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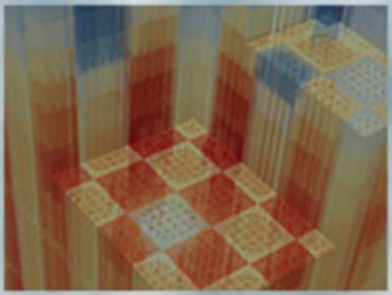

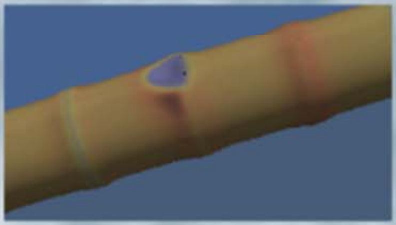

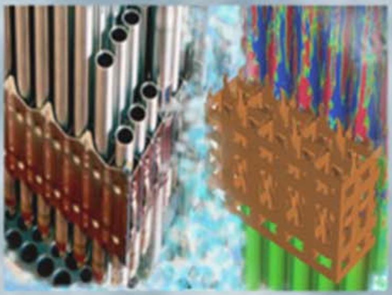

CASL Verification and Validation Plan

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EXECUTIVE SUMMARY

This report documents the Consortium for Advanced Simulation of LWRs (CASL) verification and validation plan. The document builds upon input from CASL subject matter experts, most notably the CASL Challenge Problem Product Integrators, CASL Focus Area leaders, and CASL code development and assessment teams.

This document will be a living document that will track progress on CASL to do verification and validation for both the CASL codes (including MPACT, CTF, BISON, MAMBA) and for the CASL challenge problems (CIPS, PCI, DNB).

The CASL codes and the CASL challenge problems are at differing levels of maturity with respect to validation and verification. The gap analysis will summarize additional work that needs to be done. Additional VVUQ work will be done as resources permit.

This report is prepared for the Department of Energy's (DOE's) CASL program in support of milestone CASL.P13.02.

CONTENTS

FIGURES

TABLES

ACRONYMS

BFBT	BWR Full-size Fine-mesh Bundle Tests
BOA	Boron Analysis – EPRI/Westinghouse coolant chemistry code
CASL	Consortium for the Advanced Simulation of LWRs
CC	Coolant Chemistry and CRUD
CFD	Computational Fluid Dynamics
CHF	Critical Heat Flux
CIPS	CRUD Induced Power Offset
CILC	CRUD Induced Localized Corrosion
CP	Challenge Problem
CRUD	Chalk River Unidentified Deposits
CSAU	Cod Scaling, Applicability, and Uncertainty
CTF	COBRA Two Fluid (computer code)
DAKOTA	UQ and optimization software (SNL)
DNB	Departure from Nucleate Boiling
DOE	Department of Energy
DOE-NE	Department of Energy Office of Nuclear Energy
EPRI	Electric Power Research Institute
FA	Focus Area
FMC	Fuel Materials and Chemistry (CASL Focus Area)
IET	Integral Effect Test
IFPE	International Fuel Performance Experiments
INL	Idaho National Laboratory
JFNK	Jacobian-Free Newton Krylov
JNES	Japanese Nuclear Energy Safety organization
LANL	Los Alamos National Laboratory
LOCA	Loss of Coolant Accident
LWR	Light Water Reactor
MAMBA	MPO Advanced Model for Boron Analysis (computer code)
MET	Multiple Effect Test
MIT	Massachusetts Institute of Technology
MPACT	Michigan Parallel Characteristics Transport (computer code)
M&S	Modeling and Simulation
MNF	Mitsubishi Nuclear Fuel
MV	Mixing Vane (grid spacer)
ORNL	Oak Ridge National Laboratory
NFI	Nuclear Fuel Industries
NSRR	Nuclear Safety Research Reactor
NMV	Non Mixing Vane (grid spacer)
NRC	Nuclear Regulatory Commission
NUPEC	Nuclear Power Engineering Center
OECD	Organization for Economic Cooperation and Development
PCI	Pellet Clad Interaction
PCM	Predictive Capability Maturity
PCMM	Predictive Capability Maturity Model
PIRT	Phenomena Identification and Ranking Table
PMO	Plant Measurements and Observations

PNNL	Pacific Northwest National Laboratory
POR	Plan of Record
PSBT	PWR Sub-channel and Bundle Test
PSU	Pennsylvania State University
PWR	Pressurized Water Reactor
QA	Quality Assurance
QMU	Quantification of Margin and Uncertainty
QoI	Quantity of Interest
RIA	Reactivity Insertion Accident
SET	Separate Effects Test
SLB	Steam Line Break
SLT	Senior Leadership Team
SNL	Sandia National Laboratory
S/UQ	Sensitivity and Uncertainty Analysis
TH	Thermal Hydraulics
THM	Thermal Hydraulics Methods
TK	Takahama
SQA	Software Quality Assurance
UQ	Uncertainty Quantification
V&V	Verification and Validation
VERA	Virtual Environment for Reactor Applications
VERA-CS	Virtual Environment for Reactor Applications – Core Simulator
VMA	Validation and Modeling Applications
VUQ	Validation and Uncertainty Quantification
VVUQ	Verification, Validation and Uncertainty Quantification
WALT	Westinghouse Advanced Loop Tester
WEC	Westinghouse

CASL Verification and Validation Plan

INTRODUCTION

The Consortium for the Advanced Simulation of Light Water Reactors (CASL) is developing computational modeling and simulation capabilities that are targeting operational and safety challenges for the current fleet of operating reactors. Of the set of challenges being considered, there are three that CASL aim to provide uncertainty quantification; Crud Induced Power Shift (CIPS), Pellet-Clad Interaction (PCI), and Departure from Nucleate Boiling (DNB) using the VERA core simulator (VERA-CS) capabilities [6] [7] [8]. This verification and validation (V&V) plan provides a basis to achieve that goal.

Because of the size and complexity of the CASL software, a CASL-wide document for a V&V Plan is needed. This will be a "living" document that is updated periodically. This version of the document focuses initially on validation. Verification will be addressed but is simply given lower priority for the first version of this document. This document, in combination with the code V&V plans and the challenge problem V&V plans, represents the CASL-wide V&V plan.

In general, in order to perform uncertainty quantification (UQ) in a complete sense the following list of uncertainties need to be addressed:

1. Uncertainty due to code bugs – this is addressed by documentation, regression testing, and unit testing.
2. Uncertainty due to numerical methods – this is addressed by verification
3. Uncertainty due to physics models – this is addressed by validation
4. Uncertainty in parameters due to uncertainty in the model parameters – this is addressed by UQ.

These steps provide the minimal requirement for using software with confidence for use in the region that the software has been validated.

However, there is a higher level of code quality which is based on determining the "predictive" capability of the software. This requires a much more detailed analysis to be able to predict behavior of nuclear reactors outside of the validation range.

An established approach for achieving this predictive capability is defined by the Predictive Capability Maturity Model (PCMM) [3]. In this document the application of PCMM within CASL is described.

Predictive Capability Maturity Model

The PCMM approach provides detailed analysis for determining the predictive nature of the software. Here predictive means applying the software outside of its validation range. The PCMM approach has the following components in general (for more detail see Appendix H).

1. <u>Regression Testing</u> – Part of software quality, the purpose is to provide testing to prevent code changes from having unintended changes. Ideally regression testing would cover 100% of the code.
2. <u>Unit Testing</u> – Part of software quality, unit tests are small test problems that insure that small parts of the code, units, are getting the correct answer.

3. <u>Benchmarking</u> – Part of software quality, benchmarking is when you compare one code output to another code output. It helps to improve confidence in the software but is not part of verification or validation. This is a common method in neutronics codes where results are compared to Monte Carlo codes, which are consider to be more accurate than the standard application codes.

4. <u>Code Verification</u> – Verification deals with, for example, measuring how well the numerical integration is solving the Partial Differential Equation. Depending on the code this will have a space and time or only space for steady state or only time for ordinary differential equations. Neutronics equations are often integral-differential equations where the numerical integration methods often used for angles and energy also have to be addressed. In code verification the problem has been simplified to enable an exact solution. The convergence of the code to the exact solution is measured and the convergence rate to compare with the designed convergence rate of the numerical method. There are a few numerical methods employed by CASL where the convergence rate is not known. It should be noted that the method of manufactured solutions is a powerful tool for code verification.

5. <u>Solution Verification</u> – Solution verification can be contrasted with code verification. In code verification for simplified problems, the exact solution is known as well as, in many cases, the expected convergence rate. In solution verification the problem is not simplified at all and therefore the exact solution may not be known. The mixture of different physics and numerics and length scales and times scales in multiphysics applications prevent an idealized convergence rate from being attained. The goal of solution verification is to estimate the impact of the truncation error in the numerical method caused by finite mesh spacing and time step size. Because this is an "estimate," flexibility is allowed in how this is approximated. The goal is to give a defendable quantification of the impact of numerical error on the solution.

6. <u>Separate Effects Testing (SET) Validation</u> – Validation is the comparison of the code output to "reality," where reality is measured by an experiment. Benchmarking or code-to-code comparisons are not validation. Validation plays the key role of ensuring that we are solving the correct physical models to capture the important physics. Separate effects validation are experiments designed to test specific models. Here only a single physics phenomenon is tested to prevent confusion between which physics phenomenon are causing a measured effect. Separate effects testing plays a key role in uncertainty quantification through Bayesian Calibration.

7. <u>Integral Effect Testing Validation</u> – In contrast to separate effects tests, integral effects tests measure the coupling between multiple physics phenomenon. This is the high level validation that tests the code coupling and the multiphysics coupling.

8. <u>Uncertainty Quantification</u> – The process of assessing the error or uncertainty in a quantity of interest based on distributions of model parameters. For uncertainty quantification to be accurate you need.

    a. All parameters (or at least all important parameters) exposed for study.

    b. Parameter distributions for all of the parameters, preferably from some form of calibration but at least from a defendable "expert opinion." [5]

    c. Minimal bias in the solution. This includes bias from code bugs, numerical errors, and not solving the correct physics models. In short the quality of the uncertainty quantification depends on the software quality, the verification and the validation.

Initial PCMM Assessments of CASL Codes

The PCMM approach measures maturity in each of these areas by assigning a maturity score (see Appendix H). Components 1-4 are scored in PCMM under code verification. Component 5 is solution verification and components 6 and 7 are validation. The final PCMM score comes from uncertainty quantification.

The initial PCMM analysis of the four main CASL codes CTF, MPACT. MAMBA, and BISON is provided in appendices D, E, F, and G respectively. The PCMM approach can be graded to a desired level of quality by setting a goal maturity level for each of the six PCMM. These six goals can be different for each standalone code and for the coupled code. These goals can also be different for each challenge problem. This allows the PCMM process to be customized to CASL use.

In general, the software quality of MPACT and BISON is very high. The documentation is good and the unit and regression testing are well done. CTF is a more mature code with parts of CTF that are no longer functional and parts of CTF that have limited documentation and testing. However, for a 30-year-old software, the quality of CTF has been dramatically improved in the last few years through CASL's efforts. MAMBA is a relatively software with a very small code development team, thus the software quality of MAMBA is lower than other CASL codes.

Code verification focuses on exact solutions and known convergence rates. MPACT has done a good job on code verification and BISON has some limited testing. CTF and MAMBA have no code verification work currently underway.

The solution verification work has been done in CASL applications but has not yet been formalized and documented. This high-level verification work will be given a more formal process and better documentation in the future in CASL.

Integral effects testing provides confidence that the code is getting a good solution. This work is being performed for all four CASL codes, but MAMBA needs improvement. The second part of validation is separate effects testing. This is important to insure that the right answer is produced for the right reason. The separate effects testing provides the needed support for a predictive capability. Currently separate effects testing is limited in the CASL codes.

Uncertainty quantification requires detailed knowledge of all of the code models and the entire code coupling. Although this sounds obvious, there are certain models that have been adopted with limited V&V and documentation. This limits the ability to perform detailed UQ. This level of detail is impractical for CASL. What is practical is an industry standard level of uncertainty quantification that is focused on the initial conditions and boundary conditions and code coupling. Here we have assumed that the internal models are correct and we test the uncertainty of the code inputs.

Overview of the CASL VVUQ Process

The following describes the process used to implement this high-end validation and verification uncertainty quantification (VVUQ) approach. Note that this requires significant time from the CASL

Senior Leadership Team (SLT) and the Validation Model Application (VMA) focus area. The code validation plans will be constructed based on the following steps.

1. Perform challenge problem Phenomena Identification and Ranking Table (PIRT).
2. Build challenge problem validation pyramid.
3. Initial code PCMM analysis to measure the quality and the quantity of the work that has already been done.
4. Involve SLT in the initial code PCMM analysis with the code team and set PCMM goals that are reasonable to CASL.
5. Initial challenge problem PCMM analysis to measure the quality and quantity of the work that has already been performed.
6. Involve SLT in the initial challenge problem analysis with the code teams and the challenge problem integrators to define reasonable PCMM goals for the challenge problem “delivery” given CASL resources.
7. The difference between the initial code PCMM analysis and the code PCMM goals define additional work for the code teams. Work will be done with SLT to assign milestones and resources to fill these gaps since the SLT and code teams helped define the goals for the code teams.
8. The difference between the initial challenge problem PCMM and the challenge problem goals define additional work for VMA. Work will be done with SLT to set the milestones and resources for this work since VMA, the challenge problem integrators, and the SLT defined the goals for challenge problem delivery.
9. Work is performed according to established milestones.
10. The final code PCMM analysis is done to see how close we came to the goals for the codes.
11. The final PCMM analysis is done for the challenge problem to see how close we came to our goals.

CIPS, PCI, and DNB will be the first and most complete challenge problems and will serve as examples for the other challenge problems.

The PCMM “gaps” representing the difference from the state of the code PCMM and their goals will include:

1. Software quality
2. Code verification
3. Solution verification
4. Validation and calibration
5. Uncertainty quantification and reduction

Validation and calibration will be split into two efforts; separate effects testing and integral effects testing. For integral effects testing we will use validation data that combines many models in one code or even multiple codes. All plant data fits into this type of validation. This high-level (the top of the validation pyramid) validation work will be mainly VMA’s responsibility with support from the code teams.

Separate effects testing is when validation experiments are designed to test an individual model.
These tests provide confidence that the individual models are the correct physics and that they were implemented in the software correctly. This low-level work, near the bottom of the validation pyramid will be mainly the responsibility of the code teams with support from VMA.

For separate effects validation, the work that can be achieved will vary based on the level of resources available. Note that CASL is currently considering uncertainty quantification for three the challenge problems; CIPS, PCI, and DNB. This means for important physical phenomena for these challenge problems we need enough information to support uncertainty quantification. So in addition to validation data we need:

1. Defendable range of applicability plus a range on the model or a parameter range based on expert opinion
2. Range of applicability plus the validation data from the original model paper
3. Original paper plus new validation data that is more applicable to the CASL application

Based on this information uncertainty quantification can be performed for CIPS, PCI, and DNB. The phenomena (for each code) will have different degrees of complexity. In fact, many phenomena are composite phenomena in the sense that their description/prediction contains other phenomena. There are also overlaps between listed phenomena, as well as very few tests that can be totally separate-effect tests (and often such "ideal" SET are performed under conditions not relevant/ scalable to applications).

Thus the situation can be described better as a "mix of models" validated against "mixed-effect tests". For example, a test on Chalk River Unidentified Deposit (CRUD) under flow boiling would need to describe all prior fluid flow and heat transfer regimes for it to correctly capture sub-cooled boiling that generates deposition. That "mixing/overlapping of models" makes it harder to infer about each model. This has been an obstacle in identifying experiments; sorting out data and making any conclusion about "validation" of individual models.

CASL V&V Plan Summary

For CASL we will use a graded PCMM approach which has lower PCMM maturity goals for some of the PCMM categories and focus on the key capabilities for CASL to insure the quality of the software when used inside of the validation space. This plan will consist of four key pieces.

1. Documentation – A standard level of documentation for all codes including the code coupling will be provided. Currently some codes are better documented and only limited documentation, namely milestone reports, exist to describe the code coupling. It is important that what is in the code is documented and what is in the document is in the code. Because the codes are still undergoing extensive capability addition, this document will need to be updated continuously.

2. Solution Verification – The CASL work will rely heavily on solution verification for controlling numerical error. This process will be formalized so numerical estimates of uncertainty will be included with challenge problem results. This will include, whenever possible, studies of spatial impacts, temporal impacts, and convergence criteria impacts.

3. Integral Effects Validation – Provides a basis for use of software within or near its validation range. That is, as long as the software is applied near where it is validated, it will provide useful results.

4. Uncertainty Quantification - For some CASL challenge problems, namely CIPS, PCI, and the VERA-CS (non-CFD) DNB, uncertainty quantification may also be performed. This uncertainty quantification will focus on initial conditions, boundary conditions and code coupling based on code inputs. This uncertainty quantification (UQ) approach will be based on expert opinion based parameter distributions.

This approach will provide a level of confidence that industry can use the software for its intended purposes in the ranges that it has been validated. Industry can then apply more detailed VVUQ for licensing applications and additional validation for new applications as their VVUQ processes require.

Document Organization

The rest of this document includes three sections and a conclusion. The first section discusses the challenge problem validation plans for CIPS, DNB and PCI. Depending on the specific challenge problem, these plans are documented in the challenge problem implementation plans and separate documents. As these plans are developed, they will likely all be expanded in stand-alone documents. The second section discusses the code verification and validations (V&V) plans. The third section discusses gaps or requirements in the work that need to be filled. Finally conclusions will be provided. Details will be left to other references and appendices at the end of this document.

CASL CHALLENGE PROBLEM VALIDATION PLANS

Overview

The work documented in this report considers three challenge problems and their quantities of interest (QoIs):

- CRUD-Induced Power Shift (CIPS) [9],
  - Total boron mass
  - Boron mass spatial distribution
  - Axial offset
- Pellet-Cladding Interactions (PCI) [16],
  - Maximum clad stress
  - Failure threshold distribution
- Departure from Nucleate Boiling (DNB) [13],
  - DNBR which is the ratio of the predictive heat flux over the local measured heat flux

Charters and implementation plans have been developed for the CASL Challenge problems and these documents contain significant information required for the development of V&V plans for CIPS, PCI, and DNB. The validations and qualifications for the challenge problem (CP) applications are divided into two parts: 1) code V&V are first performed by the code development team, and 2) application specific validation is coordinated and performed by the CP integrator.

The general approach used in this document is to map the important phenomena for the challenge problems to the codes that supply that capability. In that way, the important phenomena in the challenge problems can be ensured to be validated by the code teams.

Due to the multiphysics multi-code nature of the challenge problems in CASL, a higher level of V&V applies to the 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.

The approach considered is based on a validation pyramid. The validation pyramids for CIPS, PCI, and DNB are given in Appendix I. In this approach, the large scale results from the coupled code are at the top of the pyramid. The small scale individual physics are at the bottom of the pyramid. The bottom of the pyramid is covered by code validation plan. The top of the validation pyramid is covered by the challenge problem validation plan.

For multiphysics, multi-code, multiscale simulations a PIRT is as a key part of the process. The PIRT helps to identify key phenomenon that are then used to construct a validation pyramid. It should be noted that the PIRT and validation pyramid are tools to help with the construction of the validation plan. The PIRTs and validation pyramids will be used to define the integral effects validation work done in the CASL V&V plan. Basically we will use the tops of the validation pyramids as the integral effects validation plan.

Up until now, capability development has been the majority of the work on CASL. The CASL software is now becoming mature enough that Software Quality Assurance (SQA) and VVUQ can become a larger amount of the work. As such, it is important to note that we have come a long way, but there is always room for improvement. Throughout this document obvious places that can be improved will be noted.

The CASL V&V plan will, by reference, include a large number of documents. These documents will be archived in a convenient location. Likewise, a central storage of the CASL validation data will also be coordinated.

CIPS: Crud-Induced Power Shift V&V Plan

This information came from the CIPS implementation plan [9]. This will be separated out in the future as a separate document.

- Ability to do a quarter core calculation with coupled MPACT/COBRA/MAMBA for a Cycle 1 or Cycle 2 core (none of those cores would have had CIPS, so this is just a demonstration of analytical capabilities).
- Compare results to stand-alone BOA and any available plant data.
- Additional MAMBA/MAMBA BDM benchmarking completed compared to current Westinghouse Advanced Loop Testing (WALT) loop data (updated dataset).
- 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
- Expand MPACT/COBRA/MAMBA CIPS analysis to reload cores that had CIPS
    - Callaway Cycle 4 or Seabrook Cycle 5 (requires VERA models starting in Cycle 1)
    - Requires crud restart file capabilities and crud shuffling capability
    - Compare results to plant behavior, BOA 3.1 standalone
- CIPS Verification, Validation, and Uncertainty Quantification

DNB V&V Plan

Validation Plan

Validation of the multiphysics VERA-CS 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 integral test 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-CS 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-CS be considered for CASL test stand development.

Validation Experiments

Although there are no plant-scale DNB data or measurements, small-scale and separation effect test data are available for CASL VERA modeling and simulation (M&S) validation and qualification. The available test data for the DNB CP validation are listed below.

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 benchmark database and benchmark problem specifications were prepared jointly by the Pennsylvania State University (PSU) and the Japan Nuclear Energy Safety Organization (JNES) with support from the U.S. Nuclear Regulatory Commission (NRC) and OECD Nuclear Energy Agency (OECD/NEA).

2.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. The test section simulated a pressurized water reactor (PWR) 17x17 fuel design with heated rods of 0.374 inch (9.50 mm) O.D. in a 0.500 inch (12.7 mm) rod pitch. The heater rods utilized the uniform axial power shape where the hot rods were fabricated with Inconel 600 tubing. There was no simple support grid used for this series of the tests.

3.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. The test section simulated a PWR 17x17 fuel design with heated rods of 0.374 inch (9.50 mm) O.D. in a 0.500 inch (12.7 mm) rod pitch. The heater rods utilized the uniform axial power shape where the hot rods were fabricated with Inconel 600 tubing. There was no simple support grid used for this series of the tests.

4. 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 (Takahama being the basis for the TK moniker). A total of seven test segments were used, ranging in burnup levels from 37.8 GWd/MTU to 50 GWd/MTU. The seven test segments are described as TK-1, TK-2, and so on. The test segments were taken from two different fuel types: Type A, which is from Mitsubishi Nuclear Fuel (MNF) and Type B, which is from Nuclear Fuel Industries (NFI). The pellet outer diameter in Type A fuel is larger than the pellet in Type B fuel, although they both have the same fuel rod outer diameter. The difference in pellet diameters results in higher energy densities in the Type B fuel compared to Type A. Each test segment is a length of fuel that spans between two hydraulic mixing grids in a standard twelve-foot fuel assembly. The segments were then re-fabricated to fit into the Japanese NSRR test loop.

A RIA transient was simulated in the test loops by creating a highly energetic and extremely brief energy pulse to the test segment. All pulse lengths were 4.4 milliseconds and the peak enthalpies of the pulses ranged from 95-125 calories/gram. The test segment was in a pool of water (no forced coolant flow) at atmospheric pressure and room temperature.

PCI V&V Plan

The analysis of PCI is performed with VERA-CS combined with the BISON fuel performance code. VERA-CS validation is based on modeling operational reactors and comparing to plant measured data. The approach to validate BISON for use in calculating the PCI failure potential in a commercial PWR during operation consists of three key steps; 1) establishing the material property and phenomenological behavior models, 2) validating steady-state base irradiation fuel rod parameters (dimensional changes, fission gas release, temperature) using test reactor irradiations and commercial fuel rods, and 3) validating the PCI failure model using well-characterized ramp test rods. This approach along with a corollary approach for the reactor physics modeling of fuel rod power is depicted in a validation pyramids shown in Appendix I.

The PCI challenge problem leadership has transitioned in the last year. Due to this transition the PCI implementation plan [16] is being reworked. The initial draft of this document is based on a validation plan including in the PCI Charter and Implementation plan written by the previous PCI challenge problem integrator [17].

The plan contains a large number of experiments in the following areas of validation

1. Thermal Validation
2. Mechanical Validation
3. Fission Gas Release
4. Power Ramps

Code Requirements Based on V&V Plans

Based on the discussion of the V&V plans above, PIRTs and validation pyramids, requirements for the features that must be included in key CASL software to be able to model the phenomena are described below. A mapping is also provided in Table 1.

MPACT

1. Energy deposition
2. Fast flux
3. Isotopics
4. Gamma heating
5. Fission power
6. Fission product yield
7. Cross sections
8. Boron feedback to neutronics
9. Decay heat model (retards cool-down)
10. Burn up

CTF

1. Clad temperature
2. Heat transfer between clad and coolant
3. Sub-cooled, bulk, CHF, and post CHF boiling regimes.
4. Cladding surface temperature
5. Bulk coolant temperature
6. Fuel rod surface heat flux
7. Crud Erosion model
8. Crud Surface effects on boiling
9. Crud Surface effects on friction
10. Crud Surface effects on heat transfer
11. Two phase pressure drop and effect on friction
12. Turbulent mixing
13. Cross flow
14. Grid spacer heat transfer and effect on boiling
15. Grid spacer turbulent mixing
16. Grid spacer two phase pressure drop
17. Gravity effect under natural circulation and convection

BISON

1. Fuel Thermal conductivity
2. Fuel Specific heat
3. Fuel Melting temperature
4. Fuel Emissivity
5. Fuel Thermal expansion
6. Fuel Young's and shear Modulus
7. Fuel Compressive Yield Stress
8. Fuel Fracture Strength
9. Fuel Thermal/irradiation creep
10. Fuel Relocation
11. Fuel Smeared crack
12. Fuel Densification
13. Fuel Swelling
14. Fuel Steady state fission gas release
15. Fuel Transient fission gas release
16. Fuel Radial power distribution
17. Fuel High burn-up structure
18. Clad thermal conductivity
19. Clad specific heat
20. Clad melting temperature
21. Clad emissivity
22. Clad Thermal expansion
23. Clad Young's modulus
24. Clad Shear Modulus
26. Clad Meyer Hardness
27. Clad Irradiation growth
28. Clad Yield Stress
29. Clad plastic hardening
30. Clad thermal annealing
31. Clad thermal/irradiation creep

32. Clad stress corrosion cracking
33. Gap Thermal conductivity
34. Gap gas viscosity
35. Gap temperature jump distance
36. Gap open and solid gap conductivity
37. Gap contact pressure
38. Gap friction
39. Gap gas pressure
40. Temperature profile in pin
41. Temperature profile in clad given clad outer surface temperature
42. Temperature profile in clad given heat flux (heat transfer coefficient) Note complex coupling.

MAMBA

1. Clad low temperature oxidation
2. Clad hydrogen pickup model
3. Subcooled boiling in crud layer
4. Cladding surface condition (validation data exists Jacopo MIT)
5. Crud deposition rate as a function of temperature and subcooled boiling (steaming rate)
6. Boron deposition rate on the CRUD as a function of temperature
7. CRUD initial thickness
8. Solution thermo-dynamic reaction rates
9. CRUD material mass balance.

Table 1. Mapping challenge problem requirements to code capabilities

Code\CP (CPI)	**CIPS** (Jeff Secker)	**PCI** (Joe Rashid)	**DNB** (Yixing Sung)
CTF	Single-Phase heat transfer subcooled boiling wall sheer (no crud dependence) Grid spacer heat transfer and TKE Axial and azimuthal Turbulent mixing Coolant Temperature and density	Thermal and Fluid BC Coolant temperature and density	CHF (roughness) Single -Phase and Two-Phase heat transfer Two-Phase void distributions Two-Phase pressure drop subcooled boiling cross flow fuel rod heat transfer natural circulation
MPACT	Fuel rod power distributions Fuel depletion Boron Feedback and depletion	Fuel rod power distribution for operational transient conditions Fuel Depletion Xenon Fast flux Rod tip homogenization	Off-normal conditions Power distribution Moderator Feedback Control rod position Kinetics
MAMBA-1D	Subcooled boiling Crud erosion Crud growth Crud thermal resistance Boron update and removal	N/A	If considering impact of CRUD and on DNB: Surface Roughness Porosity Wettability
BISON	Fuel Temperature (to build tables for use in CTF)	Fuel, clad temperatures and behavior Azimuthal dependency Fuel Temperature	Fuel Temperature

CASL CODE V&V PLANS

The validation plans and status for codes requirement for simulating CIPS, PCI, and DNB are discussed in this section.

Code V&V Plan Requirements

A code V&V plan template has been developed for use by the code that outlines the requirements for V&V elements that must be addressed [18] [19] [29] [30]. Not all codes are currently using this template, but they are providing the information required at differently levels of completeness.

XYZ Code V&V Plan

Documentation status

1. Code Overview (brief)

- 1.1. Identification including institution, version, authors, keywords
- 1.2. Brief update of status of code development, assessment, and application
- 1.3. Model list (with connectivity)
- 1.4. Overview of code structure and modeling hierarchy
- 1.5. Other comments

2. Verification

- 2.1. Listing of verification tests (conditions; physics model; outcomes)
  - 2.1.a. Regression testing
  - 2.1.b. Unit testing
  - 2.1.c. Benchmarking
  - 2.1.d. Code verification
  - 2.1.e. Solution verification
- 2.2. Evaluation of verification (coverage, quality)

3. Validation

- 3.1. Listing of validation tests (conditions; physics model; outcomes)
  - 3.1.1. Separate-effect tests
  - 3.1.2. Integral-effect tests
  - 3.1.3. Plant tests
- 3.2. Evaluation of validation (coverage, quality)

4. **Sensitivity/uncertainty analysis**

- 4.1. Summary of S/UA
- 4.2. QPRT. Update PIRT

5. **Multiphysics code V&V**

- 5.1. Coupled code V&V
  - 5.1.1. Coupled to code #1

5.1.2. Coupled to code #2
5.2. Coupled code performance evaluation

6. Planning
6.1. Verification
6.2. Validation
6.3. Sensitivity/uncertainty analysis

References
Appendix

MPACT: Reactor Neutronics Analysis Code

The MPACT V&V plan is very complete [20]. This 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. Table 2 maps the validation work to CASL challenge problems.

Table 2. 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			

CTF: Sub-channel Analysis Code (COBRA-TF)

Being the oldest of the CASL codes, the documentation and testing in CTF is relatively mature [23] [24] [25]. The CTF V&V plan [21] contains software quality testing, which includes unit testing and validation. The unit testing is referred to as verification and results are left out. There is a significant amount of solution verification work is performed continuously but is not captured in a document as a formal procedure. Code verification work is harder in CTF but there is enabling technology that allows it to be performed and some examples from the work on rewriting some of the numerical methods used in CASL. These code verification tests will be included in future versions of this document.

This document includes four tables that show what validation problems map to VERA-CS, CIPS, DNB, and RIA. The tables also include a list of detailed unit tests that support the models being tested.

BISON: Nuclear Fuel Performance Analysis Code

The BISON V&V plan [26] validation efforts are clearly aligned with the PCI, RIA, and LOCA challenge problems where BISON is the main contributor. The verification work clearly shows convergence but in the future we may work on assessing the expected and measured convergence rates.

MAMBA: Crud build-up modeling code

The first draft of the MAMBA V&V plan is available [27]. The MAMBA software [28] is still relatively immature and work will need to be done to bring MAMBA up to the standard of MPACT, CTF, and BISON. Table 3 maps the CRUD challenge problems' MAMBA capabilities to validation studies.

Table 3. Mapping of challenge problems' MAMBA capabilities and validation studies.

		Validation Cases				
Challenge Problem	**Phenomena**	**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	

Status of MAMBA Verification

Verification of an early version of MAMBA was documented in a 2012 CASL report (CASL-I-2013-0212-000). This report listed a few steps for improving the status of MAMBA verification, including documentation of numerical procedures, studies of stability and accuracy and finally running through verification problems to demonstrate correctness of the numerical methods. The numerical schemes are being documented in the revised MAMBA manual. Studies of numerical accuracy and stability as well as solution verification have all been performed as part of the MAMBA development; however, these procedures remain to be fully documented. The MAMBA source distribution includes an extensive set of software tests to verify the code correctness. The tests are documented in the source distribution.

Status of MAMBA Validation

Several MAMBA V&V studies have been performed and reported as CASL milestones. Their connection to the validation of CASL challenge problems is summarized in Table 3 Below, we provide a brief summary of the validation work. For complete details we refer to earlier CASL reports.

- Westinghouse Walt Loop validation studies were performed of cladding temperature vs rod power and crud thickness. The Walt loop study also gives CRUD properties (porosity, chimney density, chimney diameter, bulk thermal conductivity) for use in MAMBA. This work validates MAMBA's heat transfer/chimney boiling model and crud pore fill kinetics (i.e. time dependent porosity model). This study was documented in a separate CASL report (CASL-I-2012-1121-000).
- MAMBA/BOA comparisons were made for the heat transfer/chimney boiling model, mass evaporation rate vs crud thickness and pin power (see CASL report CASL-I-2012-1121-000).

This work led to improved boiling models in BOA v3.1. MAMBA's boric acid thermochemistry was also validated against BOAs MULTEQ database.

- MAMBA/MAMBA-BDM comparisons were performed to verify the cladding temperature and boiling velocity, which gave good agreement.
- Coupled MAMBA/STAR-CCM+ comparisons were performed for plant data on oxide thickness and morphology for Seabrook Cycle 5. The measured oxide thickness correlates with the CRUD thickness. This study also showed that the local (~1 cm) TH conditions very important in determining crud deposition patterns.
- An initial CIPS study compared axial offset predicted by coupled MAMBA/CTF/MPACT with plant data for Watts Bar.

4. GAP ANALYSIS

An analysis was performed to determine the gap between the validation identified for the challenge problem and the validation being performed by code teams. This gap between expectations and what is realistically possible will be addressed by the VMA leadership and the CASL senior leadership.

The expectation is a very high level of validation that comes with very mature software. Because of the young age of the CASL software the validation level will be slightly lower leaving it up to industry to complete the validation work.

While more extensive validation is desired, the main CASL codes, CTF, MPACT, and BISON have validation coverage of all key phenomena. This is sufficient validation to provide industry with the confidence to use the software and then further validate it as they deem necessary.

For each of the challenge problems considered four types of gaps will be discussed:

1. Documentation
2. Validation
3. Verification
4. Uncertainty Quantification

CIPS Challenge Problem

Documentation

The documentation for MPACT and CTF is sufficient for CIPS. Improved documentation on how MAMBA 1D is calibrated from MAMBA 3D. If the future approach will directly use MAMBA 3D, improved documentation of MAMBA-3D will be required.

The code coupling between MPACT, CTF, and MAMBA needs to be documented in detail, including the variables 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.

Validation

The CIPS challenge problem is well validated for CTF and MPACT. CIPS does not stress the capability of either of these codes. Future validation is needed for MAMBA. There are still basic code coupling issues with MAMBA and its level of documentation and testing is significantly lower that CTF and MPACT. The selection of the use of MAMBA 1D and MAMBA 3D needs to be resolved and whatever code is chosen for CIPS it needs a well-documented pedigree.

Verification

Verification for CIPS is a challenge. Certain geometry is fixed at a single control volume like a channel for CTF. However, for solution verification we only need sensitivity information from the temporal discretization and spatial discretization. Therefore, we need to perturb whatever values can be changed and measure the impact on the CIPS quantities of interest (QoIs). This study also needs to consider convergence criteria.

Uncertainty Quantification

For uncertainty quantification expert-opinion-based distributions on the initial conditions and boundary conditions for all three codes are needed (this is already in place of CTF).

PCI Challenge Problem

Documentation

The documentation of BISON acceptable. However, the final decision on the BISON coupling with VERA-CS remains to be decided. Documentation that defines the coupling is needed with which codes and whether the coupling is one-way or two-way coupling.

Validation

The PCI validation is well covered by the BISON validation plan. The main physics, thermal mechanical, fission gas, and chemistry are the same for both. Both plans provide testing of these four phenomenon, but the PCI validation plan is significantly more extensive and is slightly different. The new PCI implementation plan written by Joe Rashid is fairly recent. In the next few months we will work to come to a compromise position on critical validation experiments and the CASL resources to complete them.

Validation of VERA-CS is similar to that for the CIPS problem and use measured data from operation reactors.

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. We need spatial discretization and temporal discretization sensitivity studies as well as sensitivity studies for all of the Jocobian-free Newton-Krylov (JFNK) solver settings.

Uncertainty Quantification

Expert-opinion-based parameter distribution for the initial conditions and boundary conditions is needed.

DNB Challenge Problem

Documentation

The documentation of CTF is acceptable for DNB. However, 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.

Validation

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.

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. In particular, the effort to develop the capability to evaluate impact of spacer grid design features effect on DNB (Sung, 2013).

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). 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.

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

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

Verification

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.

Uncertainty Quantification

Expert opinion based parameter distributions need to be given for all of the initial conditions and boundary conditions.

5. CONCLUSIONS

This document will 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.

There are still issues with the code coupling 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, this 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.

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APPENDIX A: CIPS PIRT

This document summarizes a mini-PIRT meeting held on Monday November 4, 2013 for the CASL CIPS challenge problem.

We will only be using four or five codes for this study.

1. Neutronics – MPACT or Insilico SPn
2. Thermal Hydraulics – CTF
3. Fuel performance – BISON or CTF
4. Chemistry - MAMBA

The basic physics

1. 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.
2. Conduct the energy in the fuel radially out from the center, across the gap and through the clad. The fuel is changing with burn-up and the gap is shrinking.
3. Remove the heat from the clad to the coolant and advect it out of the core.
4. Crud deposited and removed from the fuel pin surface from the coolant (boiling and non-boiling) and Boron deposited on the CRUD.

We will have three Quantities of Interest (QoIs).

1. The first is scalar and is the total Boron Mass. This is necessary but not sufficient.
2. If we can accurately predict the total boron mass we will then investigate the vector FOM which is the Boron Mass Distribution. The first QoI can be computed trivially from the second. These predictions of boron mass will be compared from inferred data from reactors.
3. The third QoI is Axial Offset.

We will list phenomenon for each of the four physics areas. Note that it may be useful to look at the VERA-CS progression problem 6 PIRT since one may consider the CIPS phenomenon list to be a superset of the VERA-CS progression problem 6 phenomenon list.

Note that the importance of phenomena and our knowledge of the phenomena will be ranked with one of the following four values

1. High (H) – very important
2. Medium (M) – important
3. Low (L) – not important
4. No Opinion (N) – not qualified to comment

The ranking will be given as an ordered pair in red **(importance, knowledge)** in parentheses in red after the phenomenon number.

Thermal Hydraulics

Here we are considering the fluid flow over the fueled portion of the pin.

1. **(H, M)** Steaming Rate (space and time integral of the subcooled boiling rate) is how much water is boiled. Note that due to condensation this is not captured by the vapor volume fraction.
2. **(H,M)** Subcooled boiling this is a dominant effect because it is the chemicals in the water that are left behind when it boils that is the dominant source of CRUD. There are two kinds of subcooled boiling
    a. **(H,H)** Subcooled boiling on a clean metal surface
    b. **(H,L)** Subcooled boiling on and in CRUD.
3. **(M,M)** Bulk coolant temperature (the boiling is a function of the fluid temperature near the rod which may be much higher).
4. **(H,H)** Heat flux, if more energy is deposited in the coolant than can be carried away by the single phase water boiling will have to occur.
5. **(L,L)** Wall roughness changes as crud builds up and effects nucleation sites for boiling and friction pressure losses in the channel.
6. **(L,M)** Single phase heat transfer determines when subcooled boiling begins and some CRUD is deposited without boiling. Because there is a large area without subcooled boiling this mass of CRUD may be significant to the total mass of crud. However, there is a minimal thickness of CRUD required for Boron deposition. Because our FOM is total Boron mass, we do not care about CRUD mass that does not absorb Boron. Thick CRUD and high boiling are needed for Boron deposition.
7. **(H,L)** Mass balance of Nickel and Iron are important. The source term from the steam generator and the sink term in the core (and other components) determine the Nickel and Iron concentration. The Nickel and Iron concentration are critical to computing the deposition rate. Once all of the Nickel and Iron source have been removed through deposition there cannot be any more crud formation. The small amount of Nickel and Iron can get "used up."
8. **(L,H)** Boron mass balance is unimportant. The large amount of Boron in the system basically gives an "infinite" source of Boron for deposition on the CRUD.
9. **(H,L)** CRUD erosion. The removal of CRUD due to shear forces is key to getting the Boron mass distribution correct.
10. **(H,L)** Initial CRUD thickness (mass) from previous fuel cycles. Impacts Nickel and Iron mass balance.
11. **(H,L)** Initial coolant Nickel and Boron Concentration.
12. **(H,L)** CRUD source term from steam generators and other surfaces.
13. **(L,M)** CRUD induced change in boiling efficiency. Thermal conductivity change and nucleation site change.
14. **(L,M)** CRUD induced change in flow area.
15. **(L,L)** CRUD induced change in friction pressure drop.
16. **(L,L)** Change in thermal hydraulic Equation of State Due to change in chemical concentrations.
17. **(H,L)** Change in local heat flux to the coolant from the fuel due to CRUD buildup.

Fuel Model

Because CRUD buildup is a long time scale effect of one to many fuel cycles fuel burnup is an important effect.

1. **(H,M)** Local changes in rod power due to burn up
2. **(H,M)** Fuel thermal conductivity change as a function of burn up
3. **(H,M)** Changes in effective CRUD conductivity due to internal fluid flow and boiling.
4. **(H,M)** CRUD removal due to transient power changes. Mechanical effects of rod contraction when rod is cooler.
5. **(H,M)** Gap conduction model
    a. **(L,M)** Fission product gas
    b. **(H,M)** Pellet swelling
    c. **(H,M)** Contact between pellet and clad

Neutronics

Due to the longer time scale of the CRUD deposition, we need to adjust our cross sections due to buildup of fission products and removal of Fissile material. This means the number of materials and therefore the number of cross sections is much larger.

1. **(H,H)** Local Boron density increases absorption
2. **(L,M)** Moderator displaced by CRUD and replaced with and absorber.
3. **(H,H)** Xenon impact on steady state and transients
4. **(L,M)** Geometry changes due to swelling, cracks, redistribution, sintering, and gaps.
5. **(H,H)** Burn up calculations that include decay chains
    a. **(H,M)** Cross section changes
    b. **(M,M)** fission products production
    c. **(H,H)** fission product decay constants
    d. **(M,M)** Simplified decay chains to make calculation more efficient. This may impact power distribution.
6. **(M,M)** Boron Induced shift in neutron spectrum
7. **(L,M)** Boron depletion due to exposure to neutron flux.
    a. **(L,L)** In the bulk coolant
    b. **(L,L)** In the CRUD (absorption and desorption may impact)
8. **(L,L)** Fuel depletion calculation being done at a different resolution than neutron flux calculation
9. **(L,L)** 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

Chemistry

This is the main mechanism for CRUD formation and Boron Deposition on the CRUD.

1. **(H,H)** Local changes (near the rod) in the equation of state due to higher concentrations of Nickel, Iron, and Boron.
2. **(M,M)** Most of the chemical reaction rates are based on lower temperature and pressures.
3. **(H,M)** Defining the list of elements and reactions assumes that other reactions not include have a small impact.
4. **(H,M)** Porous media flow. How the Borated water gets into and out of the CRUD.

    a. **(M,M)** Porosity
    b. **(M,M)** Permeability
    c. **(M,L)** Chimney density
5. **(M,M)** Water Ph effect on
    a. **(M,M)** steam generator corrosion rate
    b. **(M,M)** CRUD deposition

APPENDIX B: PCI PIRT

This document summarizes a mini-PIRT meeting held on Wednesday, November 20, 2013 for the CASL PCI challenge problem.

We will only be using three codes for this study:

1. Neutronics – MPACT or Insilico SPn
2. Thermal Hydraulics – CTF
3. Fuel performance – Peregrine

The basic physics are:

1. Compute a neutron flux that produces energy from fission (deposited in the fuel and the coolant). Fuel temperature, moderator density, and moderator temperature are all feedback mechanisms. Note that burn up plays a significant role in neutron cross sections.
2. Conduct the energy in the fuel radially out from the center, across the gap and through the clad. The fuel is changing with burn-up and the gap is shrinking.
3. Remove the heat from the clad to the coolant and advect it out of the core.

We will have two Quantiies of Interest:

1. The first is maximum cladding stress. This will be a surrogate for failure probability. Failure will be based on the maximum clad tress exceeding a given failure threshold.
2. If we can accurately predict the maximum cladding stress distribution, we will then predict the failure threshold distribution. The failure probability is then the intersection of these two distributions.

We will list phenomenon for each of the three physics areas. Note that it may be useful to look at the VERA-CS progression problem 6 PIRT since one may consider the PCI phenomenon list to be a superset of the VERA-CS progression problem 6 phenomenon list.

Note that the importance of phenomena and our knowledge of the phenomena will be ranked with one of the four values:

1. High (H) – very important
2. Medium (M) – important
3. Low (L) – not important
4. No Opinion (N) – not qualified to comment.

The ranking will be given as an ordered pair in red **(importance, knowledge)** in parentheses in red after the phenomenon number.

This calculation can be done on a section of a fuel rod. There may need to be core wide searches to determine which section of which fuel rod needs to be investigated.

Thermal Hydraulics

(H, M) Heat transfer boundary condition
(H,M) coolant temperature
(L,M) Boiling

(H,M) Clad temperature (important to creep rate)
(L,L) Flow induced vibration
(M,M) Azimuthal variation in temperature (important near edges and water rods)

Fuel Performance Model

There may be a problem due to a lack on consistence between the Peregrine burn-up model and the scale burn-up model. This inconsistency may cause uncertainty.
(H,H) Prior irradiation time
(H,H) Power maneuvers (ramp rate)
(H,M) Cladding creep
(H,M) Pellet cracking
(H,M) Pellet swelling
(H,M) Pellet densification
(H,H) Operating history (power profile)
(H,M) Fission gas release (internal pressure in the fuel rod)
(H,M) Gap model
(H,H) Pellet thermal expansion caused by power increase
(H,M) Thermal creep in pellet and clad
(M,M) Friction between pellet and clad
(M,M) Clad
(M,L) chemical interactions in the clad
(H,L) microstructure impact on stress driven cracking
(L,M) Corrosion
(L,L) Hydrides
(M,M) Material properties for time varying heterogeneous fuel pellet
(M,M) thermal expansion
(M,M) thermal conductivity

Neutronics

Because the time scales are slow the quasi-static assumptions for neutronics are good enough.
(H,H) Energy deposition (fission rate as a function of space and time)
(H,H) Fast flux (as a function of space and time)
(M,L) Gamma heating
(M,M) Isotopics impact the fuel performance model but they are currently computed by the fuel performance model. In the future these should be provided by the neutronics code which has a much more detailed calculation. Not the same isotopes are important to neutronics and fuel performance.
(M,M) Xenon impact on local power transients impacts stress
(L,L) change in pellet and clad geometry
Chemistry
(M,M) Water-clad corrosion rate (current model empirical future model lower length scale)
(H,M) Fuel pellet chemistry (current model empirical future model lower length scale)

APPENDIX C: DNB CTF PIRT

The table below summarizes a mini-PIRT for VERA-CS M&S of the reactor ore during DNB-limiting accidents (Sung 2016)

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		

APPENDIX D: INITIAL CTF PCMM ANALYSIS

The initial PCMM analysis of CTF can be summarized in the radar plot in Figure 1.

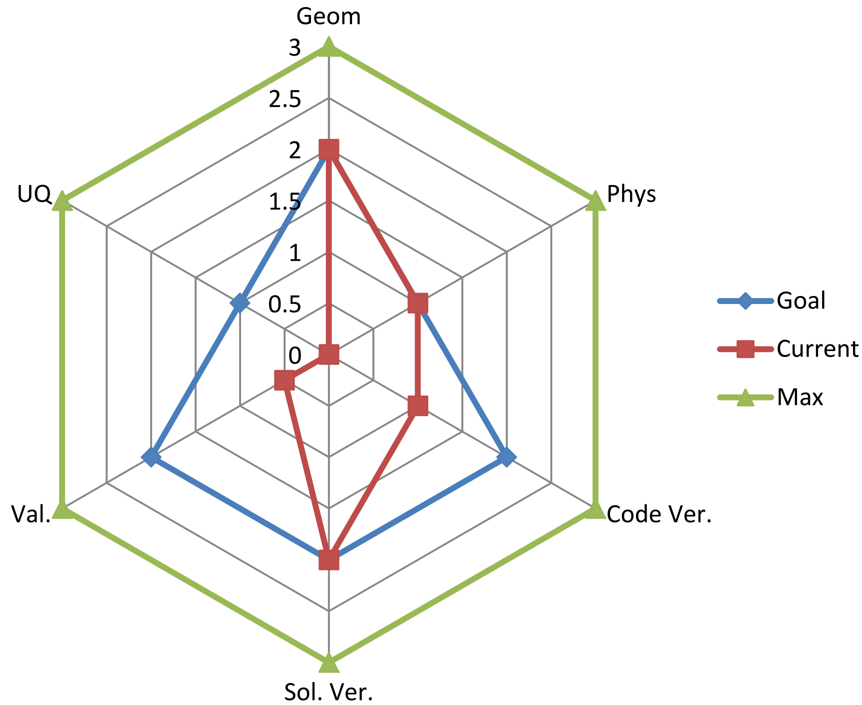

Figure 1. CTF PCMM

As can be easily seen from Figure 1, CTF is doing a good job in:

1. Geom – Representation and Geometric Fidelity
2. Phys – Physics and Material Model Fidelity
3. Sol. Ver. – Solution Verification

More work needs to be done in:

1. Code Ver. - Code Verification
2. Val. – Model Validation
3. U.Q. – Uncertainty Quantification and Sensitivity Analysis.

Representation and Geometric Fidelity

Although this documentation seems to be spread over the CTF theory manual, the CTF user manual, and the VERAIN manual it was well covered and seems to be accurate enough for the application. We were never able to find a simple picture to describe the geometry of the four pins attached to a channel and the geometry of the four channels attached to a pin, these two pictures would help.
The CTF input was far to general and relies heavily on the code user to get the correct information. However, the combination of VERAIN and the CTF preprocessor provide for a very accurate and error free description of the CTF relevant geometry.

The score was set at a value of 2 based on the fact that there are limited simplifications (namely the grid spacers) of major components.

The geometry fidelity in CTF is appropriate for a channel thermal hydraulic code so no additional work in this area is needed.

Physics and Material Model Fidelity

Because it is a channel code, CTF is highly empirical. That is to say most important physics are modeled with empirical correlations. The correlations are calibrated to match specific data sets. The coupling between correlations is based on artificial ramps and under-relaxation or ad hoc coupling. Based on this the CTF score was a one. The CASL strategy is to have Hydra move the state of the art forward so there is no reason to improve the CTF models other than possibly calibrating them with hydra computations. Because of this the goal is a one.

Code Verification

The Software Quality practices employed by the CTF team are very good. The manuals are in good shape, they have version control and regression testing. Unit testing is employed. Based on the good SQE practices the Code Verification score is a one. However, there is no actual code verification work done in CTF. The team is beginning to define test problems but there has been no work to implement them.

It was agreed that CTF should have some level of code verification. This work is not currently funded or planned but we all agreed that it should be done. To bring CTF up to a low level of code verification we set the goal at 2.

Solution Verification

Russell Hooper created two reports that describe solution verification studies for progression problem 6. The first one documents the initial study that shows first order convergence on problem 6 when the grid spacers are not included. This report shows the initial results on mesh convergence when the grid spacers are included.

In the second study, Russell performed sensitivity studies on the size and location of the grid spacers. Based on this sensitivity study it was determined that small changes in the size and location of the grid space resulted in minimal changes in the total pressure drop. Russell then created an "equivalent" problem 6 CTF nodalization, and clearly demonstrated the expected first order convergence.

Based on these two reports, the current score is 2. It was determined that this was an appropriate level of solution verification for problem 6 so the goal was also set at 2.

Model Validation

The validation work done in CTF is based on Integral Effects Tests (IET) called PSBT. These tests are designed to be appropriate for PWR conditions so they are relevant to the problem 6 application. There is currently no Separate Effects Test (SET) employed to validate the individual closure models in CTF. Because of this lack of SET validation, the model validation score is 0.5.

It is recognized that validation testing is important to CTF so the goal value is set at 2. This work is considered important but there is currently no budget or milestones that address this work.

Uncertainty Quantification and Sensitivity Analysis

It was determined that some uncertainty quantification work was done in the past with the PSBT data. This work was with a pre-CASL version on CTF and was based on “hardwired” code changes. Because of this, this work could not be reproduced with the current version of CTF. For that reason, the current uncertainty quantification score for CTF is a zero.

It did not appear that there would be an effort to separate aleatory and epistemic uncertainties in the future so the uncertainty quantification goal was set at 1.

APPENDIX E: INITIAL MPACT PCMM ANALYSIS

The initial PCMM analysis of MPACT can be summarized in the radar plot Figure 2 representing the initial (or current) and goal PCMM scores for each V&V category as listed in Table 4.

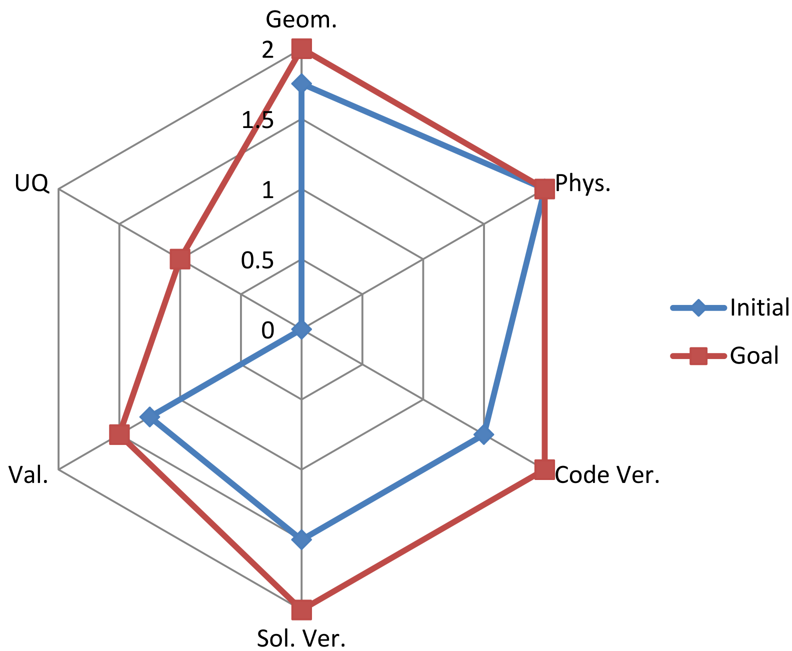

Figure 2. MPACT PCMM

Table 4. Scores of initial and goal PCMM

Element \ score	Initial	Goal
Geom.	1.75	2
Phys.	2	2
Code Ver.	1.5	2
Sol. Ver.	1.5	2
Val.	1.25	1.5
UQ	0	1

The justifications for initial scores are listed as followings:

Representation and Geometric Fidelity: Current score 1.75 versus Goal 2

a. Limited simplification or stylization of major components and BCs
b. Geometry or representation is well defined for major components and some minor components
c. Some peer review conducted
d. Pin bow ignored, gap geometry not represented.
e. Represent crud geometry

Physics and Material Model Fidelity: Current Score 2 versus Goal 2

a. Physics-based models for all important processes
b. Significant calibration needed using separate effects tests (SETs) and integral effects tests (IETs)
c. One-way coupling of models
d. Some peer review conducted
e. Very mature for single physics, less mature for coupled physics.

Code Verification: Current Score 1.5 versus Goal 2

a. Some algorithms are tested to determine the observed order of numerical convergence (evidence)
b. Some features & capabilities (F&C) are tested with benchmark solutions
c. Some peer review conducted
d. Need improved documentation

Solution Verification: Current Score 1.50 versus Goal 2

a. Numerical effects are quantitatively estimated to be small on some SRQs (evidence)
b. I/O independently verified
c. Some peer review conducted

Model Validation: current score 1.25 versus Goal 1.50

a. Quantitative assessment of predictive accuracy for some key SRQs from IETs and SETs
b. Experimental uncertainties are well characterized for most SETs, but poorly known for IETs
c. Some peer review conducted
d. Additional validation needed

Uncertainty Quantification and Sensitivity Analysis: Current score 0 versus Goal 1

a. Judgment only
b. Only deterministic analyses are conducted
c. Uncertainties and sensitivities are not addressed
d. Add cross section UQ

APPENDIX F: INITIAL MAMBA PCMM ANALYSIS

There is a basic problem with MAMBA 1D, that was revealed by this discussion. For each new application MAMBA 1D needs to be recalibrated to MAMBA 3D applied to the same application. MAMBA 1D cannot be applied to a new application without recalibration. The other option is to use MAMBA 3D and stop using MAMBA 1D. The initial PCMM analysis of MPACT can be summarized in the radar plot Figure 3.

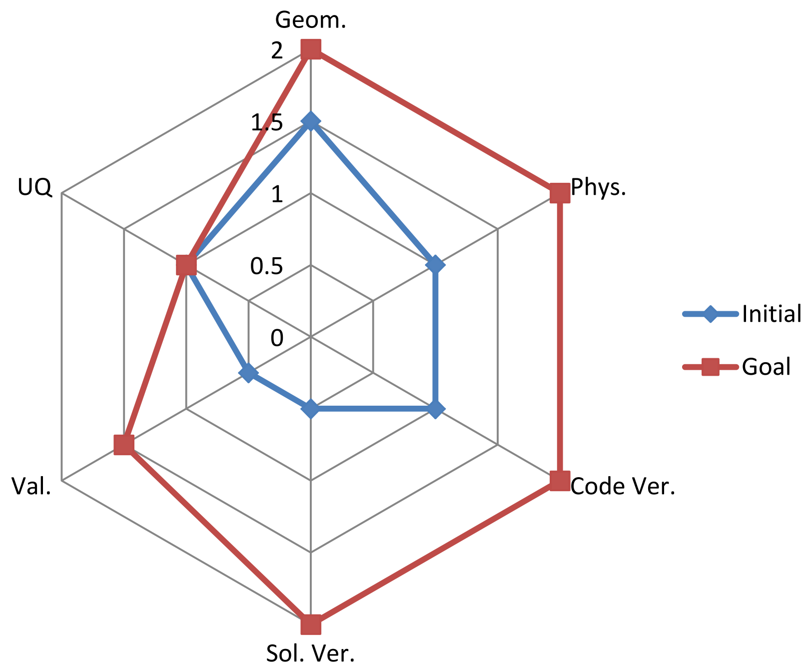

Figure 3. MAMBA PCMM

The justifications for initial scores are listed as followings:

Representation and Geometric Fidelity (1.5)
The geometric description of the CRUD is idealized but the resolution is consistent with the neutronics and thermal hydraulics. The main geometry, the crud thickness is resolved. The lower level geometry like chimneys is not resolved and is modeled with simplifications. This is why the score is less than two.

Physics and Material Model Fidelity (1.0)
The physics is a combination of empirical models and calibrations from MAMBA 3D. There is still some ad hoc coupling of models. In MAMBA 1D, we do not have "physics based models for all important physics.

Code Verification (1.0)
There is a low level of SQE in MAMBA that has been steadily improving. The SQE is now being done at ORNL. There is clearly benchmarking exercises with Boa and MAMBA 3D. There is also

benchmarking between MABA 3D and MAMBA 1D. Peer review of the numerical methods has not been done.

Solution Verification (0.5)
There was an effort to do solution verification on a MAMBA test problem a few years ago. This was never done on a challenge problem. There are still very large uncertainties in the MAMBA input parameters. This score can be improved by documenting some of the sensitivities to the numerical methods in MAMBA for the CASL challenge problems.

Model Validation (0.5)
Although it appears that MAMBA 3D has a good validation pedigree the MAMBA 1D code is highly empirical and its quality is based on benchmarking. The Walt loop validation is done with MAMBA 3D. The only validation of MAMBA 1D is the CIPS comparison with Watts Bar I. The benchmarking has already been accounted for in the code verification section.

Uncertainty Quantification and Sensitivity Analysis (1.0)
There is ongoing work on sensitivity analysis in MAMBA 3D and MAMBA 1D. The MAMBA 1D-sensitivity applies directly and the MAMBA 3D studies can be employed to impact the MAMBA 1D calibration work. There needs to be work to provide parameter distributions to improve the quality of the uncertainty quantification work.

APPENDIX G: INITIAL BISON PCMM ANALYSIS

The initial PCMM analysis of MPACT can be summarized in the radar plot Figure 4. This plot indicates that the BISON code is mature for the CASL challenge problems.

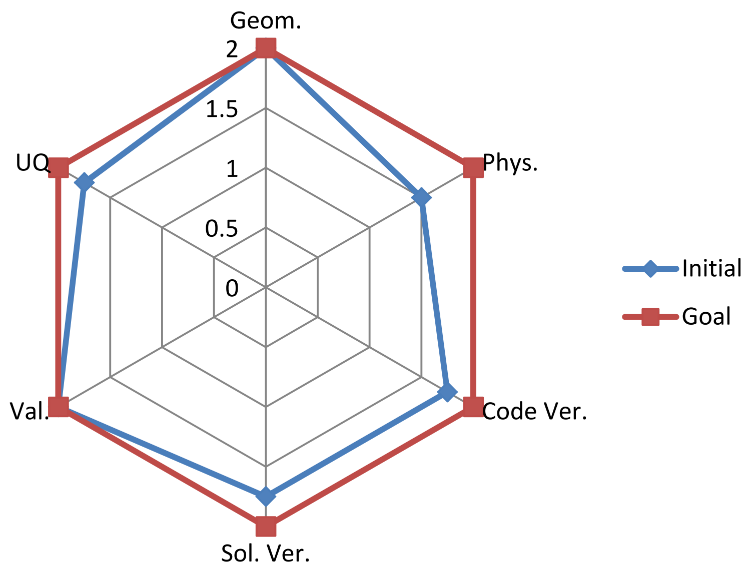

Figure 4. BISON PCMM

The justifications for initial scores are listed as followings:

Representation and Geometric Fidelity (2.0)
Compared to its counterparts FRAPCON and FRAPTRAN, BISON has high fidelity geometry descriptions when used in 3D mode. Simplifications can be done to make the code run faster, but when fidelity is required, the 3D discretization is there. There is not yet “as-built” or independent peer review of the geometry description, it is still idealized.

Physics and Material Model Fidelity (1.5)
BISON still depends on some empirical models for some important processes. This is steadily being improved but they are not there yet. Otherwise, the score would be a 2. Calibration of model parameters is still required.

Code Verification (1.75)
The software quality work in BISON is high level. Unit testing and regression testing is in continual use. The documentation is also in good shape. There has been extensive benchmarking with FALCON. The only thing keeping the score from a 2 is the lack of testing of designed order of accuracy. Independent peer review of the numerical methods has not been done.

Solution Verification (1.75)

This score would have been a 2, except of independent verification of the I/O. This score will go up when we get more BISON users inside of CASL and outside of INL. There is a nice section in the BISON V&V plan where solution verification is done and numerical errors are estimated.

Model Validation (2.0)
The BISON V&V manual includes IET and SEI validation work on the key physical phenomenon associated with the CASL quantities of interest. Better characterization of the experimental uncertainties will help to improve this score.

Uncertainty Quantification and Sensitivity Analysis (1.75)
Bison has done work on uncertainty quantification and has published these results and participated in industry benchmark studies. The Aleatory and Epistemic uncertainties are not currently separated in the BISON UQ work. This is preventing a score of 2.0.

APPENDIX H: PCMM Matrix

Table 5 PCMM Matrix

ELEMENT \ MATURITY	Maturity Level 0 Low Consequence, Minimal M&S Impact, e.g. Scoping Studies	Maturity Level 1 Moderate Consequence, Some M&S Impact, e.g. Design Support	Maturity Level 2 High-Consequence, High M&S Impact, e.g. Qualification Support	Maturity Level 3 High-Consequence, Decision-Making Based on M&S, e.g. Qualification or Certification
Representation and Geometric Fidelity What features are neglected because of simplifications or stylizations?	• Judgment only • Little or no representational or geometric fidelity for the system and BCs	• Significant simplification or stylization of the system and BCs • Geometry or representation of major components is defined	• Limited simplification or stylization of major components and BCs • 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 BCs • Geometry or representation of all components is at the detail of "as built", e.g., gaps, material interfaces, fasteners • Independent peer review conducted
Physics and Material Model Fidelity How fundamental are the physics and material models and what is the level of model calibration?	• 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 hoc coupling 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 SETs and IETs • Sound physical basis for extrapolation and coupling of models • Full, two-way coupling of models • Independent peer review conducted
Code Verification Are algorithm deficiencies, software errors, and poor SQE practices corrupting the simulation results?	• Judgment only • Minimal testing of any software elements • Little or no SQE procedures specified or followed	• Code is managed by SQE procedures • Unit and regression testing conducted • Some comparisons made with benchmarks	• 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 and human procedural errors corrupting the simulation results?	• 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
Model Validation How carefully is the accuracy of the simulation and experimental results assessed at various tiers in a validation hierarchy?	• Judgment only • Few, if any, comparisons with measurements from similar systems or applications	• 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 and SETs • Experimental uncertainties are well characterized for most SETs, but poorly known for IETs • Some peer review conducted	• Quantitative assessment of predictive accuracy for all important SRQs from IETs and SETs at conditions/geometries directly relevant to the application • Experimental uncertainties are well characterized for all IETs and SETs • Independent peer review conducted
Uncertainty Quantification and Sensitivity Analysis How thoroughly are uncertainties and sensitivities 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 • Some strong assumptions made • Some peer review conducted	• 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 • Independent peer review conducted

APPENDIX I: VALIDATION PYRAMIDS

Validation Pyramid Methodology

Introduction

Validation pyramid as a conceptual framework for visualizing, planning and implementing validation activity dated back to the AIAA CFD V&V Best Practice guideline (1998). The knowledge-based system pyramid in general and validation pyramid in particular, builds on hierarchical structure that appeal to human mind in analyzing a complex system. In fact, hierarchical decomposition is often used to describe goals-oriented functional systems. This includes their application to multiscale, multiphysics systems, characteristic of modern engineering applications such as challenge problems in CASL.

Despite inherent drawbacks due to simplification, hierarchical treatments are popular and attractive for engineering decision-making thanking to easiness for understanding, modeling and control. The fundamental principles that govern the successful use of hierarchical system are scale separation, and physics decoupling which manifest system's weak nonlinearity (Herbert A. Simon, 'The Architecture of Complexity", 1962).

It is noted that such assumptions are not valid in a rigorous sense for general complex (nonlinear) systems, where the physics and scales of participating elements (phenomena, sub-systems) are tightly coupled (and hence strong nonlinearity). However, system decomposition can be made along the line of weak nonlinearity. The practical use of validation pyramid thus follows George Box's guide: "All models are wrong. But how wrong do they have to be to not be useful?"

For CASL, the validation pyramid was adopted as a framework for validation in the original proposal for the U.S. Department of Energy's Energy Innovation Hub on Nuclear Energy Modeling and Simulation (CASL, 2010) [6].

Evolution of concepts

Validation pyramids are very useful means to visualize and communicate validation activity. It stresses the notion that fundamental tests and system tests are equally foundational to the confidence in prediction.

The original AIAA (1998) validation pyramid (Figure 5) follows a system decomposition into subsystem, and units. As it can be seen, upper level like subsystems and benchmark cases may include several lower level e.g., unit problems. The decomposition appears to be largely driven by geometrical partitioning. The decomposition does not make a clear demarcation between physical system and phenomena involved. To a large extent, this is because the guide is focused on V&V of Computational Fluid Dynamics (CFD) simulation, dominantly, of single-phase turbulent flow in aerospace applications. Thus fluid flow is the overarching phenomenon, rendering the complex CFD problem a "homogeneous" model.

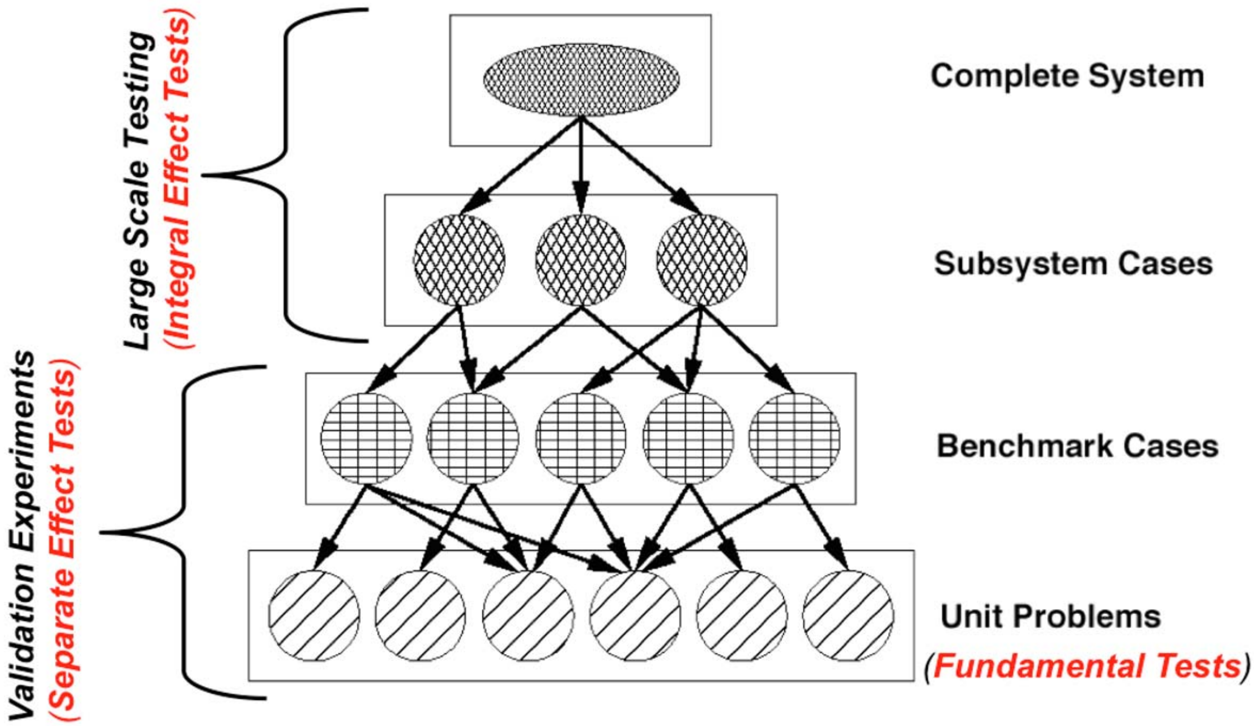

Figure 5. Validation pyramid (AIAA, 1998).

The “unit problems” represent different flow configurations, from channel flow of different channel geometry, to orifice, to jet impingement, and flow regimes (natural, mixed, forced convection). In parallel to the terminology used in nuclear thermal-hydraulics, unit problems and benchmark cases can be classified as separate-effect tests (SET), while integral-effect tests (IET) would include subsystem cases and testing on complete system. Application of the AIAA (1998) pyramid to multiphysics challenge problems in CASL is hampered by the need to handle heterogeneous models, including a large number of phenomena (from nucleation of vapor bubbles, to material chemistry).

In the CASL (2009) proposal, the validation pyramid equates to a full system decomposition into so-called “components” through a component identification/ ranking process (CIRP).

As seen from the Figure 6, the validation pyramid represents complexity in four levels: for system, it decomposes from (S1) full system, to (S2) scaled prototypes, to (S3) multiphysics components and subsystems, and (S4) single physics components. In the same pyramid, four levels of evidence (data) are gathered (E1) plant measurements and observations (PMO, which are rare, incomplete); (E2) integral effects testing (IET), (E3) mIET, or small IETs, and (E4) many separate-effect tests.
Note that (S)-line describes a functional system decomposition. The (E)-line describes an experimental data support. While the decomposition goes top-down, uncertainty propagates upwards. To relate component behaviors are processes that are expected to occur in prototypic reactor systems, scaling is a significant issue, as shown in the pyramid.

Given “full system” as a phenomenon in a nuclear power plant, the CIRP is phenomena identification and ranking table (PIRT). The PIRT process was developed as part of the U.S. Nuclear Regulatory Commission’s Code Scaling, Applicability, and Uncertainty (CSAU) methodology (CSAU, 1988 [1]). The PIRT also plays a central role in the U/S. NRC’s Regulatory Guide 1.203

"Evaluation Model Development and Assessment Process". (EMDAP, 2005 [2]). It should be noted that PIRT product is in the form of table of phenomena P([I],[K]), where [I] denotes level of importance, and [K] denotes level of knowledge about the phenomena. As such, PIRT does not follow, or necessarily lead to a hierarchical system.

For application under consideration, each phenomenon P_j is characterized by:

- a set of quantities of interest (QoI) [QoI(P_j)],
  - a set of system conditions [$SysCond_m$ (P_j)], n = (1, N), where N is number of system condition, each condition is characterized by
    - a set of M dimensional and/or non-dimensionalized parameters, each has an operating range for the given application (scenario)
      - $Par_{(n,,m),} = (Par,_{(n,m,min),}, Par_{(n,m,max)})$.

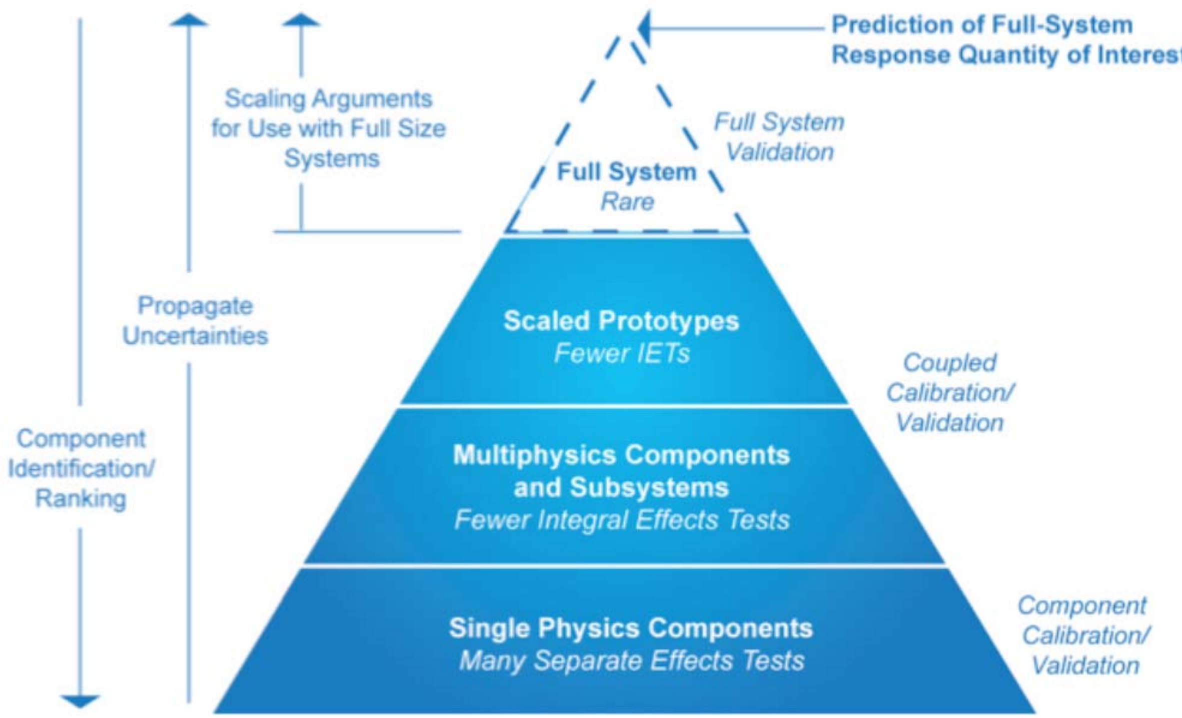

Figure 6. Validation pyramid for CASL (2009)

While designed to represent CASL multiphysics challenge problems, the CASL (2009) pyramid (Figure 6) did not make the distinction between physical phenomena that are expected to occur in the system (Px), and components/subsystem in the plant system (Sx), and data from available experiments (Ex). Notably, experiments for certain separate-effect characterization do not confine within "single physics components". Having [Px], [Sx] and [Ex] in one pyramid constrains the application of such pyramid to systems where system components have their respective physics and respective experiments to support the physics within the component.

Validation pyramid as a tool for assessing coverage

For CASL codes and challenge problems, the V&V process is guided by the Predictive Capability Maturity Model (PCMM), which was introduced by Oberkampf, Pilch and Trucano (2004). PCMM is a decision model that facilitates decision-making about maturity (appropriateness, applicability, trustworthiness) of a predictive capability (a code, or a system of coupled cods) for a given application.

Within PCMM, validation is a critical component. The validation process is illustrated in the Figure 7 below. Although "system" is shown as a pyramid, it is not necessarily for a generalized case. For a given system [Sys] under a given operating or accident scenario [Cond], PIRT process will help generate a PP, a PIRT-based phenomenology pyramid.

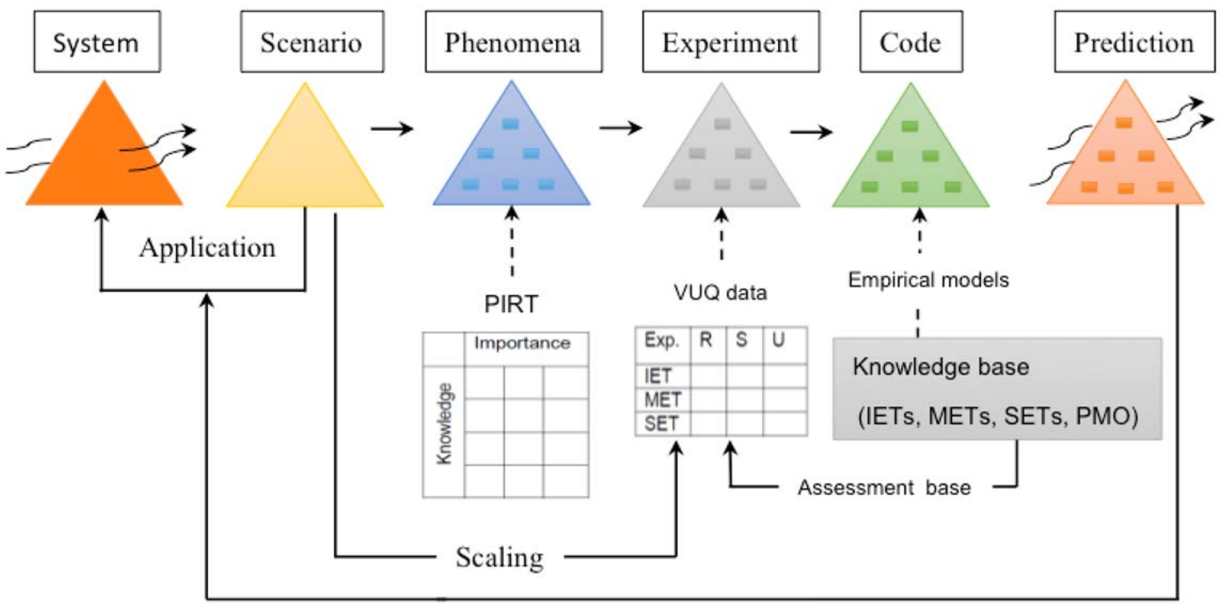

Figure 7. Validation process illustrated through a sequence of validation pyramids (PP, PE, and PM)

Generally speaking, knowledge base and capability including experiments, models, and codes are developed for a scope broader than for specific applications. Therefore, models and experiments do not necessarily be structured in hierarchy. However, given the phenomenology pyramid (PP), we can identify relevant models (which affect the prediction of QOIs) and experiments to build a code-based model pyramid (PM) and experiments-based data pyramid (PE). Figure 8 shows the relationship between these three pyramids applied for a challenge problem.

The predictive capability of a computer code or a system of coupled codes is determined based on a set of models of phenomena, processes, mechanisms, and factors of relevance to the application under consideration. The maturity of the predictive capability can be characterized by

- [CMP] - phenomenological coverage of (PP) [P_j] by models in (PM)
- [CME] - validation coverage of (PE) by models in (PM)
- [CEP] - experimental coverage of (PP) by experimental data in (PEE)

- [QPIRT] expresses quality of the PIRT process that results in phenomenology pyramid (PP). The quality depends on organization of the PIRT, expertise of participants, their depth and coverage. [QPIRT] < 1.
- [QVer] expresses quality of simulation codes as characterized through the SQA, depth and coverage of code verification and solution verification for relevant conditions. [QVer] < 1.
- [QExp] expresses quality of experiments used, including measurement uncertainty, data acquisition and data processing. [QExp] < 1.
- [CMP] characterizes degree of coverage of models in the codes used for phenomena identified in phenomenology pyramid. [CMP] < 1.

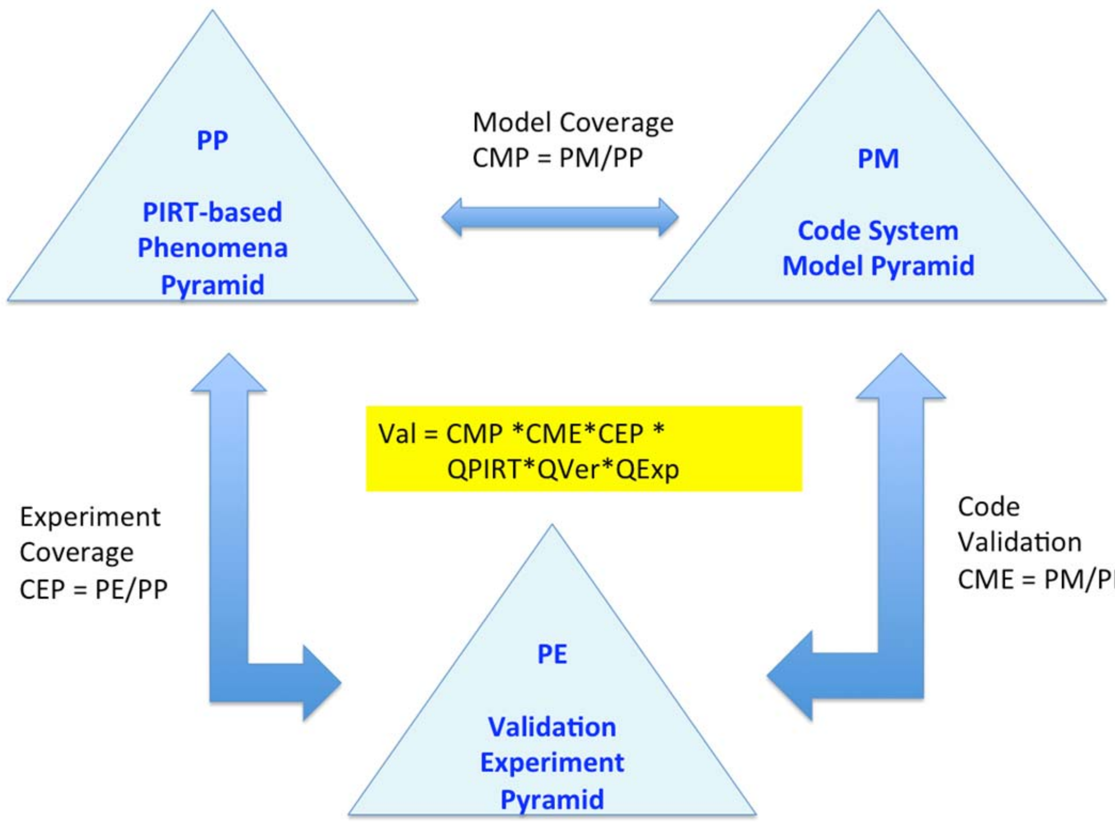

Figure 8. Relationships of pyramids.

CIPS Validation Pyramid

Figure 9 depicts the CRUD multiphysics and multi-scale phenomenological decomposition, indicating the importance of coupling of phenomena at different scales.

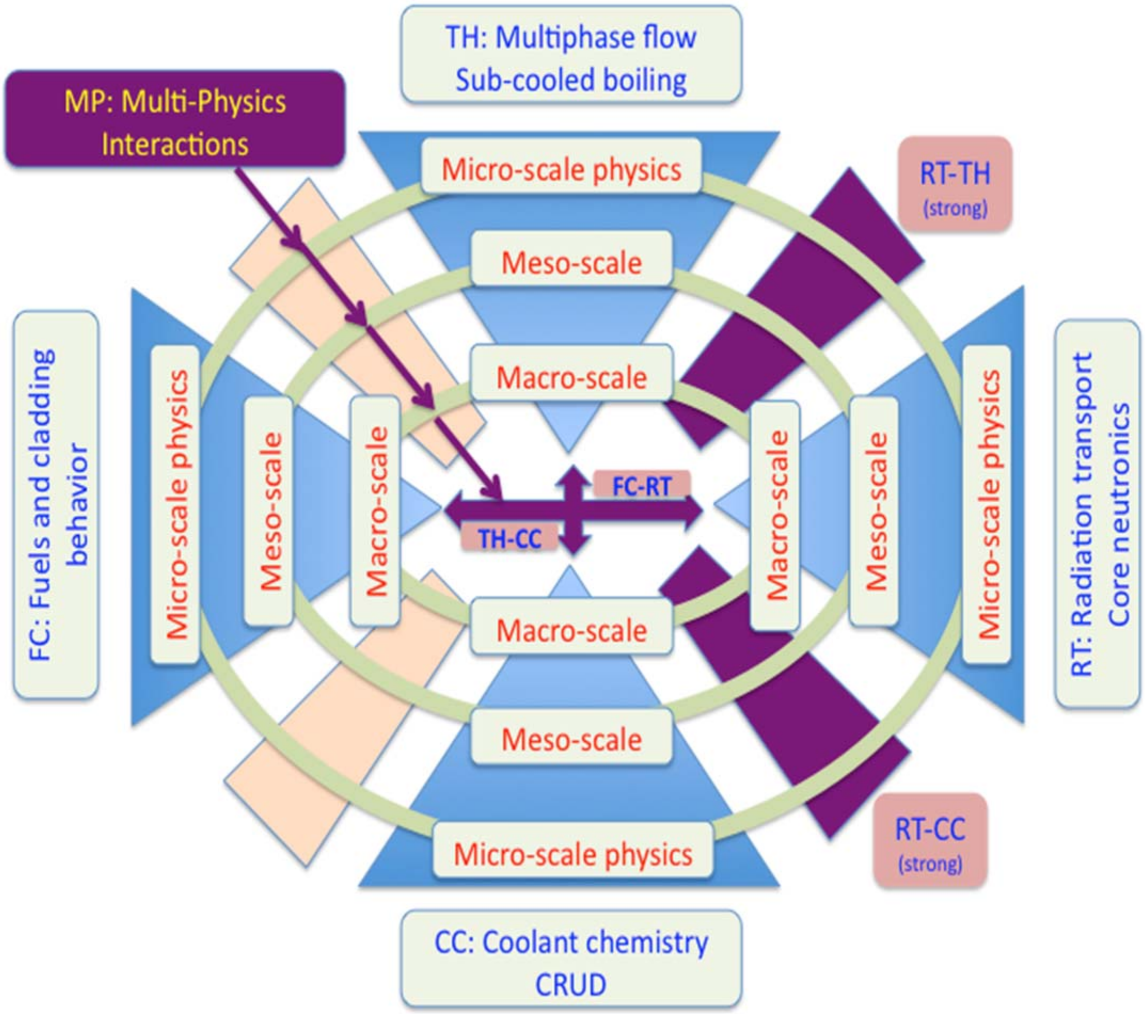

Figure 9. CRUD multiphysics and multi-scale phenomenology pyramid.

Figure 10 presents the color-coded validation pyramid for the CIPS measured axial offset problem. The font colors represent importance of the phenomena while the background colors represent knowledge level of each phenomenon such as Red is high, Black is medium, and Blue is low. These validation assessments are results of the V&V analysis described in above section. For example, the steaming rate is very important for the thermal-hydraulics model and has medium level of knowledge. At the same time, the CRUD mechanical structural properties are not important and have low level of knowledge for the CRUD coolant chemistry model.

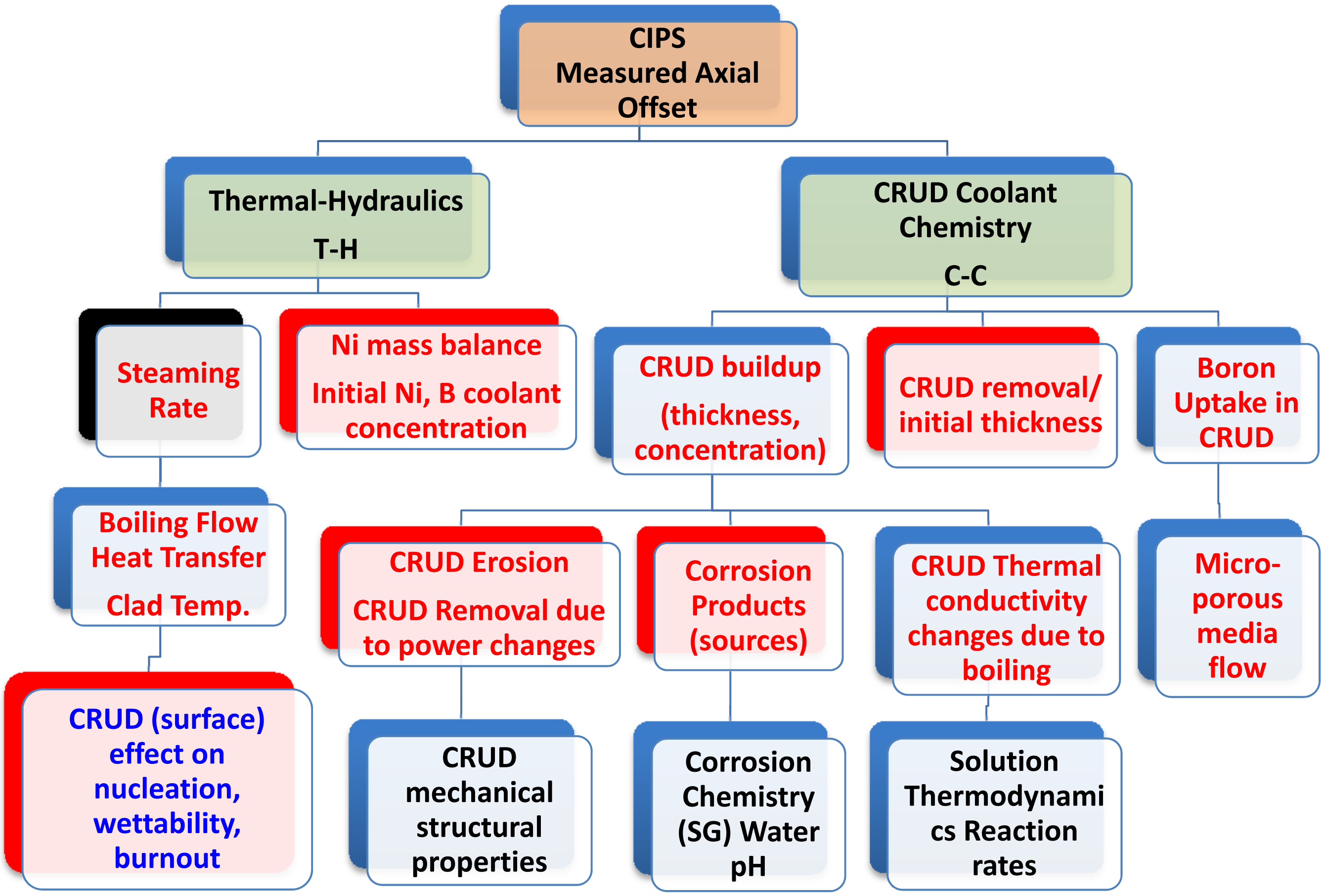

Figure 10. CIPS validation pyramid

PCI Validation Pyramid

Figure 11 presents the validation pyramid for the PCI failure calculation in LWRs.

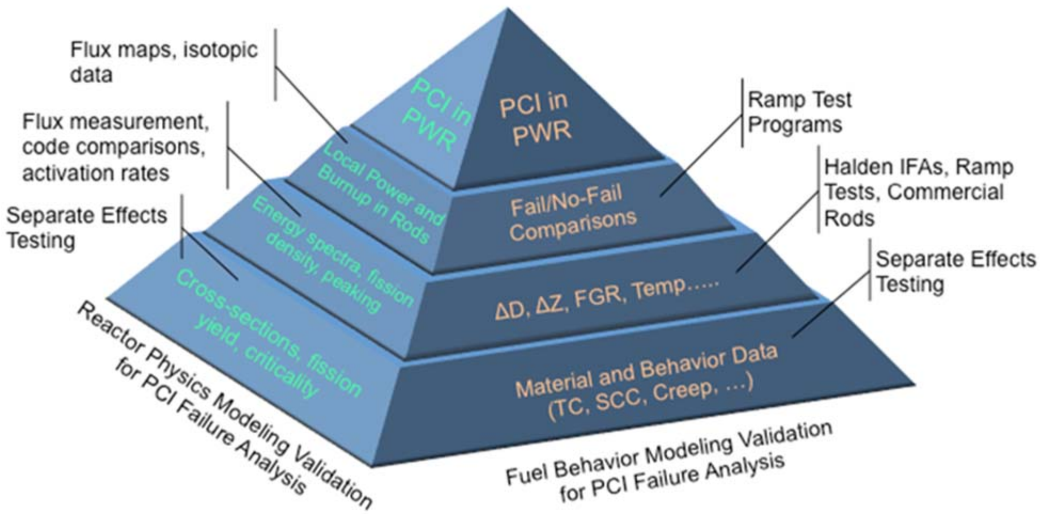

Figure 11. Validation Pyramid for Calculating PCI Failure in LWRs

Figure 12, Figure 13, and Figure 14 present the color-coded validation pyramid for the PCI reactor physics, thermal-hydraulics, and fuel performance codes, respectively. The font colors represent importance of the phenomena such as Red is high, Orange is medium, and Blue is low while the background colors represent knowledge level of each phenomenon such as Red is high, Yellow is medium, and Blue is low. For PCI problems, knowledge about reactor physics and thermal hydraulics are moderate, but fuel performance needs additional data for better understanding.

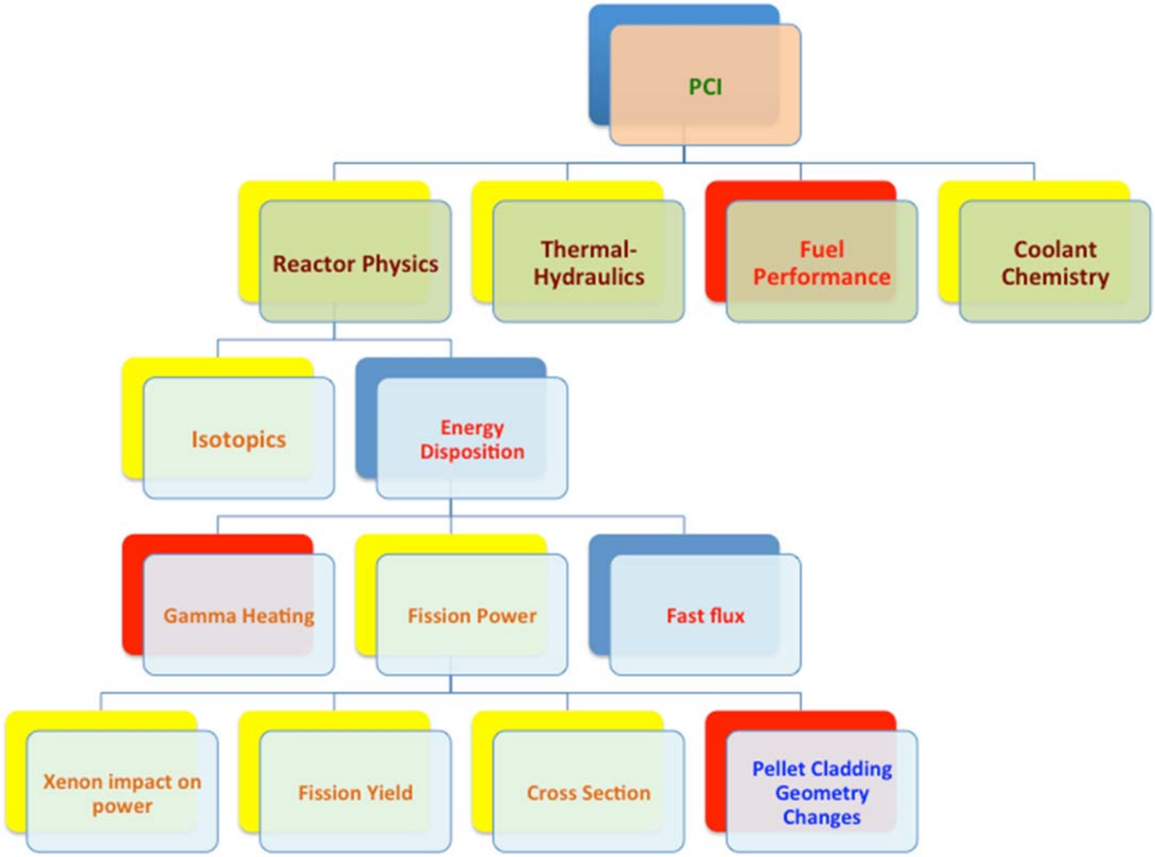

Figure 12. Validation Pyramid for reactor physics codes used for PCI calculation

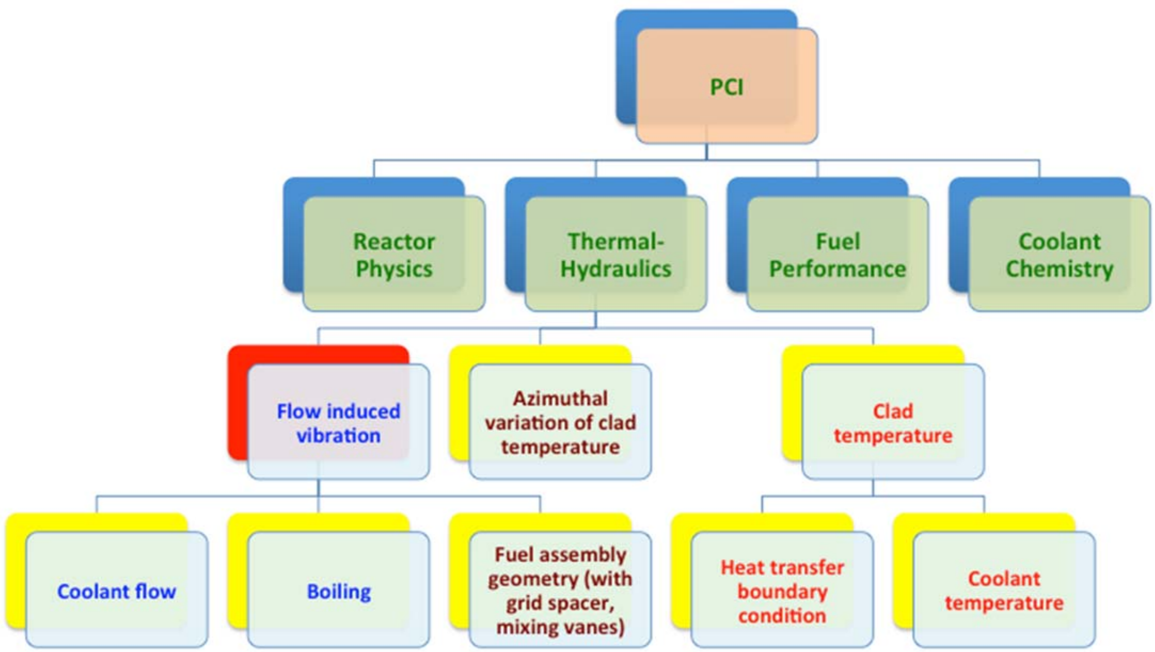

Figure 13. Validation Pyramid for the thermal-hydraulics codes used for PCI calculation

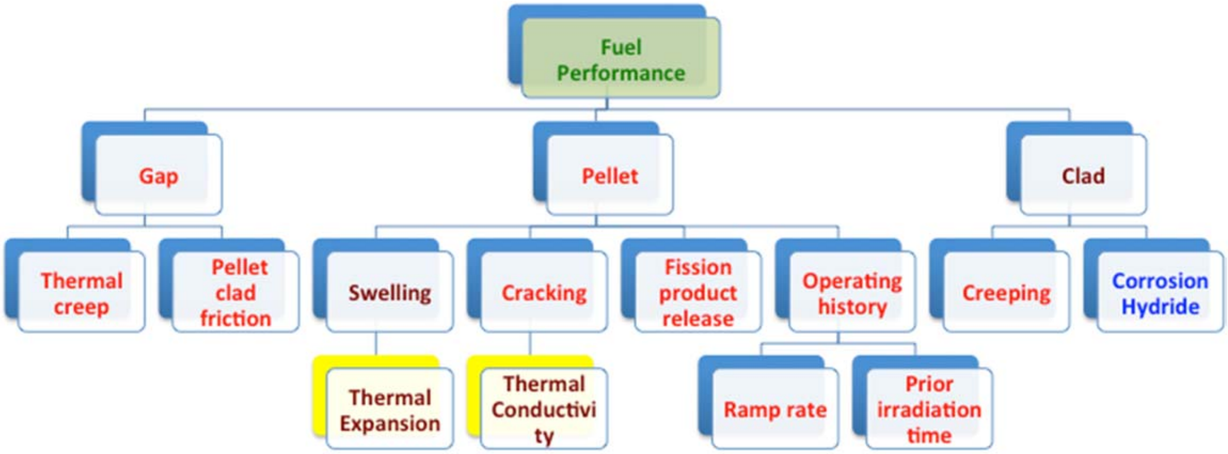

Figure 14. Validation Pyramid for fuel performance codes used for PCI calculation

DNB Validation Pyramid

Figure 15 depicts the DNB multi-scale phenomenological decomposition, indicating the important phenomena at different scales.

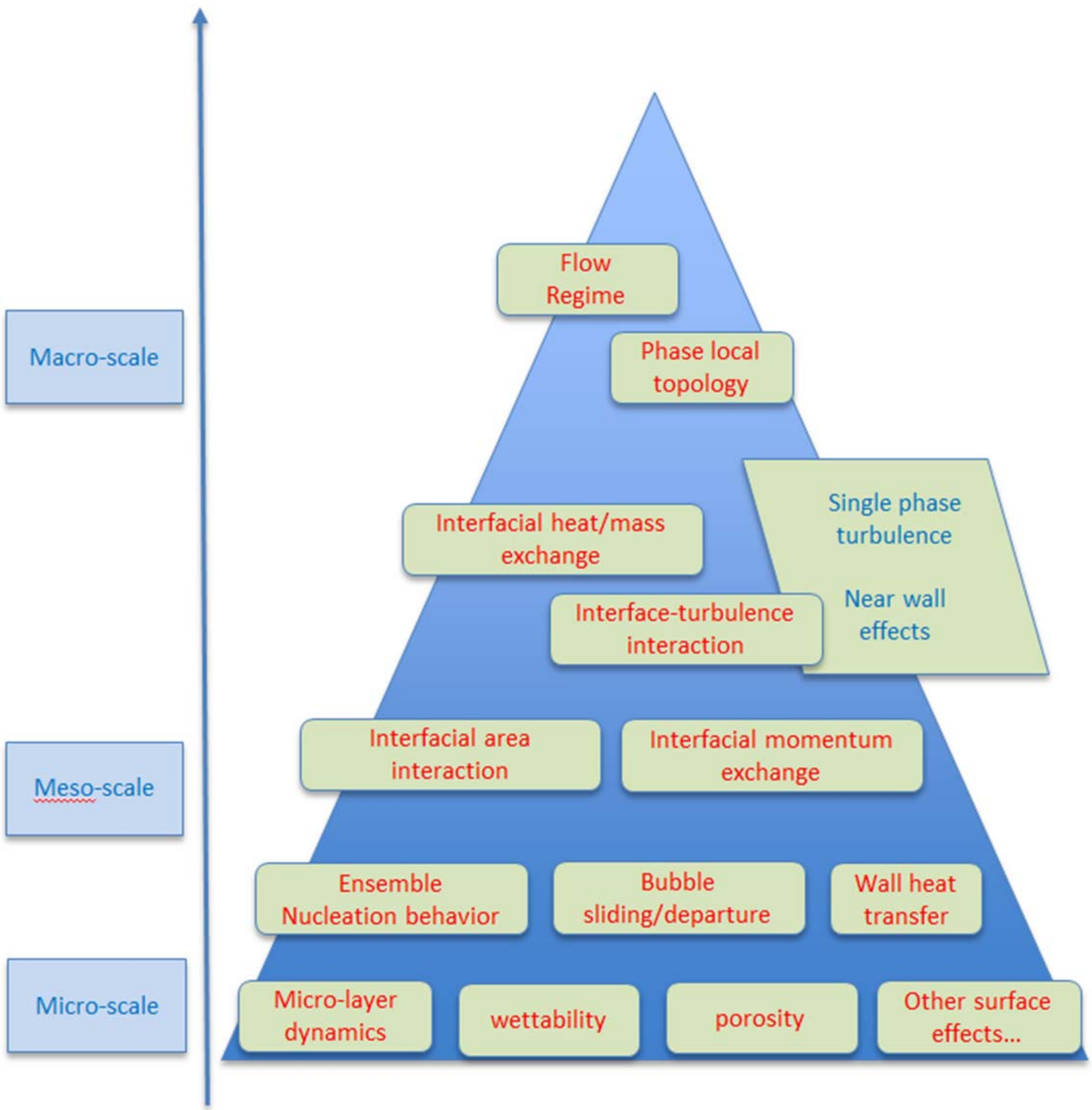

Figure 15. Phenomenology pyramid of two-phase thermal hydraulics.

Figure 16 presents a phenomena pyramid for DNB challenge problem, which provides links between separate phenomena layer and integral phenomena layer to simulate the DNB challenge problem. Figure 17 presents the phenomena pyramids for low pressure subcooled flow boiling application and Figure 18 presents the phenomena pyramids for high pressure subcooled flow boiling application. Figure 19 presents the model pyramid for two-phase thermo-hydraulics. Figure 20 shows experimental validation pyramid for two-phase flow thermo-hydraulics.

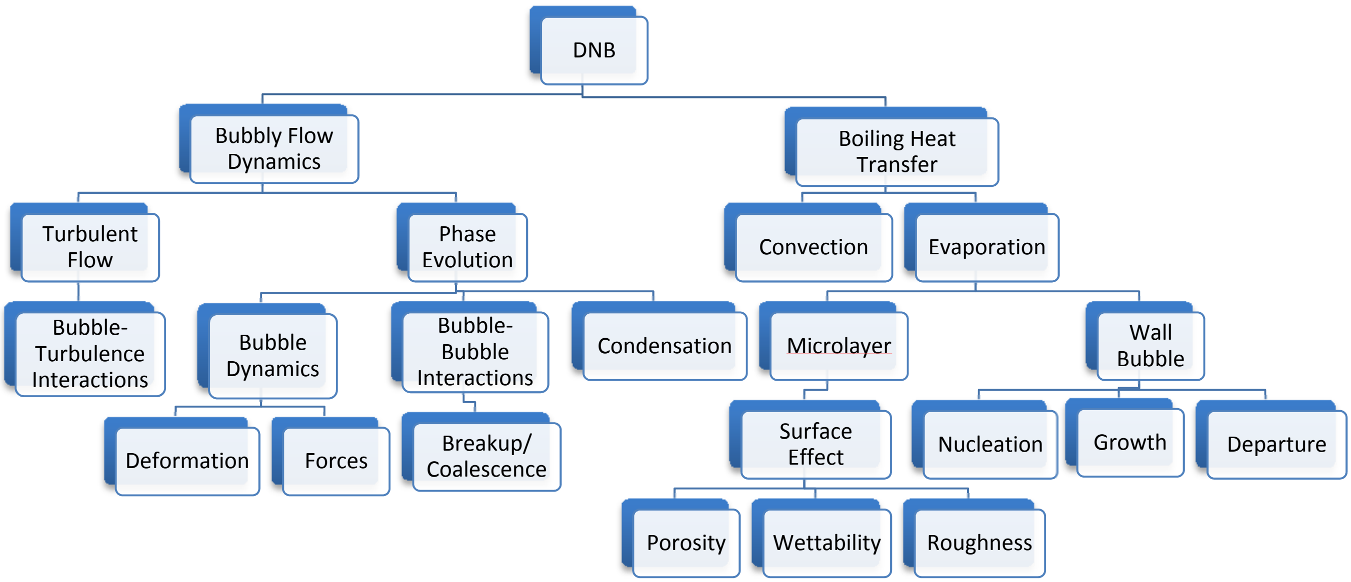

Figure 16. Phenomena pyramid for DNB challenge problem.

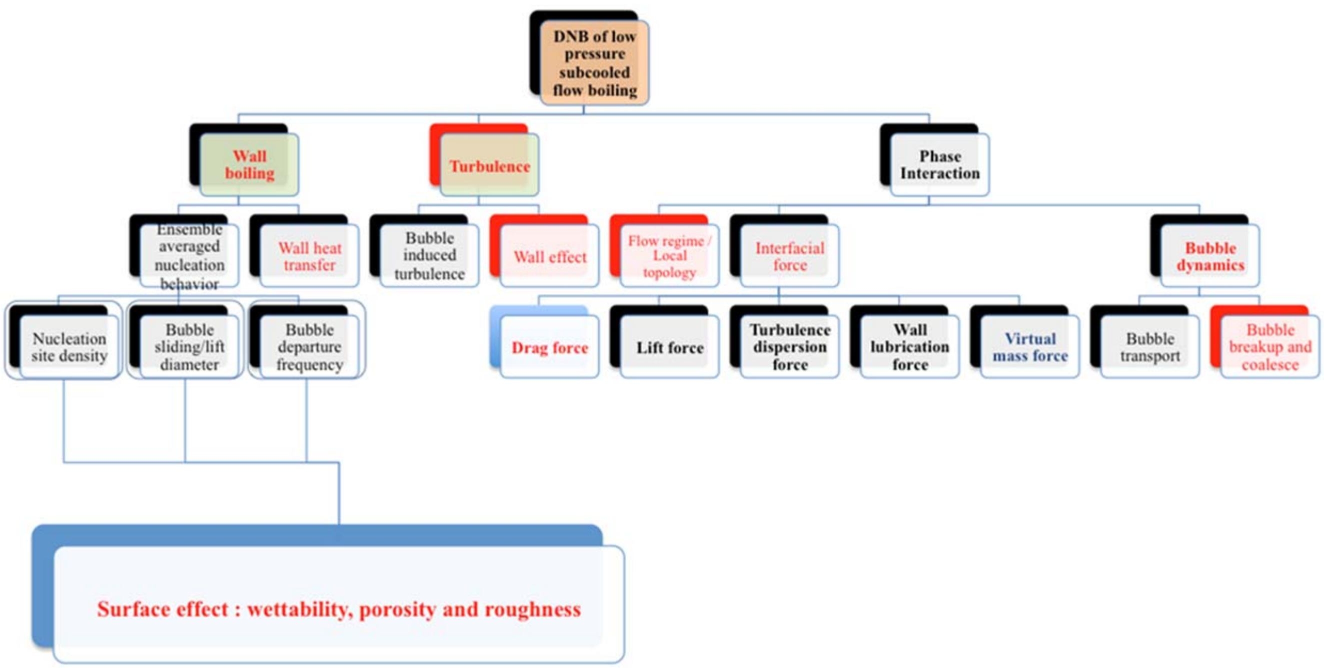

Figure 17. DNB of low pressure subcooled flow boiling (Importance font color: H=Red; M=Black; L=Blue; Knowledge background: L=Red; M=Black; H=Blue).

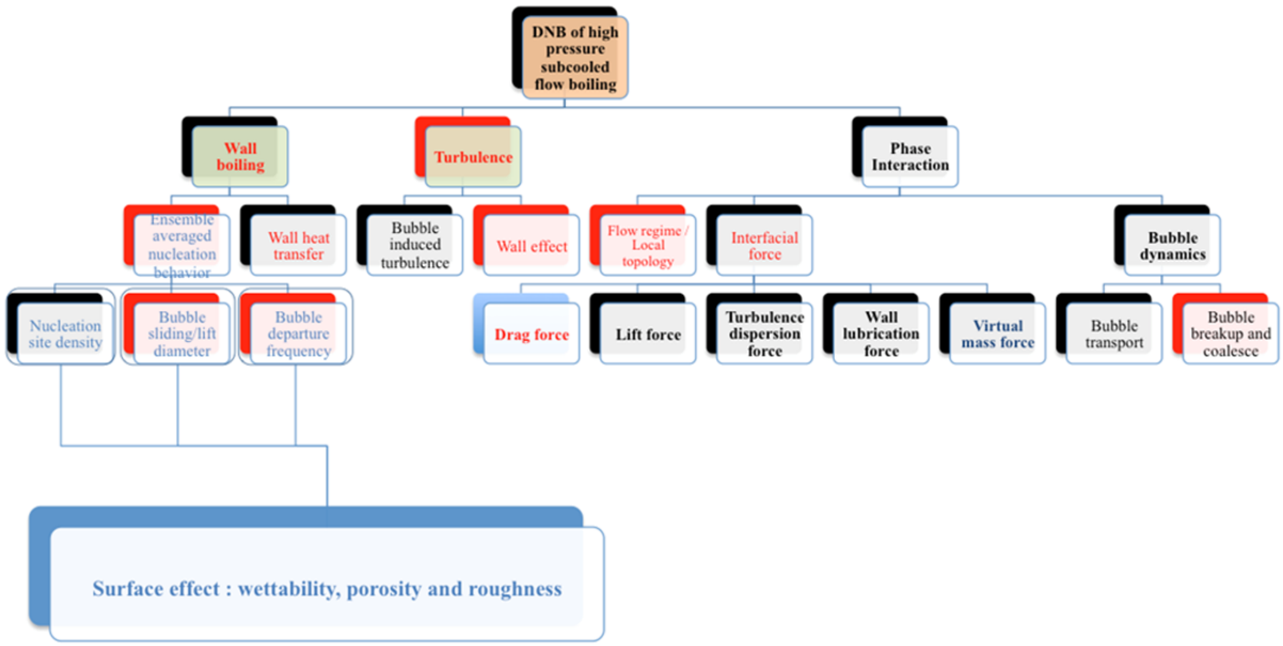

Figure 18. DNB of high pressure subcooled flow boiling (Importance font color: H=Red; M=Black; L=Blue; Knowledge background: L=Red; M=Black; H=Blue)

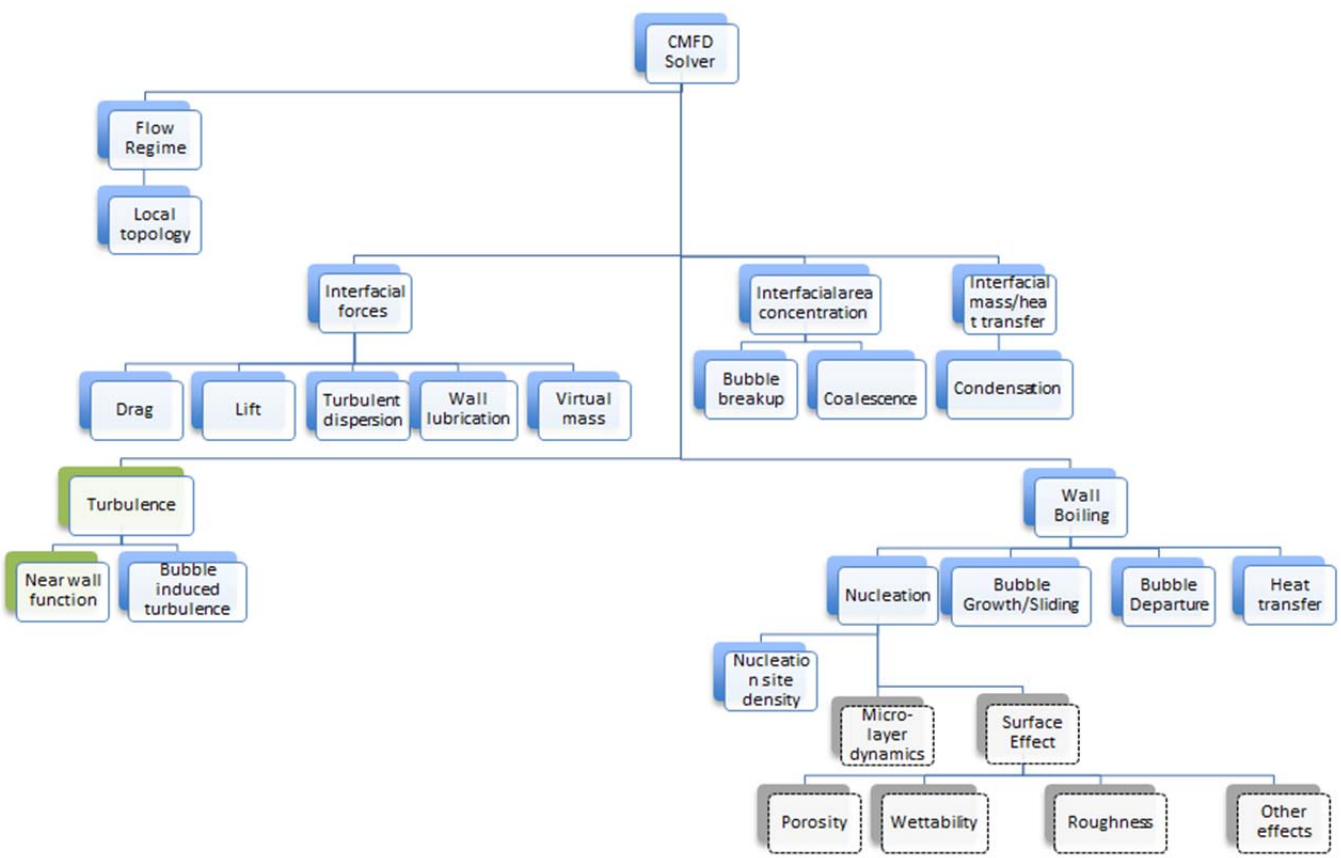

Figure 19. Model pyramid of two-phase flow thermos-hydraulics (Green means models from single phase flow). The micro-scale model is still missing in current solver (shown in grey).

Table 6 A selected set of physical and numerical experiments to provide data for validation of CASL two-phase thermos-hydraulics models

Phenomena coverage	Contributors/sources
1:flow regime and local topology (MET)	MT-Loop / DEBORA
2:Interfacial forces (MET)	NCSU Bolotnov (DNS numeric data)
3:Interfacial concertation(MET)	Purdue (Leung, et al)/ KAIST (Thai, et al)
4:Wall boiling (MET)	BETA / MIT Buongiorno
5:Nucleation site density (SET)	Wang-Dhir / Lemmert-Chawla / …
6: Bubble departure and growth (SET)	Cole / Basu-Dhir/ Tolubinsky
7: Micro-layer dynamics (SET)	Yabuki / Utaka
8: Surface effect (SET)	MIT O’hanley
9: IET	Bartolamaj

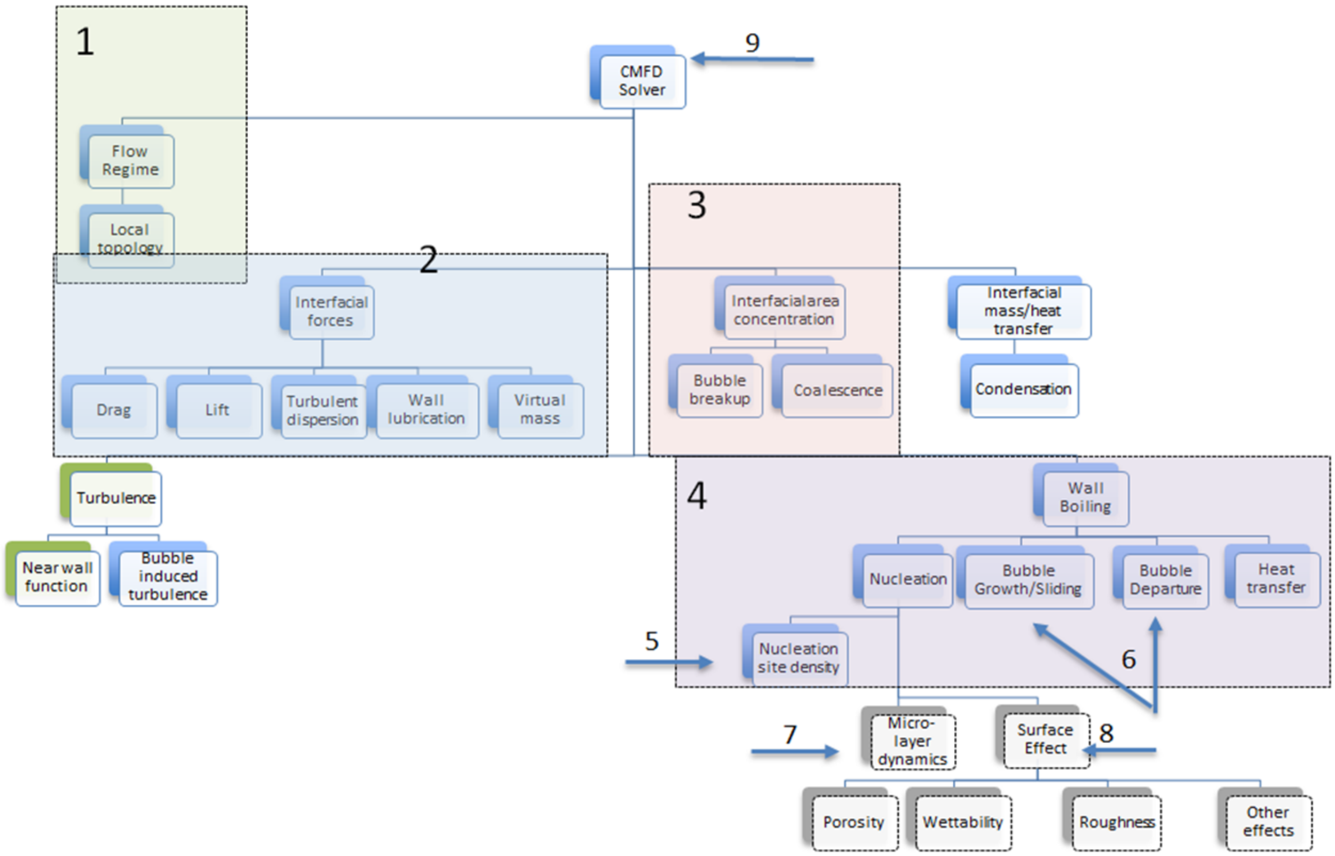

Figure 20. Experimental validation pyramid for CASL two-phase flow thermos-hydraulics. The number corresponds to the numeration in Error! Reference source not found.**.**