants) including the 2017 PIRT Update and the 2014 Mini-PIRT

Phenomena	Importance	Knowledge	Importance	Knowledge
	PIRT Update (2017)		Mini-PIRT (2014)	
Heat Transfer Boundary Condition	2.6	2.4	3.0	2.0
Coolant Temperature	2.6	2.8	3.0	2.0
Boiling	1.8	1.8	1.0	2.0
Clad Temperature	3.0	2.4	3.0	2.0
Flow Induced Vibration	0.6	1.2	1.0	1.0
Azimuthal Variation in Temperature	1.6	2.0	2.0	2.0
Prior Irradiation Time	2.7	2.5	3.0	3.0
Power Maneuvers	3.0	2.5	3.0	3.0
Cladding Creep	2.8	2.2	3.0	2.0
Pellet Cracking	2.8	2.0	3.0	2.0
Pellet Swelling	2.8	2.6	3.0	2.0
Pellet Densification	2.4	2.6	3.0	2.0
Operating History (Power Profile)	2.5	2.8	3.0	3.0
Fission Gas Release (Internal Pressure in the Fuel Rod)	2.2	1.8	3.0	2.0
Gap Model	2.5	2.0	3.0	2.0
Pellet Thermal Expansion Caused by Power Increase	3.0	2.4	3.0	3.0
Thermal Creep in the Pellet and Clad	2.6	2.0	3.0	2.0
Friction Between Pellet and Clad	2.6	1.8	2.0	2.0
Chemical Interactions in the Clad	2.4	1.8	2.0	2.0
Microstructure Impacts on Stress Driven Cracking	2.4	1.2	3.0	1.0
Corrosion	2.0	1.8	1.0	2.0
Hydrides	1.8	1.4	1.0	1.0
Material Properties for Time Varying Heterogeneous Fuel Pellet	2.4	2.2	2.0	2.0
Thermal Expansion	2.8	2.8	2.0	2.0
Thermal Conductivity	2.5	2.3	2.0	2.0
Energy Deposition (Fission Rate as a Function of Space and Time)	2.2	2.3	3.0	3.0

Table 21 (continued). PCI PIRT results (Averaged Responses for all participants) including the 2017 PIRT Update and the 2014 Mini-PIRT

Phenomena	Importance	Knowledge	Importance	Knowledge
	PIRT Update (2017)		Mini-PIRT (2014)	
Fast Flux (As a Function of Space and Time)	2.0	2.3	3.0	3.0
Gamma Heating	1.0	1.7	2.0	2.0
Isotopics Impact on Fuel Performance Model	1.2	2.3	2.0	2.0
Xenon Impact on Local Power Transients Impacts Stress	2.7	2.0	2.0	2.0
Change in Pellet and Clad Geometry	1.5	1.7	1.0	1.0
Water Clad Corrosion Rate (Current Model Empirical Future Model Lower Length Scale)	1.4	1.6	2.0	2.0
Fuel Pellet Chemistry (Current Model Empirical Future Model Lower Length Scale)	1.8	1.6	3.0	2.0

5.2 Mapping to code capability

Capability of VERA code to provide adequate treatment of key phenomena identified in PCI PIRT is summarized in Table 22 below. The level H-M-L is provided to reflect an evaluation of the adequacy of the capability and is based on the authors' understanding of the PCI CP and informal conversation with code owners, focus area leads, and other CASL researchers. Specifically, H refers to capability that has high maturity for accurate predicting the phenomenon while L corresponds to maturity for prediction. For a few of the fuel rod related requirements, capability for modeling was identified in both BISON and in CTF. The decision to utilize the functionality in one code or the other may be made based on balancing runtime efficiency with fidelity.

Table 22. Mapping PCI challenge problem requirements to VERA capabilities

Physics	Phenomena	MPACT	BISON	CTF
Sub channel thermal hydraulics	Heat Transfer Boundary Condition			H
	Coolant Temperature			H
	Boiling			M
	Clad Temperature			H
Fuel modeling	Prior Irradiation Time		H	
	Power Maneuvers		H	
	Cladding Creep		L	
	Pellet Cracking		L	
	Pellet Swelling		L	
	Pellet Densification		L	
	Operating History (Power Profile)		H	
	Fission Gas Release (Internal Pressure in the Fuel Rod)		M	
	Gap Model		M	
	Pellet Thermal Expansion Caused by Power Increase		H	
	Thermal Creep in the Pellet and Clad		L	
	Friction Between Pellet and Clad		L	
	Chemical Interactions in the Clad		M	
	Microstructure Impacts on Stress Driven Cracking		L	
	Corrosion		M	
	Material Properties for Time Varying Heterogeneous Fuel Pellet		L	
	Thermal Expansion		H	
	Thermal Conductivity		H	
Neutronics	Energy Deposition (Fission Rate as a Function of Space and Time)	H		
	Fast Flux (As a Function of Space and Time)	H		
	Xenon Impact on Local Power Transients Impacts Stress	M		

5.3 Phenomena Importance and Code Capabilities

Table 23 summarizes PIRT-identified phenomena and material properties of importance for PCI prediction by eliminating unimportant items (e.g., those with PIRT importance scores < 2.0). The column "VERA Capability" shows a simplified evaluation of VERA code capability to address the respective phenomena based on the authors understanding of the PIRT discussions and the authors' perception of the VERA capability. This assessment is necessarily subjective and is representative of the authors' views and perception but should be discussed with other CASL researchers. The "gap" column describes the gap between the phenomenological importance for

PCI and the perceived VERA capability. This gap is "quantified" as the scalar difference between the importance and the capability with results greater than zero indicating a gap and larger numbers indicating a larger gap. Finally, the Gap "Description" column provides specificity on the nature of the perceived shortcoming. Note that this evaluation is tentative and open to review and update by subject matter experts, particularly VERA application engineers and challenge problem integrators.

Table 23. Phenomena of importance for the PCI CP

Physics	Phenomena	Importance for PCI	VERA capability	Gap	Gap Description
Sub channel thermal hydraulics	Heat Transfer Boundary Condition	2.6	3.0		
	Coolant Temperature	2.6	3.0		
	Boiling	1.8	2.0		
Fuel modeling	Clad Temperature	3.0	3.0		
	Prior Irradiation Time	2.7	3.0		
	Power Maneuvers	3.0	3.0		
	Cladding Creep	2.8	1.0	1.8	Lack of SET data to assess the effect
	Pellet Cracking	2.8	1.0	1.8	Lack of SET data to assess the effect
	Pellet Swelling	2.8	1.0	1.8	Lack of SET data to assess the effect
	Pellet Densification	2.4	1.0	1.4	Lack of SET data to assess the effect
	Operating History (Power Profile)	2.5	3.0		
	Fission Gas Release (Internal Pressure in the Fuel Rod)	2.2	2.0		
	Gap Model	2.5	2.0	0.5	Lack of SET data to assess the model's components
	Pellet Thermal Expansion Caused by Power Increase	3.0	3.0		
	Thermal Creep in the Pellet and Clad	2.6	1.0	1.6	Lack of SET data to assess the effect
	Friction Between Pellet and Clad	2.6	1.0	1.6	Lack of SET data to assess the effect
	Chemical Interactions in the Clad	2.4	2.0		
	Microstructure Impacts on Stress Driven Cracking	2.4	1.0	1.4	Lack of SET data to assess the effect
	Corrosion	2.0	2.0		
	Material Properties for Time Varying Heterogeneous Fuel Pellet	2.4	1.0	1.4	High uncertainty in data
	Thermal Expansion	2.8	3.0		
	Thermal Conductivity	2.5	3.0		
Neutronics	Energy Deposition (Fission Rate as a Function of Space and Time)	2.2	3.0		
	Fast Flux (As a Function of Space and Time)	2.0	3.0		
	Xenon Impact on Local Power Transients Impacts Stress	2.7			

5.4 Discussion and Gap Identificaiton

Certain phenomenology gaps are identified in Table 24 and for reader convenience are repeated below inTable 36. Qualitatively, the phenomenological gaps for the CIPS problem lie in the fuel rod and thermal-hydraulics modeling areas.

Table 24. Phenomenological Gaps for PCI

Physics	Phenomena	Importance for PCI	VERA capability	Gap	Gap Description
Fuel Modeling	Cladding Creep	2.8	1.0	1.8	Lack of SET data to assess the effect
	Pellet Cracking	2.8	1.0	1.8	Lack of SET data to assess the effect
	Pellet Swelling	2.8	1.0	1.8	Lack of SET data to assess the effect
	Pellet Densification	2.4	1.0	1.4	Lack of SET data to assess the effect
	Gap Model	2.5	2.0	0.5	Lack of SET data to assess the model's components
	Thermal Creep in the Pellet and Clad	2.6	1.0	1.6	Lack of SET data to assess the effect
	Friction Between Pellet and Clad	2.6	1.0	1.6	Lack of SET data to assess the effect
	Microstructure Impacts on Stress Driven Cracking	2.4	1.0	1.4	Lack of SET data to assess the effect
	Material Properties for Time Varying Heterogeneous Fuel Pellet	2.4	1.0	1.4	High uncertainty in data

For the PCI challenge problem, fuel performance modeling and simulation capability plays a critical role. This capability provided by BISON embodies complex multi-physics on its own right, making it a formidable challenge to verify and validate. The complexity also dictates the modeling be phenomenological (as opposed to mathematical), and this is the main reason for difficulty in both code verification and solution verification.

The BISON verification work has been initiated but both solution and code verification need to be improved. Solution verification work has begun in BISON. This needs to include all quantities of interest for the PCI challenge problem. The verification needs to include spatial discretization and temporal discretization sensitivity studies as well as sensitivity studies for all the Jacobian-free Newton-Krylov (JFNK) solver settings.

The BISON coupling with VERA is an area that needs clarification and verification support. Documentation that defines the coupling is needed with which codes and whether the coupling is one-way or two-way coupling.

The PCI validation plan is structured to address the main physics, thermal mechanical, fission gas, and chemistry. However, separate-effect test (SET) validation is limited in BISON, largely attributed to lack of data. Observations on fuel and material behaviors in irradiated environment are typically limited to post-irradiation examination that exhibits integrated and hence convoluted effects.

A substantial body of work on Integral-Effect Test (IET) validation was performed, including OECD/NEA PCMI benchmarks. A reasonably good comparison between predicted and measured fuel centerline temperature was obtained. It is noted that this centerline temperature is rather conservative that it may hide the compensating effects of various contributing processes. Notably, large uncertainty exists in key models (e.g., relocation, fuel (swelling) and clad creep, frictional contact, gaseous swelling (at high temperature)), leading to large errors in predicted rod diameter. These topics identified through the V&V process are considered in the BISON capability development plan.

5.5 V&V Requirements

The code requirements for PCI are defined as the aggregated PIRT phenomena (above, Table 23). The most current PCI CP Implementation plan does not include any V&V requirements and the phenomenological requirements are substantially similar to those presented in Table 23. Reference [28] discusses a handful of lower-length-scale simulations and hypothesizes that these could be used to inform continuum level modeling for PCI. The authors believe that these type of upscaling techniques are still in the research realm and are excluded from the current description of requirements. As with the other CPs, it is worth noting that these requirements do not include many important practical requirements such as operating system, hardware configuration, memory constraints, communication interfaces, etc. Currently this is beyond the scope of this more physics-based assessment, but a more complete list of software requirements should include these practical aspects in addition to the more capability driven ones presented here.

5.6 V&V activities and evidence collection and evaluation

V&V evidence is distilled from various CASL documents and organized according to the index system as in the Appendix where low level evidence (LLE) corresponds to detailed, narrow statements or activities while high level evidence (HLE) refers to global or top-down activities or statements. These various pieces of evidence have varying degrees of significance to the PCMM level descriptors in Figure 3. Evidence is thus classified by their relevance to PCMM attributes and level of significance (L-Low, M- Medium, H-High). Note that this evidence classification is different than the evidence levels discussed in Section 3. Table 25 summarizes this evidence. Finally, the overall evaluation of the PCMM score is based on how well the evidence matches the descriptors in Figure 3. Since the original V&V activity was not portrayed in a system that would lend itself in PCMM attributes, the classification necessarily involves subjective approach, but the process is traceable and open for review, dispute, and update.

Table 25. V&V evidence for PCI challenge problem

PCMM attribute	Significance H	Significance M	Significance L	Gap/ Overall Evaluation
RGF: Representation and Geometric Fidelity	MP.1.3. 2 MP.2.3. 1 MP.2.3. 2 VE.1.3. 1 VE.1.3. 2 VE.1.3. 3	MP.3.3. 1 MP.3.3. 3 MP.3.3. 4 MP.3.3. 5 CT.2.2. 2 BI.2.3. 1 MP.3.2. 2 MA.1.3. 9 MA.1.3. 8 CT.2.3. 2 CT.2.3. 3 VE.1.3. 10 VE.1.3. 11	MP.3.3. 6 MP.3.3. 7 MP.3.3. 9 MP.3.3. 10	Good [2.5]
PMMF: Physics and Material Model Fidelity	MP.2.3. 3 MP.2.3. 4 VE.1.3. 1 VE.1.3. 2 VE.1.3. 3	MP.3.3. 1 MP.3.3. 3 MP.3.3. 4 MP.3.3. 5 BI.2.3. 1	MP.3.3. 6 MP.3.3. 7 MP.3.3. 9 MP.3.3. 10	Good [2.5]
SQA: Software Quality Assurance (including documentation)	MA.1.3. 1 MA.1.3. 2 MP.1.1. 3 MA.1.2. 3 CT.1.1. 1	MP.1.1. 2 MP.1.1. 4 CT.1.2. 1 CT.1.2. 2 CT.1.3. 1 CT.1.3. 2 CT.1.3. 5 CT.1.3. 6 CT.1.3. 7 BI.1.1. 1 BI.1.1. 2	MP.1.1. 1 MP.1.2. 1 MP.1.2. 2 MP.1.3. 1 MP.1.3. 2 BI.1.2. 1 BI.1.2. 2 BI.1.3. 1	CT.1.1. 2 BI.1.3. 4 Good [2]
CVER: Code Verification	MP.1.2. 2 MP.1.2. 3 MP.2.3. 4 MP.1.3. 3 MP.1.3. 4 CT.1.2. 3 CT.1.3. 8 CT.1.3. 10 CT.1.3. 12 BI.1.1. 3 MA.1.3. 4 MA.1.3. 5	MP.1.3. 1 MP.1.3. 2 CT.1.3. 3 BI.1.3. 2		MP.2.2. 2 CT.1.1. 3 CT.1.2. 3 BI.1.2. 3 VE.1.3. 4 Need improvement [1]

SVER: Solution Verification	MP.2.1. 1 MP.2.1. 4 MP.2.3. 5 CT.1.1. 4 CT.1.2. 4 CT.1.3. 9 CT.1.3. 10 CT.1.3. 11 BI.1.1. 4 MA.1.3. 5	MP.2.1. 2 MP.2.1. 3 MP.2.3. 3 MP.2.3. 4 CT.1.3. 4	MP.2.2. 1 MP.2.3. 1 MP.2.3. 2 MP.3.2. 4 BI.1.2. 4	MP.2.2. 2 CT.1.2. 4 VE.1.3. 4 Need improvement [1]
SVAL: Separate Effects Validation	MP.3.1. 3 BI.2.1. 1 BI.2.3. 1	MP.2.3. 1 MP.3.1. 3 CT.2.2. 1	MP.3.2. 1 MP.3.2. 1 MP.3.3. 1 MP.3.3. 7 MP.3.3. 8 MP.3.3. 9 MP.3.3. 10	MP.3.1. 3 CT.2.1. 1 Marginal [1.5]
IVAL: Integral Effects Validation	MP.3.1. 1 BI.1.3. 3 BI.2.1. 1 BI.2.3. 1 MA.1.3. 1	MP.3.1. 2 MP.3.1. 3 CT.2.1. 2 BI.2.2. 1 BI.2.2. 2	MP.3.2. 2 MP.3.2. 2 MP.3.3. 3 MP.3.3. 3 MP.3.3. 5 MP.3.3. 6 CT.2.2. 2 BI.2.3. 1 MA.1.3. 6 MA.1.3. 7	MP.3.1. 3 BI.2.3. 2 BI.2.3. 3 CT.2.3. 1 Good [2]
UQSA: Uncertainty Quantification & Sensitivity Analysis			BI.2.3. 4 VE.1.3. 5 VE.1.3. 6 VE.1.3. 7 VE.1.3. 8 VE.1.3. 9	None [0]

5.7 PCMM Assessment

PCMM assessment for PCI challenge problem is given in the table below. It is noted that:

- The assessment for MPACT and CTF remains consistent with that for CIPS challenge problem. In fact, the PCI challenge problem requires only a subset of CTF capability for an operating reactor core thermal-hydraulics (compared to a more intricate capability required in the CIPS and DNB challenge problems). Detailed discussion of MPACT and CTF is not repeated here.

- BISON is central to PCI. Built upon MOOSE software development platform, BISON inherits a modern "best practice" in software engineering and software quality assurance. The BISON documentation is adequate.

- Although selected capability of BISON (e.g., fuel rod heat transfer) may also be used in CIPS and DNB challenge problem, the PCI challenge problem requires BISON capability in its fullest (including fuel and cladding thermo-mechanics, fission gas behaviors, and chemistry).

- BISON V&V manual and plan include extensive efforts in validation in the regime of PCI as well as under LOCA and RIA conditions.

- Verification for BISON is non-negligible but could be improved. More efforts in code and solution verification are planned.

Table 26. PCMM scoring for PCI challenge problem

PCMM attribute	MPACT	CTF	BISON
Representation and Geometric Fidelity	3	2	2
Physics and Material Model Fidelity	3	2	2
Software Quality Assurance	2	2	2
Code Verification	2	2	1
Solution Verification	2	2	1
Separate Effects Validation	2	1	1
Integral Effects Validation	2	2	2
Uncertainty Quantification	0	0	0
V&V Manual	Good	Good	Good

6 DEPARTURE FROM NUCLEATE BOILING

DNB as a challenge problem for CASL has been articulated in "DNB Challenge Problem Charter" [25].

DNB is central to safety performance of Light Water Reactors (LWRs). Local clad surface dry-out causes dramatic reduction in heat transfer during transients (e.g., overpower and loss of coolant flow) leading to high cladding temperatures. It is noted that current tools for thermal-hydraulics and DNB analysis do not model detailed flow patterns and mixing downstream of mixing / spacer grids. They use simplified pin models and steady-state developed DNB correlations for analysis of DNB transients, resulting in loss of DNB margin. Power uprates require improved quantification and increased margins for DNB.

There is a single quantity of interest for DNB: Departure from Nucleate Boiling Ratio defined as the ratio of the predicted critical heat flux to the local heat flux. When this ratio drops below unity, DNB is expected.

CASL has developed an improved mixing method downstream of mixing grids using CFD tools for single- and two-phase flow, as well as detailed coupled pin-resolved radiation transport models for application to DNB transients. More broadly, according to the DNB Challenge Problem Charter, the CASL focus on DNB has multiple targets. CASL aims to develop capability to predict DNB utilizing more advanced methods to reduce margin and enhance understanding, and validate tools to available mixing and DNB data. The effort to develop the capability to evaluate impact of spacer grid design features effect on DNB [25].

As mentioned previously, the DNB CP seeks to improve predictive capability for the accident related transition between nucleate or subcooled boiling through the critical heat flux into a regime where heat transfer from the cladding into the coolant is significantly impacted due to the insulating effect of the high fraction of vapor near the clad surface. This CP principally involves CTF and Star CCM+, but also requires MPACT to generate the power and subsequently the heat in the fuel. For a shutdown reactor (SCRAM), only decay heat drives the boiling. A fuel model is needed to describe heat transfer from fuel pellets to the cladding and coolant.

6.1 PIRT

At high level, the prediction of DNB in a reactor core involves neutronics, fuel heat transfer and coolant thermal-hydraulics. The fundamental physics involved in DNB are heat transfer from the clad surface into the coolant and the increasing boiling rate up to and past the critical heat flux. The selection of modeling approach for DNB (sub-channel thermal-hydraulics vs computational fluid dynamics) tremendously affects the quantities of interest for the DNB problem. For sub-channel thermal-hydraulics codes, the boiling is represented using an equation of state that predicts the quality and flow regime of water (film, slug, etc.) as a function of temperature, pressure, and potentially other quantities. For CFD, the boiling is modeled explicitly as discrete bubbles of steam in the bulk liquid coolant. For this approach, a great number of physical quantities are required (that will be identified below).

6.1.1 Phenomenology considered

The phenomenology considered for the DNB CP are identified below in Table 27.

Table 27. Thermal-hydraulic phenomenology considered for the DNB Challenge Problem

Phenomena	**Description**
Nucleation Site Density	The spatial density of the specific bubble nucleation sites on the surface of the heated clad
Bubble Sliding Lift Diameter	The critical bubble diameter when the bubble will begin to slide along the surface of the clad due to buoyancy
Bubble Departure Frequency	The frequency of bubbles releasing from the surface of the clad as a function of time
Average Dry Area	The surface area of the clad that is not wetted by liquid water
Nucleation Site Interaction	Information on how two nearby nucleation sites may impact the bubble production of one another
Wall Heat Transfer	The heat transfer between the clad surface and the coolant
Bubble Induced Turbulence	As bubbles form on the surface of the heated clad the flow characteristics become less laminar and more turbulent
Wall Effects	The several wall effects including roughness and the associated drag and pressure drop
Flow Regime / Local Topology	The characteristics of the flow in the channel: laminar, turbulent, bubbly, slug, etc.
Drag Force	The force acting on a discrete bubble from drag associated with moving through liquid water
Lift Force	The buoyant force acting on a discrete bubble
Turbulence Dispersion Force	The force associated with bubbles interacting with one another and with eddies in the liquid coolant
Wall Lubrication Force	For bubbly flow, gas bubbles tend to move near but slightly away from the clad surface and the wall lubrication force is maintains this small separation
Virtual Mass Force	The component of drag associated with accelerating bubbles
Bubble Transport	The propagation of bubbles through the liquid in the channel
Bubble Breakup and Coalescence	Bubbles can interact with one another and coalesce or can break up into smaller bubbles that do not have sufficient lift force to be transported
Turbulent Mixing	The mixing associated with turbulence, usually near a spacer grid
Crossflow	The directed flow associated with mixing vanes commonly found on spacer grids
Nucleate Boiling	Boling confined to the surface of the clad below the critical heat flux
Two-Phase Flow	A continuum description of phase change associated with boiling; a volume average of liquid and vapor
Pressure Drop	The change in pressure along the length of flow associated with frictional resistance
Natural Circulation	Convection associated with fluid moving from a region of higher density (cooler) to a region of lower density (warmer)
Clad Surface Heat Transfer	The heat transfer between the clad surface and the coolant.

6.1.2 DNB PIRT Results

The table below summarizes a Mini-PIRT for VERA M&S of the reactor core during DNB-limiting accidents. This mini-PIRT considered three aspects for each phenomenon: importance, code adequacy, and data availability. The PIRT update, recently conducted includes the more typical aspects of importance and knowledge.

Table 28. Summary table for DNB Mini-PIRT conducted in 2014

Mini-PIRT for VERA-CS Modeling and Simulation of DNB Predictions (Based on Notes of June 27, 2014 Meeting)												
Summary		**Sum of Input**										
Subcategory	**Phenomenon**	**Importance**				**Code Adequacy**				**Data Availability**		
		H	**M**	**L**	**U**	**H**	**M**	**L**	**U**	**H**	**M**	**L**
Subchannel	Turbulent Mixing	X				X				X		
	Crossflow	X				X					X	
	Nucleate Boiling	X					X			X		
	Two-phase flow	X				X				X		
	Pressure drop		X			X					X	
	Natural circulation		X			X				X		
Fuel Rod	Cladding surface heat transfer	X				X					X	
	Fuel pellet heat transfer	X					X				X	
	Pellet-to-cladding heat transfer	X					X					X
	Cladding heat transfer	X				X					X	
	Fuel rod growth or densification		X				X					X
	Fuel rod bowing		X				X				X	
Neutronics	Power distribution	X				X					X	
	Core power	X				X				X		
	Moderator feedback	X				X					X	
	Doppler feedback	X					X				X	
	Boron transport and feedback		X				X				X	
	Gamma heating		X					X				X
	Depletion	X				X				X		
	Decay heat	X						X			X	
Explanation of Categories	Phenomena identified by PIRT team. Additional phenomena may be added if necessary.	Importance: In this column, rank the importance of the phenomenon to the prediction of DNB in Reactor Core. H = High M = Medium L = Low U = Not Important or Unranked				Code Adequancy: In this column, rank the adequacy of the generation I model implemented in VERA-CS to address each phenomenon. H = High M = Medium L = Low U = No capability or Unranked				Data Availability: In this column, rank the availability of experimental or operational data to support validation and/or calibration of models associated with each phenomenon. H = High M = Medium L = Low		

The recently completed PIRT update was conducted in two parts. First CASL researchers with perceived expertise for the DNB problem were requested to complete a survey that reviewed the previously considered phenomenology but did not provide any previous result. Additionally, an opportunity was provided to identify any missing phenomenology. Once the survey results were received an approximately two-hour teleconference was conducted to review the results of the survey and to discuss any items with particularly large variability in responses. Table 29 lists the CASL researchers that completed the DNB survey.

Table 29. DNB PIRT Survey Participants

Date Completed	CASL Researcher	Institution
3/16/2017	Nam Dinh	NCSU
3/18/2017	Yixing Sung	WEC

The DNB PIRT update phone call was conducted on March 24, 2017 and included the following CASL researchers:

- Christopher Jones
- Nam Dinh
- Yixing Sung
- Emilio Baglietto
- Jim Wolf
- Jess Gehin

Figure 6 shows a graphical representation of the PIRT update survey results. The survey responses for each participant are plotted in Cartesian space with importance and knowledge values quantified numerically from zero to three with a higher number corresponding to a higher ranking for either importance or knowledge thus creating an ordered pair. For example, the ordered pair for a phenomenon with high importance and high knowledge would be (3.0, 3.0). The average value for importance and knowledge from all survey responses is also presented.

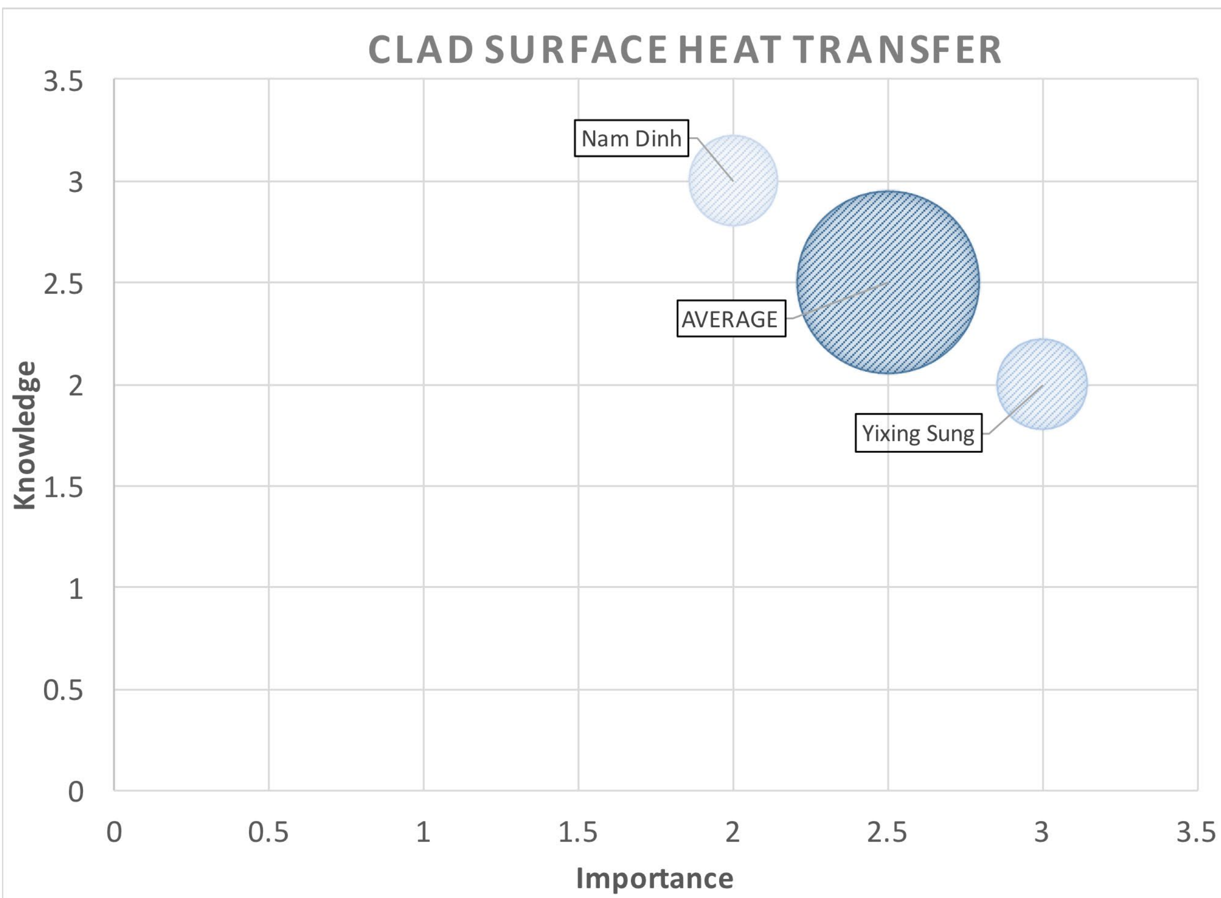

Figure 6. Graphical presentation of DNB PIRT update results for the phenomenon 'Clad Surface Heat Transfer'

Table 30 below documents the DNB PIRT Survey results for importance and knowledge. Since the 2014 mini-PIRT includes different phenomenology, and, as noted above, a different scheme for capturing the knowledge level for each phenomenon, a direct comparison is obscured.

Table 30. DNB PIRT Results (Averaged Responses for all participants)

Phenomena	**Importance**	**Knowledge**
	PIRT Update (2017)	
Nucleation Site Density	3.0	1.0
Bubble Sliding Lift Diameter	2.0	0.5
Bubble Departure Frequency	3.0	1.5
Average Dry Area	3.0	1.0
Nucleation Site Interaction	3.0	1.0
Wall Heat Transfer	3.0	2.0
Bubble Induced Turbulence	2.0	1.5
Wall Effects	3.0	1.0
Flow Regime / Local Topology	3.0	1.0
Drag Force	2.0	1.5
Lift Force	2.0	1.5
Turbulence Dispersion Force	1.5	1.0
Wall Lubrication Force	1.5	1.0
Virtual Mass Force	1.5	1.5
Bubble Transport	2.0	1.5
Bubble Breakup and Coalescence	2.5	1.5
Turbulent Mixing	3.0	2.0
Crossflow	3.0	2.0
Nucleate Boiling	3.0	2.5
Two-Phase Flow	3.0	2.0
Pressure Drop	2.5	2.0
Natural Circulation	1.5	2.5
Clad Surface Heat Transfer	2.5	2.5

6.2 Mapping to code capability

Capability of VERA code to provide adequate treatment of key phenomena identified in DNB PIRT is summarized in the table below. The level H-M-L is provided to reflect a tentative evaluation of the capability. Specifically, H refers to capability that has high maturity for accurate predicting the phenomenon while L corresponds to maturity for prediction.

Table 31. Mapping DNB challenge problem requirements to VERA capabilities

Physics	Phenomena	MPACT	BISON	CTF	Star CCM+
Neutronics	Core power	H			
	Power distribution	H			
	Moderator feedback	H			
	Doppler feedback	H			
	Boron transport and feedback	M			
	Gamma heating	H			
	Depletion	H			
	Decay heat	H			
Fuel rod	Fuel pellet heat transfer		H		
	Pellet-to-cladding heat transfer		H		
	Cladding heat transfer		H		
	Cladding surface heat transfer		M		
	Fuel rod growth or densification		L		
	Fuel rod bowing		L		
Sub channel thermal hydraulics	Turbulent mixing ○ single phase flow ○ two-phase flow			 M L	
	Cross flow			M	
	Nucleate boiling			M	
	Two-phase flow			L	
	Critical Heat Flux			M	
	Natural circulation			M	
	Pressure drop			M	
	Flow regime			M	
CFD (CMFD)	Two-phase dynamics				H
	Turbulent mixing				H
	Bubble-turbulence interactions				M
	Bubble dynamics				M
	Bubble break-up and coalescence				M
	Nucleation site density				M
	Nucleation site interaction				M
	Wall bubble growth				M
	Condensation (subcooled boiling)				M
	Wall Heat Transfer				M
	Surface effects				L
	Microlayer dynamics				L
	Spacer grid, MV effect				M
	Bubble transport				M
	Lift force				M
	Bubble departure frequency				M
	Drag force				M
	Average dry area				L

6.3 Phenomena Importance and Code Capabilities

Table 32 below summarizes PIRT-identified phenomena and material properties of importance for DNB prediction by eliminating unimportant items (e.g., those with PIRT importance scores < 2.0). The column "VERA Capability" shows a simplified evaluation of VERA code capability to address the respective phenomena based on the authors understanding of the PIRT discussions and the authors' perception of the VERA capability. This assessment is necessarily subjective and is representative of the authors' views and perception but should be discussed with other CASL researchers. The "gap" column describes the gap between the phenomenological importance for DNB and the perceived VERA capability. This gap is "quantified" as the scalar difference between the importance and the capability with results greater than zero indicating a gap and larger numbers indicating a larger gap. Finally, the Gap "Description" column provides specificity on the nature of the perceived shortcoming. Note that this evaluation is tentative and open to review and update by subject matter experts, particularly VERA application engineers and challenge problem integrators.

Table 32. Physical quantities and importance ranking thereof, required for DNB

Physics	Phenomena	Importance for DNB CP	VERA Capability	Gap	Gap Description
Neutronics	Core power	3	3	-	
	Power distribution	3	3	-	
	Moderator feedback	3	3	-	
	Doppler feedback	3	3	-	
	Boron transport and feedback	2	2	-	
	Gamma heating	2	3	-	
	Depletion	3	3	-	
	Decay heat	3	3	-	
Fuel rod	Fuel pellet heat transfer	3	3	-	
	Pellet-to-cladding heat transfer	3	3	-	
	Cladding heat transfer	3	3	-	
	Cladding surface heat transfer	2.5	2	1	Surface effect is not represented
	Fuel rod growth or densification	2	1	1	OECD benchmark results show biases
	Fuel rod bowing	2	1	1	Lack of data for assessing bowing
Sub channel thermal hydraulics	Turbulent mixing single phase flow two-phase flow	3 2	2 1	1 1	Lack of data to quantify mixing coefficients in spacer grids and mixing vanes
	Cross flow	3	2	1	Lack of SET data
	Nucleate boiling	3	2	1	Model not capturing surface effect
	Two-phase flow	3	1	2	Lack of data to support transient and transition flow patterns
	Critical Heat Flux	3	2	1	Lacking predictive capability for different surfaces and fuel bundle geometry
	Natural circulation	2	2	-	
	Pressure drop	2	2	-	
	Flow regime	3	2	1	Lack of data to support transient and transition flow patterns

Table 32 (continued). Physical quantities and importance ranking thereof, required for DNB

Physics	Phenomena	Importance for DNB CP	VERA Capability	Gap	Gap Description
CFD (CMFD)	Two-phase dynamics	3	3	-	
	Turbulent mixing	3	3	-	
	Bubble-turbulence interactions	2	2	-	
	Bubble dynamics	2	2	-	
	Bubble break-up and coalescence	2.5	2	0.5	Lack of data at high pressure
	Nucleation site density	3	2	1	Lack of understanding of the effect of surface nanomorphology on nucleation, and inter-site interactions
	Nucleation site interaction	3	2	1	Data only recently emerged. Lack mechanistic understanding
	Wall bubble growth	2	2	-	
	Condensation (subcooled boiling)	2	2	-	
	Wall Heat Transfer	3	2	1	Lack of data for quantifying separate components
	Surface effects	3	1	2	Lack of controlled tests under reactor prototypic conditions
	Microlayer dynamics	3	1	2	Lack of high-fidelity data
	Spacer grid, MV effect	3	2	2	Lack of high-fidelity data
	Bubble transport	2	2	-	
	Lift force	2	2	-	
	Bubble departure frequency	3	2	1	Lack of data in flow boiling particularly subcooled boiling and high pressure
	Drag force	2	2	-	
	Average dry area	3	1	2	Lack of high-fidelity data

6.4 Discussion and Gap Identification

Certain phenomenology gaps are identified in Table 32 and for reader convenience are repeated below in Table 36 through Table 39. Qualitatively, the phenomenological gaps for the DNB problem lie in the fuel rod and thermal-hydraulics modeling areas.

Table 33. Phenomenological Gaps for DNB in VERA

Physics	Phenomena	Importance for DNB CP	VERA Capability	Gap	Gap Description
Fuel Modelling	Cladding surface heat transfer	2.5	2	1	Surface effect is not represented
	Fuel rod growth or densification	2	1	1	OECD benchmark results show biases
	Fuel rod bowing	2	1	1	Lack of data for assessing bowing
Sub channel thermal hydraulics	Turbulent mixing single-phase flow two-phase flow	 3 2	 2 1	 1 1	Lack of data to quantify mixing coefficients in spacer grids and mixing vanes
	Cross flow	3	2	1	Lack of SET data
	Nucleate boiling	3	2	1	Model not capturing surface effect
	Two-phase flow	3	1	2	Lack of data to support transient and transition flow patterns
	Critical Heat Flux	3	2	1	Lacking predictive capability for different surfaces and fuel bundle geometry
CFD (CMFD)	Flow regime	3	2	1	Lack of data to support transient and transition flow patterns
	Bubble break-up and coalescence	2.5	2	0.5	Lack of data at high pressure
	Nucleation site density	3	2	1	Lack of understanding of the effect of surface nanomorphology on nucleation, and inter-site interactions
	Nucleation site interaction	3	2	1	Data only recently emerged. Lack mechanistic understanding
	Wall Heat Transfer	3	2	1	Lack of data for quantifying separate components
	Surface effects	3	1	2	Lack of controlled tests under reactor prototypic conditions
	Microlayer dynamics	3	1	2	Lack of high-fidelity data
	Spacer grid, MV effect	3	2	2	Lack of high-fidelity data
	Bubble departure frequency	3	2	1	Lack of data in flow boiling particularly subcooled boiling and high pressure
	Average dry area	3	1	2	Lack of high-fidelity data

In the CTF-based approach to DNB, the prediction of critical heat fluxes largely depends on steady state, empirical correlations, which are based on measured data in flow boiling experiments in tubes, channels, and rod bundles. It is worth noting that these correlations are not highly relevant for RIA-type DNB events that are associated with a rapid transient, though they are likely conservative. Characteristically, the CHF experiments (and flow boiling experiments in general) are performed on out-of-pile test sections, using deionized, distilled water and stainless steel or copper as heater materials. The experimental conditions thus deviate from reactor prototypic conditions (e.g., using reactor water chemistry, nuclear fuel cladding (e.g., Zircaloy), and irradiated environment), which are known to affect surface nanomorphology, and hence roughness, wettability, and nucleation energy barrier. In general, separate-effect tests (SET) validation is a weaker link in the DNB challenge problem. To date, the validation is more advanced in the single-phase flow regime (including simple and complex flow channel geometries), while limited in the two-phase (boiling) flow regime. The existing datasets have been used for fuel design improvement and DNB prevention, as well as for assessment of sub-channel codes. However, the data quality is not adequate for validating DNB simulations under the plant design conditions, and for calibration and validation of advanced mechanistic DNB and/or two-phase flow CFD models. Areas where additional data are most needed include the effect of rod surface characteristics (e.g., roughness) on DNB, turbulent mixing and void measurements in subcooled flow boiling in rod bundles.

In the CFD-based (STAR-CCM+) approach to DNB, the model involves treatment of many mesoscale physical processes that allow for considering the potential effects of surface characteristics. However, the treatment has so far been ad hoc, due to lack of data on mesoscale processes.

Further effort is needed to validate the capability to evaluate impact of spacer grid design features effect on DNB.

DNB calculations use boundary conditions from system codes and computational fluid dynamics (CFD) codes. Detailed descriptions of these boundary conditions and key assumptions need to be documented.

Sensitivity studies on the axial nodalization need to be done for all DNB QoIs. Where applicable, time step sensitivities should be performed as well. Finally, the sensitivity to iteration convergence criteria needs to be studied.

6.5 V&V Requirements

The code requirements for DNB are defined as the union of the aggregated PIRT phenomena (above, Table 32) and the DNB Validation Plan [21] requirements. In other words, the requirements for DNB are the ability to model the physical phenomena in Table 32 and the additional requirements from [21]. A summary of these requirements is provided below. For DNB the additional requirements relate primarily to validation. It is worth noting that these requirements do not include many important practical requirements such as operating system, hardware configuration, memory constraints, communication interfaces, etc. Currently this is beyond the scope of this more physics-based assessment, but a more complete list of software requirements should include these practical aspects in addition to the more capability driven ones presented here.

Validation of the multiphysics VERA code system will be based on code V&V of MPACT, CTF, BISON and coupled code system using experimental and test data available and accepted by the industry. A good example of the code V&V is the CTF code, which is based on the test data previously used for validating other sub-channel codes such as VIPRE-01. V&V of a coupled multiphysics code system is challenging and may require application of advanced and new VVUQ techniques. Furthermore, there is no plant or data available for code validation, since the plants are currently well protected to avoid any DNB occurrence. Any application specific validation at the present will be based on benchmark and comparison with the existing coupled code system such as the Westinghouse RAVE code system. Such code-to-code benchmarks are incorporated in each VERA application. There are also code benchmark exercises for DNB applications such as the Organization for Economic Cooperation and Development (OECD) Steam Line Break (SLB) and Reactivity Initiated Accident (RIA) code benchmark problems. It is recommended that such benchmark exercise using VERA be considered for CASL test stand development.

Although no actual plant data exists, in-pile measurements and observations of DNB are available, so relevant datasets do exist. These include Integral-Effect Tests (IETs) from the Columbia University test loop, Freon test loops, NUPEC bundle tests, and the ODEN (Westinghouse) loop, and SETs (rod surface roughness tests, MIT; and flow visualization tests, Texas A&M). It is noted that most test data on turbulent mixing and DNB from small scale rod bundles (e.g., 5x5 bundle) simulating actual PWR fuel designs are proprietary to fuel vendors. Important, but limited data on void measurements are available from OECD benchmark programs (BFBT and PSBT).

Specifically, the DNB V&V plan identified:

(1). OECD PSBT Rod Bundle Tests

Test data from the PWR Sub-channel and Bundle Test (PSBT) were made available for thermal-hydraulic modeling and benchmark through the OECD. The mixing and DNB test data for CASL VERA modeling and simulation.

(4). Westinghouse NMV Grid Tests

5x5 rod bundle mixing and Critical Heat Flux (CHF) tests were performed on an Inconel non-mixing vane (NMV) grid design at the Columbia University’s Heat Transfer Research Facility in the 1980’s.

(5). Westinghouse MV Grid Tests

5x5 rod bundle mixing and CHF tests were performed on a mixing vane (MV) grid design at the Columbia University’s Heat Transfer Research Facility in the 1980’s.

(6). RIA Tests for DNB Evaluation

RIA transient tests were performed at the NSRR in Japan. The TK test cases used fueled segments from commercial 17x17 fuel rods taken from the Takahama-3 reactor. A total of seven test segments were used, ranging in burnup levels from 37.8 GWd/MTU to 50 GWd/MTU.

The validation data that is used by industry has been made available to CTF. To that end, the validation of the VERA (non-CFD) version of DNB is on par with the industry standard.

Special effect test data (e.g., rod surface roughness effect) exists, but they are obtained under conditions (e.g., system pressure, surface characteristics) far from the prototypic PWR reactor environment. High quality data are not available for transient DNB because the existing testing facilities are designed for steady state tests.

6.6 V&V activities and evidence collection and evaluation

V&V evidence is distilled from various CASL documents and organized according to the index system as in the Appendix where low level evidence (LLE) corresponds to detailed, narrow statements or activities while high level evidence (HLE) refers to global or top-down activities or statements. These various pieces of evidence have varying degrees of significance to the PCMM level descriptors in Figure 3. Evidence is thus classified by their relevance to PCMM attributes and level of significance (L-Low, M- Medium, H-High). Note that this evidence classification is different than the evidence levels discussed in Section 3. Table 34 summarizes this evidence. Finally the overall evaluation of the PCMM score is based on how well the evidence matches the descriptors in Figure 3. Since the original V&V activity was not portrayed in a system that would lend itself in PCMM attributes, the classification necessarily involves subjective approach, but the process is traceable and open for review, dispute, and update.

Table 34. V&V evidence for DNB challenge problem

PCMM attribute	Significance H	Significance M	Significance L	Gap/ Overall Evaluation
RGF: Representation and Geometric Fidelity	MP.1.3. 2 MP.2.3. 1 MP.2.3. 2	MP.3.3. 1 MP.3.3. 3 MP.3.3. 4 MP.3.3. 5 CT.2.2. 2 MP.3.2. 2 MA.1.3. 7 MA.1.3. 8 CT.2.3. 2 CT.2.3. 3 VE.1.3. 10 VE.1.3. 11	MP.3.3. 6 MP.3.3. 7 MP.3.3. 9 MP.3.3. 10 VE.1.3. 1 VE.1.3. 2 VE.1.3. 3	Good [2.5]
PMMF: Physics and Material Model Fidelity	MP.2.3. 3 MP.2.3. 4	MP.3.3. 1 MP.3.3. 3 MP.3.3. 4 MP.3.3. 5	MP.3.3. 6 MP.3.3. 7 MP.3.3. 9 MP.3.3. 10	Good [2.5]
SQA: Software Quality Assurance (including documentation)	MA.1.3. 2 MA.1.3. 1 MP.1.1. 3 MP.1.2. 3 MA.1.2. 3 CT.1.1. 1	MP.1.1. 2 MP.1.1. 4 CT.1.2. 1 CT.1.2. 2 CT.1.3. 1 CT.1.3. 2 CT.1.3. 5 CT.1.3. 7 ST.1.1. 1 ST.1.1. 2	MP.1.1. 1 MP.1.2. 1 MP.1.2. 2 MP.1.3. 1 MP.1.3. 2 ST.1.2. 2	CT.1.1. 2 Good [2]
CVER: Code Verification	MP.1.2. 2 MP.1.2. 3 MP.2.3. 4 MP.1.3. 3 MP.1.3. 4 CT.1.2. 3 CT.1.3. 10 CT.1.3. 12 MA.1.3. 4 MA.1.3. 5	MP.1.3. 1 MP.1.3. 2 CT.1.3. 3 ST.1.1. 3	ST.1.2. 3	MP.2.2. 2 CT.1.1. 3 CT.1.2. 3 VE.1.3. 4 Need improvement [1]
SVER: Solution Verification	MP.2.1. 1 MP.2.1. 4 MP.2.3. 5 CT.1.1. 4 CT.1.2. 4 CT.1.3. 9 CT.1.3. 11 MA.1.3. 5	MP.2.1. 2 MP.2.1. 3 MP.2.3. 3 MP.2.3. 4 CT.1.3. 4	MP.2.2. 1 MP.2.3. 1 MP.2.3. 2 MP.2.3. 4	MP.2.2. 2 CT.1.2. 4 VE.1.3. 4 Need improvement [1]
SVAL: Separate Effects Validation	MP.3.1. 1 BI.2.3. 5	MP.2.3. 1 MP.3.1. 3 CT.2.2. 1	MP.3.2. 1 MP.3.2. 4 MP.3.3. 1	MP.3.1. 4 CT.2.1. 1 Marginal [1.5]

			MP.3.3. 7 MP.3.3. 8 MP.3.3. 9 MP.3.3. 10	
IVAL: Integral Effects Validation	MP.3.1. 1	MP.3.1.3 CT.2.1. 2	MP.3.2. 2 MP.3.2. 3 MP.3.3. 3 MP.3.3. 4 MP.3.3. 5 MP.3.3. 6 CT.2.2. 2 MA.1.3. 6 MA.1.3. 7	MP.3.1. 4 ST.1.1. 4 ST.1.3. 1 ST.1.3. 2 CT.2.3. 1 Good [2]
UQSA: Uncertainty Quantification & Sensitivity Analysis			ST.1.3. 3 VE.1.3. 6 VE.1.3. 7 VE.1.3. 8 VE.1.3. 9	ST.1.2. 4 None [0]

6.7 PCMM Assessment

PCMM assessment for DNB challenge problem is given in the table below. It is noted that

- The assessment for MPACT remains consistent over CIPS, PCI and DNB. A detailed discussion of MPACT is not repeated here and can be found in the preceding sections.

- CTF is a "legacy" code, based on two-fluid model and hence inherited both software development practice of the 1980s, and limitations of the ill-posed two-phase flow models. Significant efforts were made by the CTF users community and by CASL PHI focus area researcher to improve software quality of CTF, and its theory and V&V manuals. Nonetheless, code verification and solution verification remain limited.

- STAR-CCM+ has an extensive verification and validation base. However, with respect to DNB-related physics (e.g., bubble nucleation, subcooled boiling, bubble-induced turbulence) in particular and two-phase boiling flow in general, the verification and validation are limited. This is reflected in scores for SVER, SVAL, and IVAL

Table 35. PCMM scoring for DNB challenge problem

PCMM attribute	MPACT	CTF	STAR-CCM+
Representation and Geometric Fidelity	3	2	3
Physics and Material Model Fidelity	3	2	2
Software Quality Assurance	2	2	3
Code Verification	2	2	2
Solution Verification	2	2	1
Separate Effects Validation	2	1	1
Integral Effects Validation	2	2	1
Uncertainty Quantification	0	0	0
V&V Manual	Good	Good	Good

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7 DISCUSSION AND OVERALL GAP IDENTIFICATION

The preceding discussion and evaluation of capability and credibility for VERA will be summarized here. Furthermore, the identified gaps will be organized, and for the credibility gaps, prioritized.

7.1 Capability Gaps for VERA

The capability gaps for each CP identified in Table 36, Table 37, Table 38, and Table 39 are reproduced here but are organized by code, including gaps from each CP. Table 36 through Table 39 document the capability gaps for each of the CASL codes. The authors are unable to quantify the impact or cost associated with implementing this capability however the code teams are encouraged to review and discuss these findings and prioritize development according to these gaps.

Table 36. Identified CTF Capability Gaps

Code	Phenomena	Gap Description	Challenge Problem
CTF	Subcooled Boiling In CRUD	Lack of SET data under reactor prototypic CRUD	CIPS
	Wall Roughness	Lack of SET data under reactor prototypic CRUD	
	Mass Balance of Nickel and Iron	Unclear how the calibration of system corrosion and fluid chemistry will be considered	
	CRUD Erosion	Lack of SET data under reactor prototypic conditions to assess the effect	
	Initial Coolant Nickel and Boron Concentration	Uncertainty in using this input from other analysis	
	CRUD Source Term from Steam Generators and other Surfaces	Unclear how the calibration of system corrosion and fluid chemistry will be considered	
	CRUD Induced Change in Boiling Efficiency:	Lack of SET data under reactor prototypic conditions to assess the effect	
	Heat Flux Distribution (new phenomenon)	Hi2Lo calibration of these phenomena not demonstrated for prototypic fuel designs	
	Changes in Effective CRUD Conductivity due to Internal Fluid Flow and Boiling	Limited to conditions of WALT experiments	
	Turbulent mixing single phase flow two-phase flow	Lack of data to quantify mixing coefficients in spacer grids and mixing vanes	DNB
	Cross flow	Lack of SET data; Hi2Lo calibration for non prototypic fuels	
	Nucleate boiling	Model not capturing surface effect	
	Two-phase flow	Lack of data to support transient and transition flow patterns	
	Critical Heat Flux	Lacking predictive capability for different surfaces and fuel bundle geometry	
	Flow regime	Lack of data to support transient and transition flow patterns	

Table 37. Identified Capability Gaps for BISON

Code	Phenomena	Gap Description	Challenge Problem
BISON	Cladding Creep	Lack of SET data to assess the effect	PCI
	Pellet Cracking	Lack of SET data to assess the effect	
	Pellet Swelling	Lack of SET data to assess the effect	
	Pellet Densification	Lack of SET data to assess the effect	
	Gap Model	Lack of SET data to assess the model's components	
	Thermal Creep in the Pellet and Clad	Lack of SET data to assess the effect	
	Friction Between Pellet and Clad	Lack of SET data to assess the effect	
	Microstructure Impacts on Stress Driven Cracking	Lack of SET data to assess the effect	
	Material Properties for Time Varying Heterogeneous Fuel Pellet	High uncertainty in data	
	Cladding surface heat transfer	Surface effect is not represented	DNB
	Fuel rod growth or densification	OECD benchmark results show biases	
	Fuel rod bowing	Lack of data for assessing bowing	

Table 38. Identified Capability Gaps for MAMBA

Code	Phenomena	Gap Description	Challenge Problem
MAMBA	Local changes (near the rod) in the equation of state	Need to include equation of state and properties for metastable state	CIPS
	Chemical reaction rates are based on lower temperature and pressures	Uncertainty in using data in extrapolation regime	
	CRUD Porosity	Lack of SET data under reactor prototypic conditions to assess the effect	
	CRUD Permeability	Lack of SET data under reactor prototypic conditions to assess the effect	
	CRUD Chimney Density	Lack of SET data to assess the effect	

Table 39. Identified Capability Gaps for Star CCM+

Code	Phenomena	Gap Description	Challenge Problem
Star CCM+	Bubble break-up and coalescence	Lack of data at high pressure	DNB
	Nucleation site density	Lack of understanding of the effect of surface nanomorphology on nucleation, and inter-site interactions	
	Nucleation site interaction	Data only recently emerged. Lack mechanistic understanding	
	Wall Heat Transfer	Lack of data for quantifying separate components	
	Surface effects	Lack of controlled tests under reactor prototypic conditions	
	Microlayer dynamics	Lack of high-fidelity data	
	Spacer grid, MV effect	Lack of high-fidelity data	
	Bubble departure frequency	Lack of data in flow boiling particularly subcooled boiling and high pressure	
	Average dry area	Lack of high-fidelity data	

7.2 Credibility Gaps for VERA

PCMM provides a framework for comprehensive, systematic and continuing assessment of V&V activities for CASL VERA with respect to challenge problem's mission and requirements. The addition of SQA/SQE and separation of validation into SET and IET help address specificity of VERA development history and multi-physics/ multi-scale nature of CASL challenge problems.

The PCMM score cards were obtained for three high-priority challenge problems. The numerical results, although relative, provide a basis for constructive discussions (on V&V plan, priority, and resource allocation) between VERA stakeholders, including challenge problem integrators (applications), code development teams, code assessment team, and the CASL leadership.

Several observations can be made from reviewing Table 14, Table 26, and Table 35:

- Uncertainty quantification represents the largest credibility gap and transcends all codes and CPs
- Significant progress has been made with Code and Solution Verification for MPACT and CTF since the previous assessment are underdeveloped for other CASL codes
- MAMBA is significantly less mature than the other CASL codes

The V&V assessment exercise identified the need for a CASL-wide systematic documentation, dissemination and discussion of V&V activities performed in various CASL branches. This knowledge management includes CASL researchers and analysts archiving their V&V-related data from both experiments and simulations for future use and comparison, documenting expert opinions, e.g., on quality of measured data, sources and magnitude of uncertainty, implication of V&V findings for their applications of interest as well as other potential applications.

The VERA V&V plan (updated February 2017 and described in Section 2) describes a comprehensive strategy to address gaps, both in single-physics codes and in coupled code capability. Key activities related to the challenge problems under consideration are summarized in Table 40. Ranging from verification to plant benchmarks (IET), these activities will improve maturity in corresponding PCMM categories. These proposed activities relate primarily to credibility.

Table 40. Currently Planned and in Progress V&V Activities from [62]

Index	VERA V&V planned activities for FY17 and FY18	CP Relevance	PCMM category
MPACT-P1	Develop and implement a plan to improve the overall testing of the ORIGEN API:	CIPS: H DNB: M PCI: H	SQE CVER
MPACT-P2	Update the MPACT V&V manual 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 manual. All results in the MPACT manual should be updated with the new 51-group library using the new automation scripts.	CIPS: H DNB: H PCI: H	SQE CVER
CTF-P1	The CTF V&V manual should be modified with a specific section summarizing the ongoing code verification activities:	CIPS: H DNB: H PCI: M	SQE CVER
BISON-P1	Develop a formal Fuel Temperature Tables V&V document. Include code verification with documentation of existing tests A modest expansion of unit testing and regression testing to include uncertainty analysis of various user input options.	CIPS: H DNB: H PCI: H	SQE CVER
MAMBA-P1	Enforcing source code verification with extensive unit and regression tests during the code development.	CIPS: H DNB: 0 PCI: 0	SQE CVER
MAMBA-P2	Perform all the validation cases with the refactored MAMBA3D	CIPS: H DNB: 0 PCI: 0	SVAL IVAL
MAMBA-P3	Prepare a formal MAMBA3D Verification and Validation document.	CIPS: H DNB: 0 PCI: 0	SQE
TIAMAT-P1	The verification of TIAMAT for the fully coupled BISON/VERA capability	CIPS: H DNB: H PCI: H	CVER
TIAMAT-P2	Formally document all TIAMAT V&V.	CIPS: H DNB: H PCI: H	SQE
VERA-P1	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).	CIPS: H DNB: H PCI: L	RGF PMMF SVER
VERA-P2	Verification work should be performed to quantify errors introduced by mapping CTF-channel solution to pin-based density-temperatures	CIPS: H DNB: H PCI: H	RGF SVER
VERA-P3	Assess the impact that thermal expansion on the verification of the direct MPACT-CTF coupling.	CIPS: H DNB: H PCI: H	PMMF SVER

Table 40 (continued).Currently Planned V&V Activities from [62]

Index	VERA V&V planned activities for FY17 and FY18	CP Relevance	PCMM category
VERA-P5	After the fully coupled, full core capability has been demonstrated with BISON 1.5D and VERA using TIAMAT, all the cases in the VERA validation based should be performed, beginning with the "legacy" cases of Watts Bar and BEAVRS.	CIPS: H DNB: H PCI: H	IVAL
VERA-P6	After the testing is completed on the refactored MAMBA3D and is integrated into VERA, the Watts Bar Unit I core follow cases should be performed and added to the VERA V&V manual.	CIPS: H DNB: H PCI: H	IVAL SQE

8 CONCLUSIONS

An updated V&V assessment for the CASL developed software, VERA, has been conducted and the primary findings can be summarized in a few points:

- Significant gaps in Code and Solution Verification for all three challenge problems have been addressed by the code teams and are documented here.
- Capability gaps still exist for some of the required phenomenology, defined by expert elicitation via the PIRT process, exist for all CPs considered (CIPS, PCI, DNB).
- Maturity as assessed utilizing a modified PCMM framework shows non-uniform maturity across the various maturity attributes. Uncertainty quantification are scored lower for all codes and all challenge problems.
- The assessment approach for both capability and credibility is necessarily evidence based, yet remains a large degree of subjectivity. Accordingly, the response to any identified gaps should begin with reaching consensus between all stakeholders for any gaps.

Having now been updated twice, this document will continue to be a living document that provides a description of the CASL V&V approach and plans for both the CASL codes and for the CASL challenge problems. In general, the main CASL codes CTF, BISON, and MPACT are making good progress in terms of validation work. They are aligned with the challenge problems that they support. MPACT is the most mature of the three, but BISON and CTF are close behind. MAMBA needs additional work to come up to the level of maturity of the other codes that it is coupled to for CIPS however there has been marked improvement from the initial assessment.

There are still issues with the code coupling, and the documentation thereof, that need to be solidified to help focus where validation work should be done. Because this capability is still under development, it cannot be expected to be as mature as the other older code capabilities. However, the coupling is fundamental to all CPs and, therefore, needs to be documented and reviewed.

For the codes contributing to the CASL challenge problems that will include uncertainty quantification—namely CIPS, DNB, and PCI—a higher emphasis is needed on solution verification. Additionally, a higher emphasis on parameter distributions for use in the UQ assessment. Sensitivity analyses should also be pursued with high priority and the results of these studies should be evaluated carefully in the context of the PIRT exercises presented in this document.

The assessment methodology is fundamentally empirically based and clear documentation is critical for this approach. Future assessments will be conducted on a semi-annual basis by reviewing the evidence produced in the previous six months. Ideally these assessments would occur in the middle of each period of record. The results of each assessment will then permit prioritization of effort to eliminate gaps and to improve credibility via PCMM scores. It is recommended that the prioritization of effort should be based on the perceived value (e.g., considering difficulty and payoff), but this approach is difficult for capability gaps since, by definition, all capability is required to address the challenge problems.

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APPENDIX A:

Collection and classification of V&V activity evidence and outcomes

The evidence for the current VERA-CS assessment is identified below in a series of tables and is organized in the order of codes in VERA-CS:

- MPACT (Tables 1-3)
- CTF (Tables 4-5)
- BISON (Tables 6-7)
- STAR-CCM+ (Table 8)
- MAMBA (Table 9)
- VERA-CS (Table 10)

Table A.1. Evidence related to MPACT software quality assurance (SQA) and code verification (CVER)

References: (Rider, 2013) [14]; Downar 2017 [31]; (Downar, 2018) [32]; Kochunas 2019 [33]; Pilch 2019 [35]

Index	Category	Description	Relevance/ Comments
MP.1.1. 1	HLE	Comprehensive MPACT V&V Manual [29-32, 35]	
MP.1.1. 2	HLE	Comprehensive unit tests and regression tests supports SQA of MPACT [31]	
MP.1.1. 3	HLE	Some peer review conducted	Need tracking of issues and resolution
MP.1.1. 4	HLE	Rigorous version control [31] [33]	
MP.1.2. 1	MLE	Unit test for individual functions and subroutines [33]	
MP.1.2. 2	MLE	Regression tests that involves functional tests encompassing different sections of the code with various inputs [31] [32] [33]	
MP.1.2. 3	MLE	IMPACT software test plan, requirement and test report [33]	SQA
MP.1.2. 4	MLE	Work is in progress to implement both the consistency test and MMS test in the MPACT reactor code as part of the code verification and overall quality assessment effort for MPACT [35].	
MP.1.3. 1	LLE	Unit tests for solver kernels test against analytical solutions [31]	Including CVER
MP.1.3. 2	LLE	Key capabilities tested [31]: Geometry Transports solvers: P0 and Pn 2D MOC, P0 and Pn 2D-1D with SP3 and NEM Other solvers: depletion search (boron, rod), multistate, Eq Xe/Sm, XS Shielding, CMFD, Cusping treatment	Including CVER

		Parallel solver: MPI, OpenMPI	
MP.1.3. 3	LLE	Code verification using method of exact solutions. Benchmark problem 3.4 in Ganapol15 has been used as a code verification test for MPACT [35]. MPACT agreed with all cases to within a few pcm [35].	CVER
MP.1.3. 4	LLE	Code verification using Method of Manufactured Solution (MMS) Applied MMS to the C5G7 benchmark problem to verify 2D multigroup neutron transport solver The relative error of the scalar flux of the first energy group is ~1E-8. The relative error of the scalar flux of the thermal energy group is close to ~1E-5. These close-to-zero error indicates that the scalar flux from the fixed-source problem converges to the same solution as from the eigenvalue calculation [35].	CVER

Table A.2. Evidence related to MPACT solution verification (SVER)

References: Downar 2017 [31]; Downar 2018 [32, 63]; Pilch 2019 [35]

Index	Category	Description	Relevance/ Comments
MP.2.1. 1	HLE	Supported by test involving Mesh Convergence analysis and method of manufactured solution [31] [35]	
MP.2.1. 2	HLE	Numerical effects are quantitatively estimated to be small on some SRQ (system response quantities) [31] [35]	
MP.2.1. 3	HLE	I/O independently verified [31]	
MP.2.1. 4	HLE	Some peer review conducted	Need tracking of issues and resolution
MP.2.2. 1	MLE	Mesh convergence analysis-Work is based on evaluation of sensitivity of K-eff to different MOC parameter (Flat source region mesh, angular quadrature, ray spacing) for VERA Benchmark Problems [31]	
MP.2.2. 2	MLE	Method of Manufactured Solution will be used to quantify the rate of convergence of the solution to MOC parameters [29, 32]	Gap
MP.2.3. 1	LLE	Test performed for regular pin cell (VERA-CS Benchmark Problem 1a) and assembly (VERA-CS Benchmark Problem 1a) [31]	
MP.2.3. 2	LLE	Test encompasses radial and azimuthal discretization, ray spacing, angular quadrature, coupling between discretization parameter [31]	
MP.2.3. 3	LLE	MPACT Library Generation Procedure [31]	
MP.2.3. 4	LLE	Testing (and improvement) of the ORIGEN API [31]	

MP.2.3. 5	LLE	Extensive solution verification test performed for 3D assembly geometry and 2D pin geometry [35]	

Table A.3. Evidence related to MPACT Validation, and representation and geometric fidelity (RGF)

References: Downar 2015 [30]; Downar, VERA-CS V&V, 2017[31], Downar 2018 [29, 32]

Index	Category	Description	Relevance/ Comments
MP.3.1. 1	HLE	Quantitative assessment of predictive accuracy for key SRQ from IETs and SETs[29, 32]	
MP.3.1. 2	HLE	MPACT validation is supported by [30] [31] measured data from different criticality tests, operating nuclear power plants, measured isotopes from irradiated fuel, calculation from continuous energy MC simulation Use of post-irradiation examination (PIE) tests for evaluation and validation of the isotopic depletion capability in MPACT.	
MP.3.1. 3	HLE	Demonstrated capability to support challenge problems (CIPS, PCI and DNB)	Table A.3.1
MP.3.1. 4	HLE	Additional validation is required	Gap
MP.3.2. 1	MLE	Criticality tests encompass: critical condition, fuel rod fission rate distribution, control rod burnable poison worth, isothermal temperature coefficient	
MP.3.2. 2	MLE	Operating nuclear power plants: critical soluble boron concentration, BOC physics parameter-control rod worth, temperature coefficient, fission rates	
MP.3.2. 3	MLE	Measured isotopes from post irradiation experiment: gamma scans of 137Cs, burnup based on 148Nd, full radiochemical assay of the major actinides and fission products	
MP.3.2. 4	MLE	Continuous energy Monte Carlo simulation: 3D core pin-by-pin fission rates at operating condition, intra-pin distribution of fission, capture rates, reactivity, pin power distribution, gamma transport, thick radial core support structure effects	
MP.3.3. 1	LLE	Babcock & Wilcox Critical Experiments	The successful validation shows adequate quality in RGF and PMMF

MP.3.3. 2	LLE	Development of preliminary VERA-CS Crud induced localized corrosion modeling capability (milestone: L2:PHI.P17.03) [57]	Representation and geometric fidelity

Table A.3 (Continued). Evidence related to MPACT Validation

References: Downar 2015 [30]; Downar, VERA-CS V&V, 2017[31]; Downar 2018 [29, 32]

Index	Category	Description	Relevance/ Comments
MP.3.3. 3	LLE	Special Power Excursion Reactor Test (SPERT)	
MP.3.3. 4	LLE	DIMPLE Critical Experiments	
MP.3.3. 5	LLE	Watts Bar Nuclear plant. The MPACT validation for the WB2 start-up tests (Godfrey, 2017) [64].	
MP.3.3. 6	LLE	BEAVRS	
MP.3.3. 7	LLE	Validation by Code to Code Comparisons (MCNP)	
MP.3.3. 8	LLE	Reaction Rate Analysis	
MP.3.3. 9	LLE	VERA progression problems 1-4	
MP.3.3. 10	LLE	Extensive PWR pin and assembly benchmark problems	

Table A.3.1. MPACT Validation for Challenge Problems

Challenge Problem	Phenomena	Validation Problem: B&W Critical	DIMPLE Critical	SPERT	Watts Bar	KRSKO	BEAVRS
CIPS, PCI, DNB	Fast flux	x	x	x	x		
CIPS, PCI, DNB	Isotopics				x	x	x
CIPS, PCI, DNB	Gamma heating						
CIPS, PCI, DNB	Fission power	x	x	x	x	x	x
CIPS, PCI, DNB	Fission product yield						
CIPS, PCI, DNB	Cross section data	x	x	x	x	x	x
CIPS, PCI, DNB	Boron feedback to neutronics				x	x	x
CIPS, PCI, DNB	Burn up				x	x	x
CIPS, PCI, DNB LOCA	Decay heat model (retards cool-down)						
RIA	Kinetics data			x			

Table A.4. Evidence related to SQA and verification of CTF

References: Salko et al., 2016[42]; Porter el al., 2017[40]; Salko et. al, 2017[45]; Salko et al., 2019[41]; Pilch et al., 2019[39]; Toptan et. al, 2018 [46]

Index	Category	Description	Relevance/ Comments
CT.1.1. 1	HLE	SQA is based on unit test and regression tests	SQA
CT.1.1. 2	HLE	Documentation of SQA of base code is required.	Gap
CT.1.1. 3	HLE	Code verification work is insufficient	Gap
CT.1.1. 4	HLE	Solution Verification study performed by mesh refinement study	Solution verification
CT.1.2. 1	MLE	Unit tests: tests for different classes/procedures	SQA
CT.1.2. 2	MLE	Regression tests: unit tests, verification problems and validation problem used as regression test	SQA
CT.1.2. 3	MLE	Code Verification: Few models have been verified using analytical solution	Limited CVER
CT.1.2. 4	MLE	Solution Verification by mesh refined study for progression problem 6	Limited SVER
CT.1.3. 1	LLE	(Unit test) Covers input reading, fluid properties, units, etc.	SQA
CT.1.3. 2	LLE	(Regression test) Covers both steady state and transient simulation All V&V test inputs are part of CTF repository PHI continues testing system	SQA
CT.1.3. 3	LLE	Tested phenomena: Single phase wall shear, Grid heat transfer enhancement, Isokinetic advection Shock tube Water faucet	Code verification
CT.1.3. 4	LLE	Test performed with and without spacer grids QoI: Total pressure drop across the assembly	Solution verification
CT.1.3. 5	LLE	Use validation tests as regression tests which are run on a continual basis to demonstrate code results are not changing	SQA
CT.1.3. 6	LLE	Code to code benchmarking with sub channel code, VIPRE-01	SQA
CT.1.3. 7	LLE	Comparison of CTF predicted rod surface temperature with STAR CCM+ predicted rod surface temperature	SQA
CT.1.3. 8	LLE	Details on CTF coverage by code and solution verification is provided in the latest CTF code and solution verification report. There are some gaps in the assessment (Grid shear enhancement, grid heat transfer enhancement is not tested). Convergence behavior and numerical errors needs to be quantified [39]	

CT.1.3. 9	LLE	Solution verification tests conducted [39]. • The first solution verification problem in assembly geometry is a modification of Problem 3 in the CASL's Progression Test Suite (Godfrey[1]) for decoupled codes. • The second solution verification test in assembly geometry is a modification of Problem 6 in the Progression Test Suite, which emphasizes coupled CTF and MPACT calculations using VERA-CS. These solution verification tests represent a nearly complete integration of the physics capabilities in assembly geometry.	
CT.1.3. 10	LLE	Solution and code verification of the wall friction model in CTF[18]	CVER and SVER
CT.1.3. 11	LLE	Solution verification on the governing equations for the water faucet problem [55]	SVER
CT.1.3. 12	LLE	Two phase pressure drop code verification study	CVER

Table A.5. Evidence related to validation, and representation and geometric fidelity of CTF

References: Salko et al., 2016 [42]; Salko et al., 2017 [45]; Salko et al., 2019 [41]

Index	Category	Description	Relevance/ Comments
CT.2.1. 1	HLE	Lack of separate effect test validation	Gap
CT.2.1. 2	HLE	Extensive integral effect validation done	
CT.2.2. 1	MLE	Testing of component models (correlations)	Table A.5.1
CT.2.2. 2	MLE	Integral-effect test validation	Table A.5.2
CT.2.3. 1	LLE	High to low fidelity simulation using STAR CCM+ was used to improve grid heat transfer effect or rod bundle geometry	Accuracy improvement
CT.2.3. 2	LLE	Development of preliminary VERA-CS Crud induced localized corrosion modeling capability (milestone: L2:PHI.P17.03) [57]	Representation and geometric fidelity
CT.2.3. 3	LLE	Improvement in representation and geometric fidelity of CTF was shown by the calibration study using measured plant data (Watts Bar Nuclear Plant) and experimental loop data (Westinghouse Advanced Loop Tester (WALT)) [54].	Representation and geometric fidelity

Table A.5.1. Requirement and testing for normal PWR conditions

References: Salko et al., 2016 [42]

Phenomenon	Model	Validation test status	Verification test status
Single-phase convection	Dittus-Boelter	Completed	--
Subcooled boiling heat transfer	Thom	Completed	--
Single-phase grid spacer pressure loss	Form loss	Completed	--
Single-phase wall shear	Darcy-Weisbach	Completed	Completed
Grid heat transfer enhancement	Yao-Hochreiter-Leech	--	--
Single-phase turbulent mixing	Mixing-length theory	Completed	Completed
Pressure-directed cross flow	Transverse momentum equation	--	--

Table A.5.2. CTF validation

References: Salko et al., 2016 [42]

Integral test validation experiments

Effect	Experiments
Pressure Drop	BFBT, FRIGG, Risø
Void/Quality	PSBT, FRIGG
Single Phase Turbulent Mixing	GE, CE, RPI
Turbulent Mixing/Void Drift	GE, BFBT
DNB	Harwell, Takahama
Heat Transfer	CE
Natural Circulation	PNNL
Fuel Temperature	Halden

Table A.6. Evidence related to SQA and verification of BISON

Reference: Williamson, BISON V & V plan, 2016 [51]; Williamson et al., 2016 [52] ;Hales, 2017[49]; (Update 2018) [50]

Index	Category	Description	Relevance/ Comments
BI.1.1. 1	HLE	Demonstrable SQA/SQE plan in place.	
BI.1.1. 2	HLE	Unit test and regression test are used for SQA	
BI.1.1. 3	HLE	Code verification is high level [52]	
BI.1.1. 4	HLE	Solution verification is of high level [52]	
BI.1.2. 1	MLE	Software quality is tightly controlled using issue tracking, merge requests and collaborative code review (via GitLab).	SQA
BI.1.2. 2	MLE	Recently (Nov 2015) underwent detailed software quality assessment. Deemed NQA-1 compliant for R&D software.	SQA
BI.1.2. 3	MLE	Lacks testing of designed order of accuracy	CVER Gap
BI.1.2. 4	MLE	For LWR fuel rod problem: Temporal and spatial solution verification study performed for all FOM	SVER
BI.1.3. 1	LLE	Employs patch tests to check the FEM implementation	CVER
BI.1.3. 2	LLE	Benchmark tests with other fuel performance codes- FALCON, TRANSURANUS, ENIGMA-B (Assessment of BISON, INL/MIS-13-30314 Rev. 2, September 2015)	CVER
BI.1.3. 3	LLE	Fuel temperature tables have performed well for core follow and provide confidence in the overall fuel temperature used in PWR core follow calculations.	

BI.1.3. 4	LLE	Plan the expansion and documentation of unit testing and regression testing to include an uncertainty analysis of various user input options	Gap

Table A.7. Evidence related to validation of BISON

References: Williamson, BISON V & V plan, 2016 [51]; Hales, 2017[49]; (Update 2018) [50]; Williamson et al., 2016 [52]; Williamson et al , 2019[53]

Index	Category	Description	Relevance/ Comments
BI.2.1. 1	HLE	IET and SET Validation work performed for key physical phenomenon related to CASL quantity of interest [52] [53]	
BI.2.2. 1	MLE	LWR validation (48 Cases):	
BI.2.2. 2	MLE	Validation metrics: ○ Fuel centerline temperature through all phases of fuel life ○ Fission gas release ○ Clad diameter (PCMI)	
BI.2.3. 1	LLE	LWR fuel benchmark: Reasonable prediction of centerline temperature	
BI.2.3. 2	LLE	LWR fuel benchmark: Rod diameter prediction with large errors	Gap
BI.2.3. 3	LLE	LWR fuel benchmark: Large uncertainty in key models ○ Relocation (and recovery) ○ Fuel (swelling) and clad creep ○ Frictional contact ○ Gaseous swelling (at high temperature	Gap (need SVER)
BI.2.3. 4	LLE	L3: FMC.CLAD.P13.04 – Cluster dynamics modeling of Hydride precipitation	UQ (data assessment)
BI.2.3. 5	LLE	SET (Bursting experiments) and IET validation of BISON for LOCA behavior [53] Validation of BISON to integral LWR experiment (IET validation) [52]	SVAL and IVAL

Table A.8. Evidence related to SQA, V&V and UQ of STAR-CCM+

References: Pointer, 2017 [61]

Index	Category	Description	Relevance/ Comments
ST.1.1. 1	HLE	Demonstrable SQA/SQE plan in place.	
ST.1.1. 2	HLE	Standard quality assurance is followed. ○ ISO9001 quality assurance process	
ST.1.1. 3	HLE	Code verification is high level	
ST.1.1. 4	HLE	Some validation work for boiling and DNB	Gap
ST.1.2. 1	MLE	Unit test and regression test used for SQA.	
ST.1.2. 2	MLE	Working to establish commercial grade dedication under US NRC ○ NQA-1 compliant baseline has been established ○ Readiness review successfully completed mid-2016 ○ Non-Conforming Defect process established in late 2016	
ST.1.2. 3	MLE	STAR-Test suite provides automated testing of new features and builds ○ More than 30,000 test cases with baseline data stored in data warehouse for staged automated regression testing. Testing suite currently includes ○ unit tests ○ applications verification tests Subset distributed to customers as customer verification tests for local installation Manual tests Frequently defined as part of project plan for specific feature implementation Sometimes implemented for specific customer needs Includes some MMS order of convergence tests Results recorded in the ALM system Work to maintain coverage of all code classes User verification suite (77 cases in 13 categories)	CVER

Table A.8 (continued). Evidence related to SQA, V&V and UQ of STAR-CCM+

References: Pointer, 2017 [61]

Index	Category	Description	Relevance/ Comments
ST.1.2. 4	MLE	Not sufficiently clear how to make meaningful comparisons of relative uncertainty contributions of: ○ Uncertainty related to grid convergence when GCI is not especially well-defined for necessary meshing and modeling practices ○ Uncertainty related to primary variables ○ Uncertainty related to constitutive and closure model descriptions of secondary variables	UQ Gap
ST.1.3. 1	LLE	DNB-related simulation in Westinghouse 5x5 with mixing vanes ○ Single-Phase ○ Establish Grid Convergence and a reference 1-phase grid (FY17 L1) ○ Evaluate propagation of inlet BC uncertainty (late FY17)	Gap
ST.1.3. 2	LLE	DNB-related simulation in Westinghouse 5x5 with mixing vanes ○ Two-Phase ○ In planning	Gap
ST.1.3. 3	LLE	L3:THM.CLS.P13.01 - Hydrodynamic closure evaluation in multiphase flow using STAR-CCM+ and NEPTUNE	Sensitivity analysis

Table A.9. Evidence related to SQA, V&V and UQ of MAMBA

References: Anderson, 2016 [55]; Downar, VERA CS V&V Plan ,2017; (Kendrick, 2012) [56]; (Anderson, 2016) [55], (Okhyusen, 2018) [59]; (Anderson, 2019) [60]

Index	Category	Description	Relevance/ Comments
MA.1.1. 1	HLE	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.	Gap
MA.1.1. 2	HLE	SQA needs some improvement	Gap
MA.1.1. 3	HLE	Low level code verification performed	Gap
MA.1.1. 4	HLE	Solution verification not done for CASL challenge problems	Gap
MA.1.1. 5	HLE	Some validation work performed (separate-effect, integral-effect tests and plant analysis)	Table A.9.1 Gap

MA.1.2. 1	MLE	Solution Verification and Code Verification using analytical solution are in progress[60]	
MA.1.2. 2	MLE	Simulation of Westinghouse Walt Loop Experiment Cladding temperature vs rod power and crud thickness against the WALT data	Table A.9.2
MA.1.2. 3	MLE	An initial CIPS study compared axial offset predicted by coupled MAMBA/CTF/MPACT with plant data for Watts Bar	Multiple codes
MA.1.2. 4	MLE	Plant analysis: CIPS study by coupled MAMBA(1D)/CTF/MPACT simulations compared with plant data Oxide thickness and morphology compared with an operating plant	Multiple codes
MA.1.3. 1	LLE	SQA: unit testing (water properties) Unit test coverage is good and most of the important routines are tested. The automatic test coverage reported coverage of ~98% Source properties and Steam generator properties are not tested in the assessed version of MAMBA [60]	SQA
MA.1.3. 1	LLE	Comparisons between the model in FACTSAGE and MAMBA [58]	SQA, PMMF
MA.1.3. 2	LLE	Comparison to BOA 3.0 for heat transfer/chimney boiling model, mass evaporation rate vs crud thickness, pin power and thermochemistry.	Quasi-CVER
MA.1.3. 3	LLE	Comparison to MAMBA-BDM to verify cladding temperature and boiling velocity	Quasi-SVER
MA.1.3. 4	LLE	Convergence studies for the main quantities of interest as function of the radial mesh density is completed. Convergence studies with respect to the internal time-step size is completed [60].	
MA.1.3. 5	LLE	Code verification and solution verification tests conducted [60]: • The thermal and mass transport solvers were compared to analytical solutions for a simple diffusion problem (no convection or sinks/sources). • A simplified thermal diffusion problem with a sink term was solved by introducing a few minor code changes and compared to the form of the corresponding analytical solution. • A simplified convection-diffusion problem was implemented by setting reaction rates for internal chemical reactions to zero and choosing the concentrations of Li and B to avoid precipitation of $Li_2B_4O_7$. • The solution to the CRUD growth rate equation was verified by comparison to an analytical solution.	CVER and SVER

MA.1.3. 6	LLE	Inference of CRUD model parameters from plant data [54]	IVAL (partial credit) Calibration study
MA.1.3. 7	LLE	Improvement in MAMABA source term model was achieved by calibration using measured plant data and experimental loop data. The calibration process was able to estimate thermophysical and growth rate parameters in MAMBA given experimental evidence in the form of flux maps and thermocouple measurements. The small-scale WALT loop calibration demonstrated the ability to perform statistical inference of the thermophysical crud parameters present in MAMBA given an experimental data set from a small-scale crud test loop using a Markov Chain Monte Carlo sampler [54].	IVAL (partial credit) Calibration study
MA.1.3. 8	LLE	Improvement in representation and geometric fidelity of MAMABA was shown by the calibration study using measured plant data (Watts Bar Nuclear Plant) and experimental loop data (Westinghouse Advanced Loop Tester (WALT)) [54].	Representation and geometric fidelity
MA.1.3. 9	LLE	Development of preliminary VERA-CS Crud induced localized corrosion modeling capability (milestone: L2:PHI.P17.03) [57]	Representation and geometric fidelity

Table A.9.1. MAMBA Validation

Reference: CASL-I-2012-1121-000

MAMBA 1D/3D models or parameters	Source	Validation
Permeability of crud	Walt loop report	Not beyond Walt loop calibration
Crud porosity	Walt loop report	Not beyond Walt loop calibration
Solid phase thermodynamics	BOA/MULTEQ and/or thermocalc/calphad	BOA/MULTEQ or thermocalc/calphad
Solution phase thermochemistry	BOA/MULTEQ, thermocalc/calphad	Validated in BOA/calphad
Boric acid chemistry	Literature, Mesmer 1972, Byers 2000, Wofford 1998	Validated against Mesmer 1972, Byers 2000, Wofford 1998
Water chemistry	Literature Marshall & Frank 1981 and Ho & Palmer 1998	Validated against Marshall & Frank 1981 and Ho & Palmer 1998
Diffusion coefficients, chemical kinetic rate coefficients, deposition rates	Fitted to Walt loop data	Crud growth
Mass evaporation rate	BOA comparison	BOA comparison
Local radial flow velocity	Boundary condition	Not known
CRUD erosion	Fitted, CFD	Not known
Fuel heat flux	Boundary condition	Not known
Coolant temperature	Boundary condition	Not known
Cladding temperature	Calculated	MAMBA-BDM
Coolant species concentrations/source term	From BOA or the new source term model	BOA validation

Table A.9.2. MAMBA validation using Westinghouse Walt Loop Experiment

Reference: CASL-I-2012-1121-000; [56]

MAMBA 1D/3D models or parameters	Source	Validation
CRUD skeleton thermal diffusivity	Walt loop report	Not beyond Walt loop calibration
CRUD skeleton heat capacity	Walt loop report	Not beyond Walt loop calibration
Crud skeleton density	Walt loop report	Not beyond Walt loop calibration
Coolant (water) thermal conductivity	Literature	Literature
Coolant (water) density	Literature	Literature
Coolant (water) heat capacity	Literature	Literature
Coolant (water) thermophysics (Tsat)	Literature	Literature
Chimney wall surface area	Measured, Walt loop report	Not beyond Walt loop calibration
Chimney density	Measured, Walt loop report	Not beyond Walt loop calibration
Chimney wall heat transfer coefficient	Fitted to Walt loop data	Not beyond Walt loop calibration
Pore fill rate	Fitted to Walt loop data	Not beyond Walt loop calibration

Table A.9.3. MAMBA capability for challenge problems

Reference: Mousseau and Dinh, V&V Plan, June 2016 [15]

Challenge problem	Phenomena	Validation cases				
		Watts Bar	Walt loop	Seabrook	BOA comparison	MAMBA-BDM
CIPS and CILC	Growth/erosion		X	X	X	
CIPS and CILC	Heat transfer		X		X	X
CIPS	Boron uptake	X			X	
CIPS and CILC	Soluble/particulate transport				X	
CIPS and CILC	Crud morphology		X		X	

Table A.10. VERA-CS Verification and Validation

References: (Rider, 2013) [14]; (Pernice, 2013) [16];(Godfrey, 2014) [62, 65]; (VERA,2013) [66]; (Godfrey, 2017) [64]

Index	Category	Description	Relevance/ Comments
VE.1.1. 1	HLE	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.	
VE.1.1. 2	HLE	For every new VERA-CS reactor analyzed, the metrics shown in Table A4.1 was suggested as an initial proposal (Palmtag, 2016) [36].	Table A.10.1 For CIPS
VE.1.2. 1	MLE	Specific attention / analysis would be expected for any plants/cycles/measurements that fall outside of these metrics. (VE.1.1.2)	
VE.1.2. 2	MLE	A red-flag condition would be automatically generated on the results outside this metric (VE.1.1.2) and require re-evaluation and review before that data is admitted to the validation base.	

VE.1.2. 3	MLE	The TIAMAT code for MPACT-BISON code coupling requires significant V&V work	(Clarno, 2014)**[67-69]** Gap
VE.1.3. 1	LLE	Godfrey [64, 70] successfully demonstrated VERA-CS ability to model the operating history of the Watts Bar I Nuclear Plant Cycles 1-12 and Watts Bar Unit 2. A rigorous benchmark was performed using criticality measurements, physics testing results, critical soluble boron concentrations, and measured in-core neutron flux distributions.	
VE.1.3. 2	LLE	The Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS) provided measured data 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. In general, the VERA-CS prediction results for cycle 1 are in good agreement with the plant data.	
VE.1.3. 3	LLE	Cycle 2 of BEAVRS has been completed and similar results were observed (to be documented)	
VE.1.3. 4	LLE	Need verify the MPACT-CTF 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). The impact of thermal expansion on the verification of the MPACT-CTF coupling.	Gap
VE.1.3. 5	LLE	L2:VMA.P12.01- Data assimilation and uncertainty quantification using VERA-CS for a core wide LWR problem with depletion [71]	UQ
VE.1.3. 6	LLE	L2:VMA.VUQ.P11.04 - Uncertainty quantification analysis using VERA-CS for a PWR fuel assembly with depletion	UQ
VE.1.3. 7	LLE	L2:VMA.P13.03 - Initial UQ of CIPS[20]	UQ
VE.1.3. 8	LLE	Uncertainty quantification and sensitivity analysis with CASL core simulator VERA- CS [72]	UQ/SA
VE.1.3. 9	LLE	Uncertainty quantification and data assimilation (UQ/DA) study on a VERA core simulator component for CRUD analysis[73]	UQ
VE.1.3. 10	LLE	Improvement in representation and geometric fidelity of VERA-CS (MAMABA and CTF) was shown by the calibration study using measured plant data (Watts Bar Nuclear Plant) and experimental loop data (Westinghouse Advanced Loop Tester (WALT)) [54].	Representation and geometric fidelity
VE.1.3. 11	LLE	Development of preliminary VERA-CS Crud induced localized corrosion modeling capability (milestone: L2:PHI.P17.03) [57]	Representation and geometric fidelity (MAMBA, MPACT and CTF)

Table A.10.1. Metric for evaluation of validation

Reference: Palmtag, 2016 [36]

Start-up	State point
HZP boron: ± 20 ppm	HFP boron: ±35ppm
Rodworth: ± 7 %	AO: ±3%
ITC: ±1 pcm/F	Pin Power Distribution and Peaking factors: ± 2 %