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CASL Validation Data: An Initial Review

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About this Document

This report is prepared for CASL program's VUQ Focus Area under activity VUQ.VVDA.Y1-1.02 entitled "Complete initial review of experimental data and plant observations related to CRUD and GTRF challenge problems".

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The work described in this report has benefitted from interactions with contributors and collaborators in CASL, LWR-S and NEAMS programs.

Abstract

The study aims to establish a comprehensive view of "data" needed for supporting implementation of the Consortium of Advanced Simulation of LWRs (CASL). Insights from this review (and its continual refinement), together with other elements developed in CASL, should provide the foundation for developing the CASL Validation Data Plan (VDP). VDP is instrumental to the development and assessment of CASL simulation tools as predictive capability. Most importantly, to be useful for CASL, the VDP must be devised (and agreed upon by all participating stakeholders) with appropriate account for nature of nuclear engineering applications, the availability, types and quality of CASL-related data, and novelty of CASL goals and its approach to the selected challenge problems.

The initial review (summarized on the January 2011 report version) discusses a broad range of methodological issues in data review and Validation Data Plan. Such a top-down emphasis in data review is both needed to see a big picture on CASL data and appropriate when the actual data are not available for detailed scrutiny. As the data become available later in 2011, a revision of data review (and regular update) should be performed. It is expected that the basic framework for review laid out in this report will help streamline the CASL data review in a way that most pertinent to CASL VDP.

Acronyms

	Description	*Comments/ Relationship*
AIAA	American Institute of Aeronautics and Astronautics	
AMA	Advanced Modeling Applications	CASL FA
AMS	Advanced Modeling and Simulation	
ANS	American Nuclear Society	
AOA	Axial Offset Anomaly	
ASME	American Society of Mechanical Engineers	
ASA	Adjoint Sensitivity Analysis	
BEPU	Best Estimate Plus Uncertainty	
BWR	Boiling Water Reactor	
CASL	Consortium for Advanced Simulation of LWRs	
CFD	Computational Fluid Dynamics	
CHF	Critical Heat Flux	
CIPS	Crud Induced Power Shift	
CILC	Crud Induced Localized Corrosion	
CPTS	Challenge Problem Technical Specification	AMA
CRUD	Chalk Rivers Unidentified Deposit	
CSAU	Code Scaling, Applicability, and Uncertainty	
CT	Computer Tomography	
DA	Data Assimilation	
DNB	Departure from Nucleate Boiling (CHF)	
DoE	Department of Energy	
EPRI	Electric Power Research Institute	
FA	Focus Area	CASL
FSA	Forward Sensitivity Analysis	Deterministic
FSI	Fluid-Structure Interaction	
GTRF	Grid To Rod Fretting	
IET	Integral-Effect Test	
IFPE	International Fuel Performance Experiments	IAEA-OECD Db
INL	Idaho National Laboratory	
IR	Infrared (thermometry)	
LANL	Los Alamos National Laboratory	
LIME	Lightweight Integrating Multiphysics Environment	SNL
LOCA	Loss Of Coolant Accident	
LWR	Light Water Reactor	
LWR-S	LWR Sustainability	DoE Program
MC	Model Calibration	
M-C	Monte-Carlo	
MNM	Models and Numerical Methods	CASL FA

MPO	Materials Performance and Optimization	CASL FA
NE	Nuclear Energy	
NE-CAMS	NE Computational Applications Management System	
NEAMS	Nuclear Energy Advanced Modeling & Simulation	DoE Program
NGSAC	Next-Generation Safety Analysis Code	
NPP	Nuclear Power Plant	
NRC	Nuclear Regulatory Commission	
NWP	Numerical weather Prediction	
ONB	Onset Nucleate Boiling	
ORNL	Oak Ridge National Laboratory	
PCI	Pellet-Clad Interaction	Fuel
PCI	Predictive Capability Index	ModSim
PCM	Predictive Capability Maturity	
PCMM	PCM Model	
PDE	Partial Differential Equation	
PDF	Probability Distribution Function	
PIE	Post Irradiation Examination	
PIRT	Phenomena Identification and Ranking Table	
PIV	Particle Image Velocimetry	
PMO	Plant Measurements and Observations	Plant Data
PWR	Pressurized Water Reactor	
QA	Quality Assurance	
QMU	Quantification of Margin and Uncertainty	ASC
Q-PIRT	Quantitative (quantified) PIRT	
R7	(also called RELAP-7) a NGSAC developed in LWR-S	Support RISMC
RBHT	Rod Bundle Heat Transfer	
RBTH	Rod Bundle Thermal Hydraulics	
ROAAM	Risk-Oriented Accident Analysis Methodology	
RELAP	Reactor Excursion and Leakage Analysis Program	
RISMC	Risk-Informed Safety Margin Characterization	
SA	Sensitivity Analysis	
SAMAP	Simulation-Aided Margin Analysis Process	RISMC
SFB	Subcooled Flow Boiling	
SET	Separate-Effect Test	
SNL	Sandia National Laboratory	
SQA	Software Quality Assurance	
STH	System Thermal Hydraulics (code)	e.g., RELAP
UQ	Uncertainty Quantification	
V&V	Verification and Validation	
VDP	Validation Data Plan	
VERA	Virtual Environment for Reactor Applications	
VRI	Virtual Reactor Integration	CASL FA
VUQ	V&V and UQ	CASL FA

Executive Summary

The milestone report provides a scoping review of VUQ fitness of experimental data and plant observations related to two challenge problems. In essence, the present work investigates and exploits CASL data characterization as a bridge that connects the developments in applications (AMA), tools (VRI), and validation (VUQ) focus areas.

In a top-down approach, the challenge problems are analyzed with respect to their data needs for implementing a modern VUQ process for VERA. To make the present task plausible, the analysis is carried out for (1) a (sub-)set of projected VERA tools (i.e., with capabilities and quality within the VERA development plan) and (2) an appropriate VUQ process (defined within the VUQ FA development plan). The analysis leads to (3) identification of (a range of possible) experiments and plant measurements of potential interest, and their desired VUQ-related characteristics.

In a bottom-up approach, (4) known and available sources of experiments and plant observations are reviewed and analyzed (5) for their quality (relevance, scalability, uncertainty) in the VUQ of the simulation tools to-be-applied to the selected challenge problems. In this report, (6) a graded system is used to characterize the data's quality (VUQ fitness). Potential paths for upgrading experimental methods and measurement techniques are discussed. A realistic assessment of quantity and quality of data available for VUQ, including (7) a projection of experimental and diagnostic capabilities development, lead to recommendations of both future experiments and new advances in VUQ process that take into account the CASL data characteristics.

As the project evolves, the report will be renewed in order to accommodate for extension of (1), (4), and (7) and refinement of (2) and (6), leading to updating of (3), (5), and (8).

Contents

Chapter 1. Data Support for Nuclear Reactor Analysis

1.1. <u>Data in nuclear engineering applications</u>

Data is central to development, assessment, and application of models and simulation codes in all fields, from computational physics, to computational material science, to meteorology ("numerical weather prediction"), and nuclear safety. In this report, the scope of data discussion is tied to mission, objectives, and approach of the Department of Energy's Consortium of Advanced Simulation of LWRs (CASL). This is a deterministically-minded, mechanistically-oriented slice of nuclear engineering practice.

> Remark on CASL vs RISMC: Another important class of modeling, simulation, and analysis of engineering systems (currently, not within the scope of CASL or NEAMS) has their root in probabilistic treatment of complex system. The objective of such modeling and simulation is to generate and quantify scenarios; e.g., transient or accident progression. Correspondingly, the probabilistic risk analysis involves data of different nature, e.g., reliability of systems, structures, and components, and human actions. Integration of probabilistic and mechanistic simulations, including treatment of aleatory and epistemic uncertainty, are being pursued in the Risk-Informed Safety Margin Characterization (RISMC) / R7 project in the LWR Sustainability (LWR-S) program. Despite the above-delineated difference in scope and approach between CASL/VERA and LWR-S/RISMC/R7, there are significant similarities (and potential for leveraging) in data components between these projects.

1.1.1. Validation and uncertainty quantification in nuclear reactor engineering

There exist an increasing number of documents (guidelines, standards, requirements, monographs and textbooks) on verification and validation (V&V) and uncertainty quantification (UQ), or VUQ. Notably, a majority of these documents builds on experience of application of scientific computing in aerospace (AIAA) and mechanical (ASME) engineering fields; for an overview see e.g., [Roache, 1998; Oberkampf & Roy, 2010]. In addition, nuclear weapon stockpile stewardship program has played a critical role in advancing VUQ theory [and presumably, practice] through development of QMU method. Computational mechanics, particularly Computational Fluid Dynamics (CFD) have been the main target for VUQ development. More recently, VUQ methods found their way to nuclear energy through the work performed in Nuclear Energy Advanced Modeling and Simulation (NEAMS) program; see e.g., [Nelson et al., 2010].

While VUQ theory has made important progress over the past decade, their broad adaption in engineering applications, particularly when it comes to system and multi-physics analysis, is plagued by data deficiency and inadequate treatment. The above statement applies fully to nuclear energy field (system design, safety analysis)[1].

> Remark on NE-VUQ: In fact, due to the significant role modeling and simulation play in its technology licensing and decision-making, nuclear energy practitioners (designers, analysts, regulators) were pioneer in asking and addressing questions about simulation code applicability and uncertainty quantification. US NRC developed method (e.g., Code Scaling, Applicability, and Uncertainty, CSAU) and process (Evaluation Model Development and Assessment Process, EMDAP).

Nuclear engineering applications are characteristically multi-physics, often including fluid flow, heat transfer (thermal-hydraulics), nuclear fuel performance, neutronics, structural material mechanics, coolant chemistry, material corrosion, instrumentation and control, and increasingly, human factor.

Solving a nuclear engineering problem requires treatment of phenomena and components identified as important to the problem's figure of merit. In many reactor applications in the past, it sufficed to focus developments on physical process(es) that are primary contributors of uncertainty. Thermal-hydraulics in LOCA (safety) analysis or DNB (design) analysis are well-known examples. More generally, a problem solution may be achieved through improved modeling and more accurate prediction of important physics, and by more faithful representation of coupling of different physics. More importantly, nuclear engineering system analysis necessarily invokes processes at multiple scales, from molecular-scale processes that govern material behavior or nucleation of vapor bubbles, to a large-scale dynamics of plant piping network or convection in voluminous containment atmosphere. Thus, the application requires integration of multi-scale models and data.

While "multi-physics," "multi-scale" (multi-resolution) attributes are not unique to nuclear reactor (system-level/engineering) applications, VUQ methods for multi-scale and multi-physics problems are under-developed. Additionally, there are several ways nuclear energy simulations differ from other fields. These differences reflect on data characteristics, and influence data requirements, and data treatment methods.

> Remark on CFD vs NE: In CFD applications, the question asked by VUQ is how accurately a particular turbulence model (physical simplification) and numerical scheme (computational representation) predicts an experimental "reality". Such reality presumably exists and can be measured (e.g., by PIV) or computed by a Direct Numerical Simulation (DNS) of Navier-Stokes equations. In other words, developments in VUQ help CFD modelers/users to effectively establish the degree of

[1] Exception is reactor physics (core neutronics) simulation where methods in sensitivity analysis and uncertainty quantification (both deterministic and statistical classes) have been both instrumental. Applications of VUQ methods in this case were effective for linear and steady-state processes.

approximation of simulation relative to a gold standard. Given resources and desire, VUQ-generated evaluation can be scrutinized and qualified. In [nuclear] engineering applications, VUQ task is to establish a code's (or code system's) "fitness for purpose" (e.g., certain engineering decision), without having either "gold standard" (DNS) or "true reality" (Navier-Stokes equation) to benchmark against.

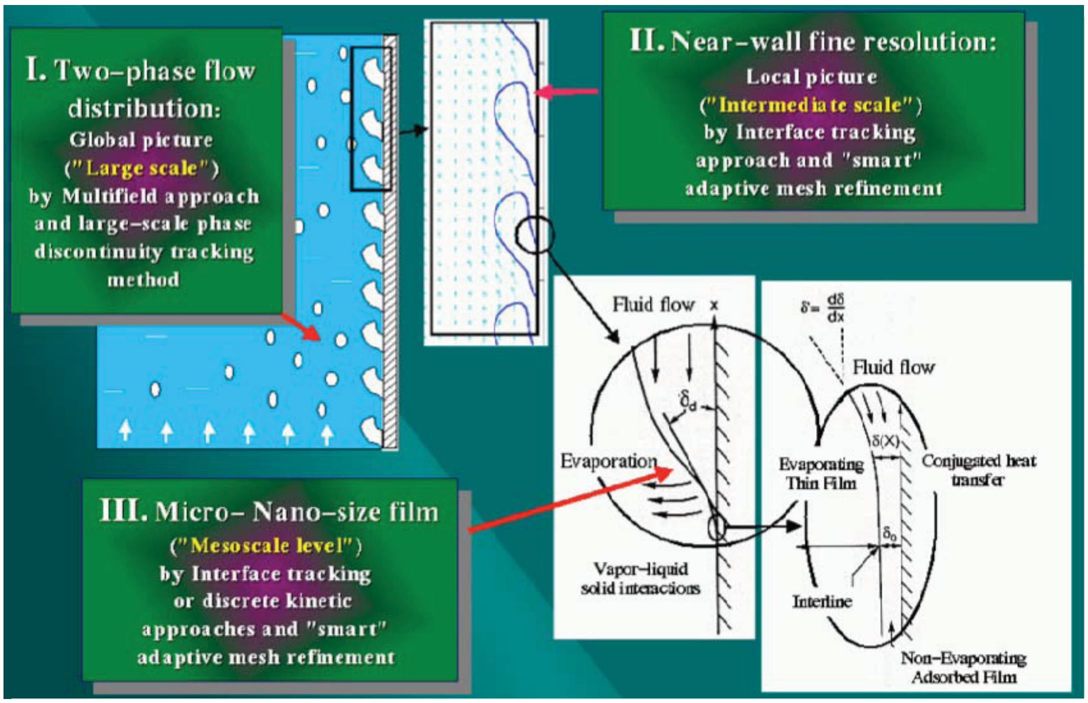


Figure 1.1. Multi-scale phenomena in a flow boiling process.

Remark on decision context: The above remark signifies a point about difference between VUQ in scientific research (where effort is designed to continually improve the predictive capability), and VUQ in engineering applications (where effort is designed to acquire decision-pertinent information at given time and resources). *Thus, value of particular data for nuclear engineering applications is determined with respect to the decision, to which predictive capability is a contributor, but the predictive capability (simulation code) by itself is not the R&D end-point. In such a decision context, it is equally valuable to have data that confirms a code predictive capability, and data that show the validity "cliff", i.e., where the give model and code cease to perform.*

Remark on NWP vs NE: Numerical weather prediction (NWP) is another field where advanced methods in VUQ (particularly data assimilation) were successfully applied. It is tempting to bring their development and experience to nuclear energy field. It is noted that in NWP highly heterogeneous data (e.g., satellite images, field measurements) are collected and assimilated to bridge the model and reality ("weather") the code tries to predict. In nuclear reactor applications, *experimental data bridge models to processes occurred in a test facility. There remains a gap between the test facility and reality (reactor behavior) that the simulation code ultimately aims to predict.*

Remark on scaling: Scaling is the instrument designed to bridge the gap between test facility and reactor behavior. Scaling is technically hard, subjective (sensitive to expert's opinion), and not easily quantifiable. While a rigor scaling was developed for many classical fluid dynamics problems, the scaling methods are far less advanced in two-phase flow, and largely non-existent for multi-physics and multi-scale problems. This adds a new dimension of complexity to nuclear engineering decision. In addition to the challenge in integrating models of different physics and resolutions, a nuclear engineering system treatment must factor in heterogeneous outcome (findings, insights, conclusions, uncertainty estimates) from analyses of a set of tests. As a matter of fact, these tests are designed and conducted by different research groups, under different assumption, scale, and quality. Assessment of a test's importance and applicability has largely relied on (and will continue to be) subjective engineering judgment.

1.1.2. Characterization of data in nuclear reactor engineering

Data for supporting development, assessment, and application of advanced modeling and simulation in nuclear engineering can be characterized in multiple ways. In this study, a two-pronged approach is used to characterize data, namely, by their sources (inheritance) and their usability (VUQ "fitness").

1.1.2.a. Characterization of data source

Data inherit characteristics of their sources, e.g., experiments. Along this line, data (sources) are characterized by

- ***Physics tested***, i.e., whether
    - Single physics, e.g.,
        - Thermal-hydraulics
        - Neutronics
        - Structural materials
        - etc.
    - Multi-physics
        - Coupled neutronics and thermal-hydraulics
        - Coupled materials and thermal-hydraulics
        - Etc.
- ***Modes of experimentation*** (data generation), i.e., whether
    - Separate-effect tests (SET), studying a physical process
        - Typically small-scale, well-controlled, well-diagnosed
    - Integral-effect tests (IET), studying a scenario or application

        - Larger scales, multiple phenomena,
        - May be performed in test reactors.
        - Increasingly multi-physics

    - Plant measurements and observations (PMO)
        - On-line plant diagnostics (flux, temperature, pressure history)
        - Samples collected during operation, refueling (e.g., crud)
        - Post-irradiation examination (PIE)

- ***Scale of experiments***, which cover small-, medium-, and large-scale experiments, and full-scale (prototypic) reactor tests.

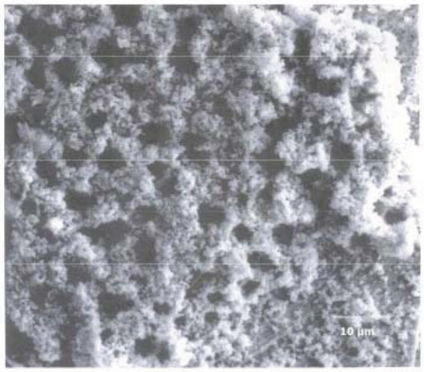
    - Parameter range covered

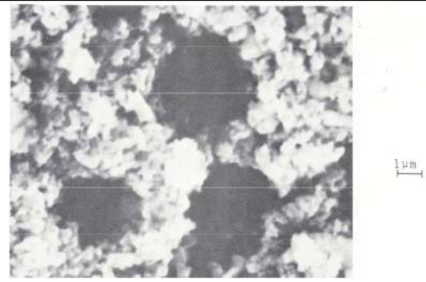
Remark: although advanced simulations increasingly aim to capture multi-physics behavior, there are very limited (may not exist for novel applications) experimental data that can be used for qualification of multi-physics models and multi-physics simulation codes. Lack of experimental infrastructure and corresponding diagnostic techniques needed for multi-physics experimentation explains the high cost and long time for planning and conducting multi-physics experiments.

Other characteristics of data source are

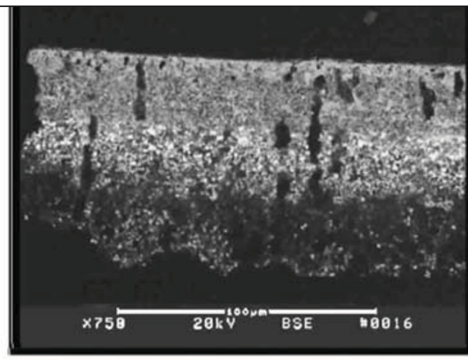
- data producer (e.g., research laboratory)
    - availability and accessibility of experimenters for additional information
- data ownership (proprietary)
    - data release and usage conditions
    - cost of the data production program
- format, conditions and cost of data maintenance

Figure 1.2. Observations on crud in PWR. [Q: how this “data” is used in VUQ of crud/AOA models?]

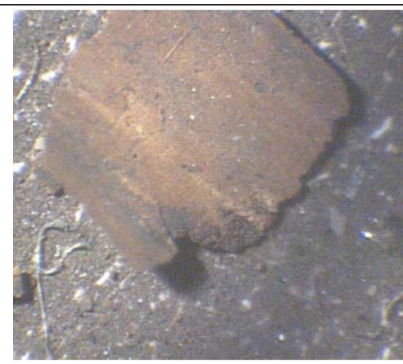




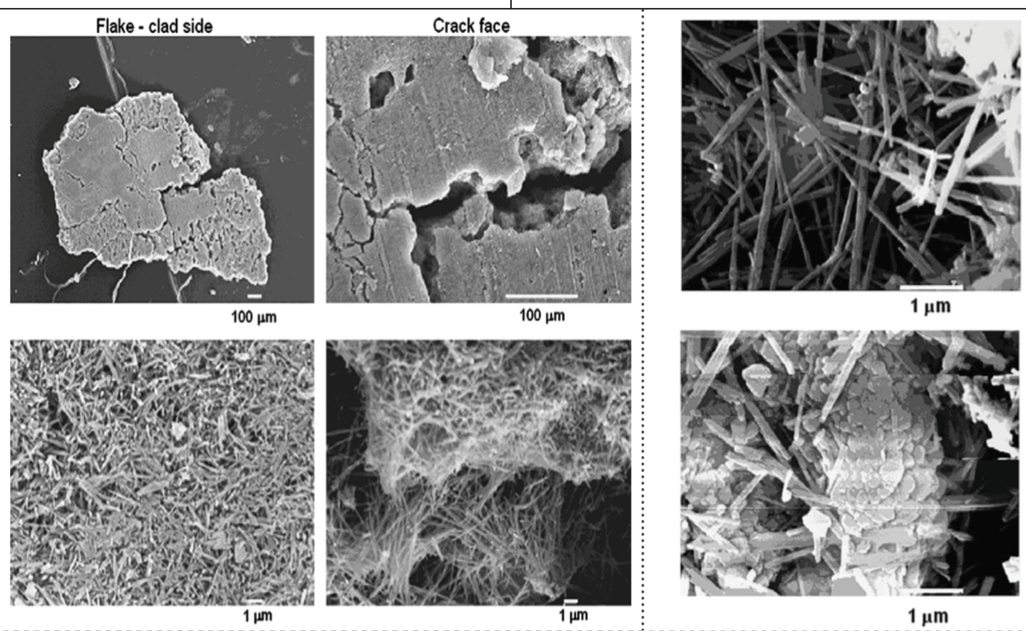
EPRI Report 1003213 (PWR AOA Guideline), Oct. 2003.



A thick crud flake showing three distinct layers. The middle white zone contains ZrO_2 (J. Henshaw et al, JNM, 2006)



Light micrograph of a small fragment of sample C1 extracted from core C after Cycle 10 (J.A. Sawicki, JNM-2010).



SEM micrographs of crud taken at various magnifications. Left: flat cladding-side of flake. Middle: crud near fissures or cracks. Right: structural details of a crud flake (J.A. Sawicki, JNM-2008).

Figure 1.3. Images obtained in experiments performed under conditions thought to be relevant to processes that govern crud growth in a nuclear reactor core. [Q: How this “data” is used for validation of models of crud-related processes?]

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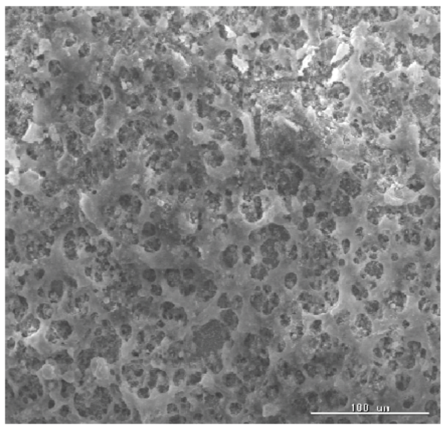
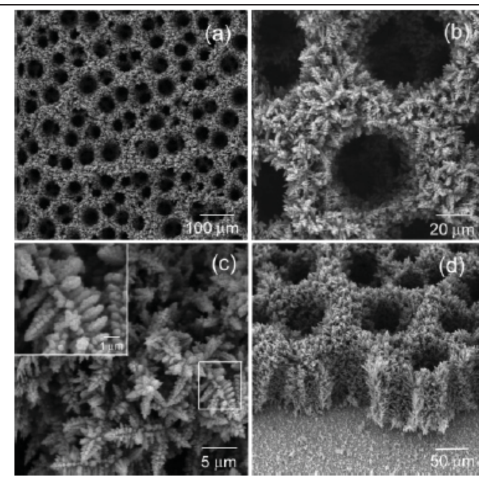
<tr>
<td>

Figure 4.4: SEM Image of Crud on Experiment Number 26 at 250x Magnification.</td>
<td>
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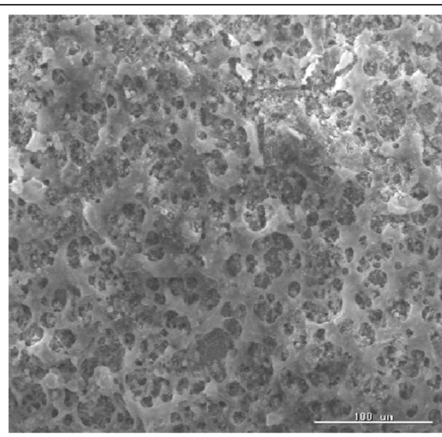
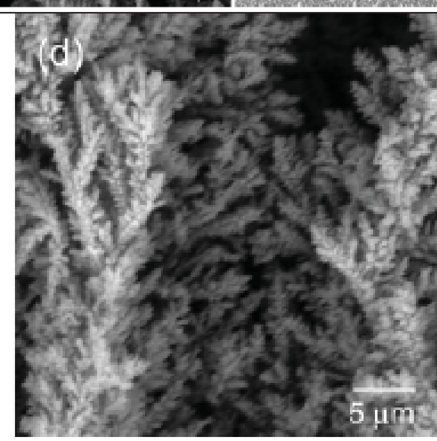
<td>

Figure 4.4: SEM Image of Crud on Experiment Number 26 at 250x Magnification.</td>
<td>
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<td>J. Hawkes, Georgia Institute of Technology, PhD Thesis, 2004.</td>
<td>Growth of nano-porous layer, Shin and Liu (2003, 2004)</td>
</tr>
</table>

1.1.2.b. Characterization by data usage

Secondly, data are characterized by their VUQ "fitness" quality. Along this line, the following categories can be considered.

- ***Quality of information*** (increasing order of value):
    - Relevance
        - Relevance/applicability of experiments / data typically reflects a preconceived (expert's) view of phenomenology / process (this view is necessarily developed through observing past experiments).
    - Scaling
        - Scaling requires simplification (often experimental scaling is devised for a dominant physics).
        - Characterization of relevance and scaling is largely subjective, leading to question how do we quantitatively account for expert opinion / biases in maturity measure.[2]
    - Uncertainty
        - Uncertainty should be considered only after "relevance" and "scaling" issues are satisfactorily resolved.
- ***Usability of information*** (increasing order of impact on application):
    - For model development
        - Qualitative (trend) and basic data
        - Basic understanding of phenomena
        - Parameter estimation
    - For model calibration and code assessment
        - Suitable for advanced methods of data assimilation
        - Suitable for predictive capability maturity measurement
    - For code applications
        - Uncertainty quantification of FOM [in challenge problems]
- ***Compatibility with VUQ*** (increasing order of VUQ user-friendliness)
    - Comprehensiveness of description of data sources, e.g.,
        - Experiment design,
        - Experimental procedure, including test control,
        - Measurement system

[2] Calibrating a model on data sets that are not representative of the scenario under study increase rather than reduce the model/code predictive capability for the conditions of interest.

    - Data acquisition and processing

  - Completeness of information about physical experiments, e.g.,
    - Initial and boundary conditions (control, error estimates)
    - Measurement device (error estimates)
    - Data are also characterized by their accessibility. Not all data that exist and owned by certain partners in the consortium are available for CASL validation tasks due to legal (proprietary) and commercial constraints.

  - Consistence with implementation of VUQ process
    - Different sources of error, bias, and uncertainty
    - Archived, meta-processed and formatted for convenient and accurate integration with VUQ methods and tools

It should be noted that the above-described categories characterize individual data sets, in reference to a solution framework. The same data set can change its value drastically when one changes solution approaches to the same problem.

1.2. CASL approach to validation data

Data have been a cornerstone consideration in CASL from the beginning (proposal stage). The author of this report provided a scoping assessment of data support for CASL (Table 1.1) and an initial structure and timeline for CASL validation data plan (Figure 1.1).

Table 1.1. A scoping review of data support for CASL [CASL, 2009].

Types of Experiments & Measurements	Phenomena and Regimes	Issues	Validation for Related VR Capability	Measures to be taken to Meet the Validation Data Needs
Plant & In-Core Diagnostics	Neutronics and T/H Data in Operational Transients	Unable to discern local effects and to reveal relationships of interest for VR validation	Core Neutronics, T/H (steady state)	Coordinate with Westinghouse and TVA to plan in-core measurements, PIE, and characterization of an used fuel assembly to obtain a complete data set for VR code validation
Fuel Post-Irradiation Examinations of LWR used fuels	Fuel performance. Crud, corrosion, fretting wear, and failures	Exhibiting only accumulative effect	Fuel performance. Chemistry Fluid-structure interactions	Apply advanced diagnostic techniques to obtain new detailed data on cladding failure modes, oxide layer and crud compositions (coordinate with LWR-S Program)
In-Pile and Out-of-Pile Testing of Prototypic Fuels	Fuel behavior under normal, abnormal transient and accident conditions	Past tests were conducted with limited diagnostics, (main data: post-test characterization)	Assembly Dynamics under normal, transient and accident conditions	Collect and qualify data sets from previous experimental programs (e.g. FLECHT, BFBT, NSSR, CABRI) Coordinate with the planning of fuel tests in OECD Studsvik and Halden Reactor Project and INL's TREAT (if restarted)
Separate-Effect Tests	Thermal hydraulics-structural mechanics in Fuel Assembly	Exhibiting only differential relationships under potentially non-prototypic conditions	Multiphase T/H, fluid structure interactions	Coordinate with V&V activity in other DOE-NE programs as well as basic research experiments using advanced diagnostic capabilities at MIT, TAMU, OSU, and INL.
Integral-Effect Tests	System dynamics	Scaling distortions. Limited set of scenario and range of test conditions.	Coupling to a system code	Coordinate with the INL-led development of database for validation of CFD in nuclear reactor safety applications

It is noted that also at the very beginning, the CASL team recognizes the critical importance of multi-scale nature of engineering challenge problems CASL intends to tackle. As shown in Figure 1.2, an initial validation process proposed for CASL (2009) is built on "triangular representation". Recognized in AIAA and ASME community (see e.g., AIAA V&V guidance [AIAA, 1998])[3], the triangular representation of validation process was more recently brought to nuclear energy

[3] AIAA V&V Guide (1998) uses the term "validation pyramid", where different hierarchy levels are called, in a bottom-up order, as "unit problems", "benchmark cases", "subsystem cases", and "complete system". The bottom two levels are addressed by validation experiments, while the upper two levels are addressed by large-scale testing.

discussion [Unal et al, 2007], and further developed in NEAMS program [e.g., Nelson et al, 2010].

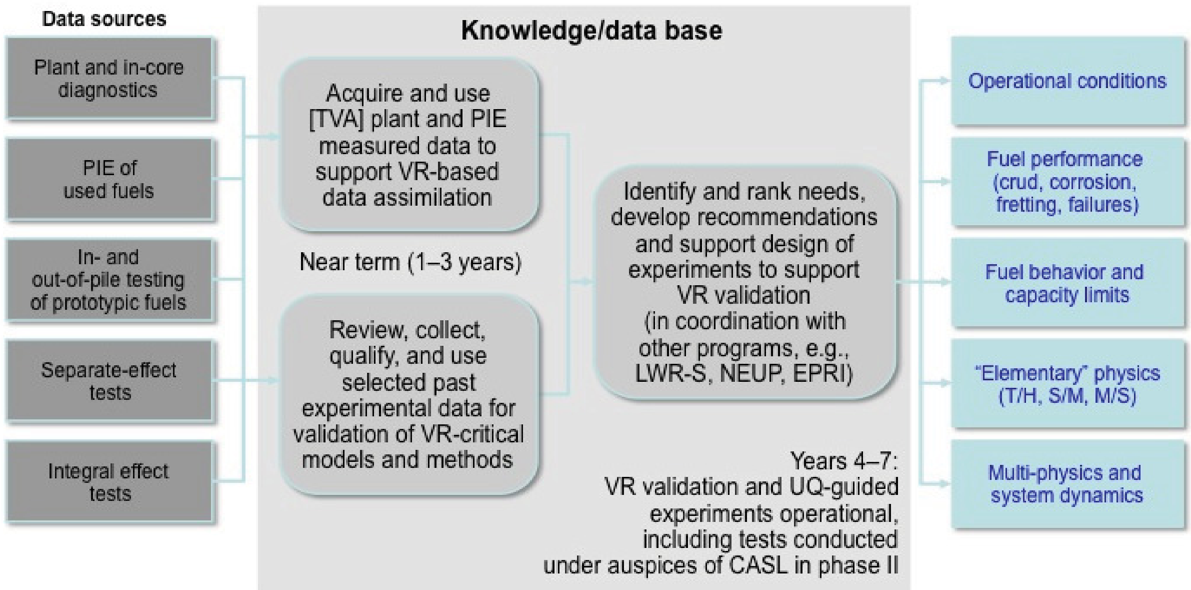

Figure 1.4. An initial structure and time line for CASL validation data plan [CASL, 2009].

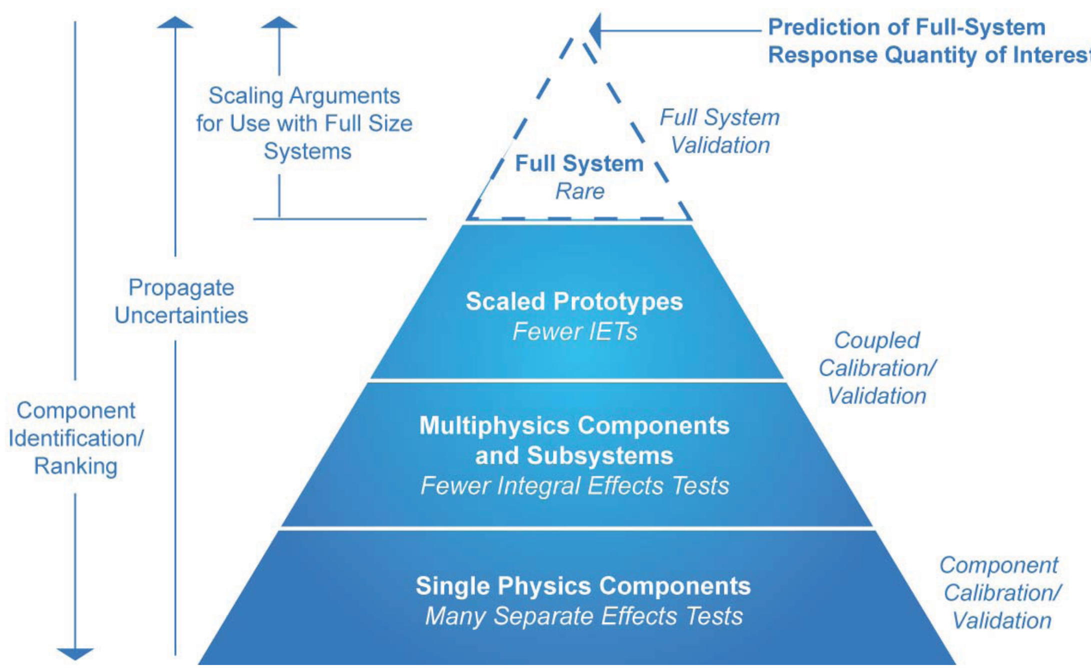

Figure 1.5. Validation process [CASL, 2009].

Over the first half year of CASL operation (since July 2010), the initial view of data has evolved substantially, thanking to many workshops and interactions between subject domain experts, VUQ methodologists, model developers, and computational scientists. Nonetheless, as it can be seen from the remaining of this report that the initial scoping of data assessment, structure/timeline and process served a sound platform for further discussion on validation data.

1.2.1. Product and process objectives

In CASL, challenge problems of interest (e.g., CRUD/CIPS/CILC, GTRF, DNB) are highly complex, e.g., inherently nonlinear and transient, with multiple time scales and length scales. Consequently, the data support for CASL is broad and heterogeneous. In formulating CASL approach to validation data, we keep in mind that CASL aims to lower the barrier for integrating high-performance computing in nuclear energy applications, and it doing so by improving usability and predictive capability of advanced simulation codes. Thus, CASL success is to be measured relative to two objectives, namely,

– (product) establishing a set of functional simulation capabilities that can be used to significantly advance solution of the specified challenge problems. Capabilities and solutions are equally important measures. Although this part of the success is an absolute must, the resulting "capability/solution" outcome has definitive/narrow impact (limited to the specified problems). The solution is eventually reflected by an application (design, licensing) decision, such as issue resolution (in ROAAM style). Generally speaking, CASL (design, operation, safety) challenge problems can be formulated as a margin problem. Even a hypothesis can be cast in term of margin. Along the line of methods like BEPU, QMU, or RISMC, a system's margin is found through computing and comparing ***probabilistic load*** vs. a ***probabilistic capacity*** [4]. In some cases, it suffices for the challenge problem's success to obtain one-sided margin information about the loading or the capacity, which are the problem's figure of merit (e.g., power shift level, or critical heat flux distribution).

– (process) establishing and demonstrating a collaborative VUQ-guided process by which development of advanced modeling and simulation capabilities can be efficiently streamlined and integrated to effectively help solving hard and practical nuclear-engineering problems. The "process" goal is to align and streamline efforts on developing "capabilities" with "solutions". Although this part of the success is less tangible, its impact can be broad and foundational in reducing barriers to innovation in nuclear reactor technology. In addition, the "process" is enabled by a set of VUQ

[4] The "probabilistic" attribute manifests the notion of uncertainty in margin. In general case, the PDF of margin integrates aleatory and epistemic uncertainty.

tools, which are developed or adopted and demonstrated by the CASL. As a result, the CASL successful use of VUQ-guided simulation tools will motivate industry and a broader community to adopt both the VUQ process and the associated VUQ tools.

1.2.2. Product-oriented data support

As outlined in the previous subsection, "product" is defined in term of both simulation capabilities (codes) and solution of a given challenge problem defined for an engineered system or sub-system. Within a margin-oriented problem solution framework, the simulation codes compute the system's physical behavior and propagate uncertainty toward the FOM's margin.

In the case of CASL, the simulation code system is built on VERA (Virtual Environment for Reactor Applications) enabled by Lightweight Integrating Multiphysics Environment (LIME). LIME integrates panoply of existing codes, and in future, also codes that are currently under development or to be developed within CASL, NEAMS, LWR-S and other programs. The current code class includes industry codes, such as ANC, RETRAN, VIPRE, BOA, codes developed in national laboratories and universities like RELAP5, DENOVO, DeCART, and commercial codes like STAR-CCM.

Computer codes integrated in VERA system can also be categorized by its intended functionality, i.e., what physics does the code is designed to capture (neutronics, thermal-hydraulics, chemistry, materials), and even more specifically, [within a given physics] what models/equations the code solves, etc.

Each of the simulation components (existing codes) comes with their own pedigree in "legacy" verification and validation. The remaining questions are:

(i) To what extent the "legacy" validation cover the need in CASL applications; both in term of the required VUQ process, and in term of coverage of conditions relevant to application's decision;

(ii) To what extent (if any) the legacy validation domain covers performance in "coupled code" regime.

Remark: Both questions implicitly point to a critical role for measuring the validation adequacy. While this (adequacy) issue has been part of discussion in CSAU and EMDAP (see Appendices A.1-A.2, there is no formal procedure and metrics developed and applied in nuclear engineering applications.

Inversely, for simulation codes or code systems, which are in planning or under development for CASL/VERA, the validation plan should foresee the timely availability of data to support the functionality and VUQ process required for the new code, or code system.

The product-oriented data support adopted in CASL thus focuses on data needed to characterize and enhance, as appropriate, the validation status of computer codes selected (by the CASL VRI/AMA) to be components of the VERA-based simulation engine (for the given challenge problem).

1.2.3. Process-guided data support

To meet the "process" objective, it is envisioned that in "data domain", CASL operation is guided by "value-of-information" (or information entropy in decision context). Specifically, value of data, models (developments), and capabilities (codes) is measured by the extent they help reduce uncertainty in challenge problem's figure of merit (FOM). In case where no data will be available for evaluating a model impact on FOM, the model is of no value in CASL decision framework.

Given the methodological challenges in VUQ support for such problems as discussed in "remarks" in subsection 1.1.1, CASL approach to validation data planning and implementation is necessarily "phased" and "multi-pronged".

The term "phased" refers to a gradual process of development, assessment, and application of analysis tools. Such a "phased" approach is even more so necessarily for CASL while advanced issues on VUQ methodology are being addressed. More detailed description of one such "phased development" process (called SAMAP, or Simulation-Aided Margin Analysis Process) is given in Appendix A.3. It builds on experience and guidance from CSAU (Appendix A.1) and EMDAP (Appendix A.2). Notably, SAMAP is intended for a broader range of (nuclear engineering) applications, including but not limited to issues in public safety.

The term "multi-pronged" refers to parallel activities, as discussed in a validation data plan outlined in the next Chapter. There are also cross-cutting needs for different challenge problems and different activities, such as infrastructure (e.g., NE-CAMS) for supporting databases, methods and tools for VUQ (e.g., QPIRT and PCMM).

Chapter 2. Validation Data Plan

2.1. What is Validation Data Plan for?

Validation Data Plan (VDP) is a ***dynamic planning*** instrument to guide (potentially, optimize) activities on data production (e.g., new experiments or plant measurements), collection, management (i.e., analysis, qualification, archiving), and usage so that they enable effective support for development, assessment and application of simulation tools intended for a challenge problem.

> The term "dynamic" in the above definition reflects VDP as part of learning curve in a developmental / application project (such as CASL or R7, when predictive capability is developed). In this sense, validation is organic part of the "born-assessed" code development effort (as opposed to having validation as an afterthought evaluation exercise).
>
> The term "guide" is given in the context that data activities are complex and constrained by other factors (as discussed in the next subsection 2.2).
>
> The term "optimize" here refers to the use of limited resources available to data-related activity to achieve maximum impact on the project goal (e.g., maximum reduction of uncertainty in predicting a figure(s) of merit in the selected challenge problem).
>
> Remark: Generally, the referred optimization should be taken in qualitative sense, since expert judgment remains to play the most significant role in VDP development and implementation. Success criteria in a project management, as a rule, include not only "accuracy" (i.e., uncertainty reduction) but also "timeliness" of the simulation result (i.e., when the tools become available for applications). In a simulation-aided engineering decision-making context, ***value of information*** generated by the simulation tends to decrease with time (e.g., there is diminishing value in having an accurate simulation many years late for the relevant decision).

As defined, in order to serve as guidance for data activities, VDP development must build on insights derived from substantial tasks of

(a) identification of data gaps (data needs), including specification of required characteristics of data that would fill the gaps;

(b) evaluation of means, time and resources needed to acquire the data identified / specified;

(c) selection and prioritization of data (production, collection, analysis) tasks that most cost-effectively and timely fill the gaps.

2.2. Factors that influence VDP

Development of VDP for CASL is faced with substantial challenges, methodologically because there is no ready-to-use recipe (CASL VDP will provide one for other programs), and programmatically because of uncertainties and constraints (time, resources, intellectual property and data accessibility) in CASL execution arrangement.

Methodologically, CASL is pioneering a novel approach (still exploratory in nature) to advanced simulation and VUQ in nuclear reactor engineering applications. As discussed in Chapters 1 and 2, nuclear reactor applications, especially those involving multi-physics and transient processes, differ from other fields (e.g., aerospace or meteorology) or problems (e.g., core neutron physics) for which many advanced VUQ methods were developed and applied[5].

A VDP development is influenced by a number of factors, several of which e.g., (ii), (iv), and (vii) are in early formative stage or under selection.

(i) Challenge problem specification (mission and success criteria)

(ii) Problem solution framework and approach (which and how simulation codes are used and their applicability assessed)

(iii) Status of required capabilities in available and selected analysis tools

(iv) VUQ techniques and method for assessment of predictive capability

(v) Types, quality, availability, and accessibility of existing data

(vi) Projected time and resources for generating new data

(vii) Decision model that integrates information from (i) through (vi) and prioritizes data activities, based on cost-benefit analysis of possible activities.

Relative to (i) [challenge problem], VDP must first be developed for each challenge problem (i.e., a given nuclear power plant, a well-defined technical issue/scenario, analysis objective, solution approach, success criteria). This does not exclude possible use of elements developed for one VDP for another, but consistency should be maintained throughout the individual VDP.

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[5] Perhaps developments in ASC (Accelerated Scientific Computing) initiative under auspice of DOE-NNSA nuclear weapon stockpile stewardship program (including weapon aging management) can provide closer examples to nuclear energy applications, although information and experience from that and other defense applications are not accessible for comparison.

Figure 2.1 shows the challenge problem specification receives input from outcome of the analysis work ("solution framework"). Most importantly, having well-defined, preferably quantifiable success criteria ("goal")[6] is crucial for making possible a systematic quantification of uncertainty and a global sensitivity analysis [item (iv)]. If the so-defined goal is not achievable within resources and time allowed, then the challenge problem specification, the solution approach, the choice of tools, the data support, and the VUQ techniques used – all need to be reconsidered in the "Project Execution Decision Making", which includes VDP.

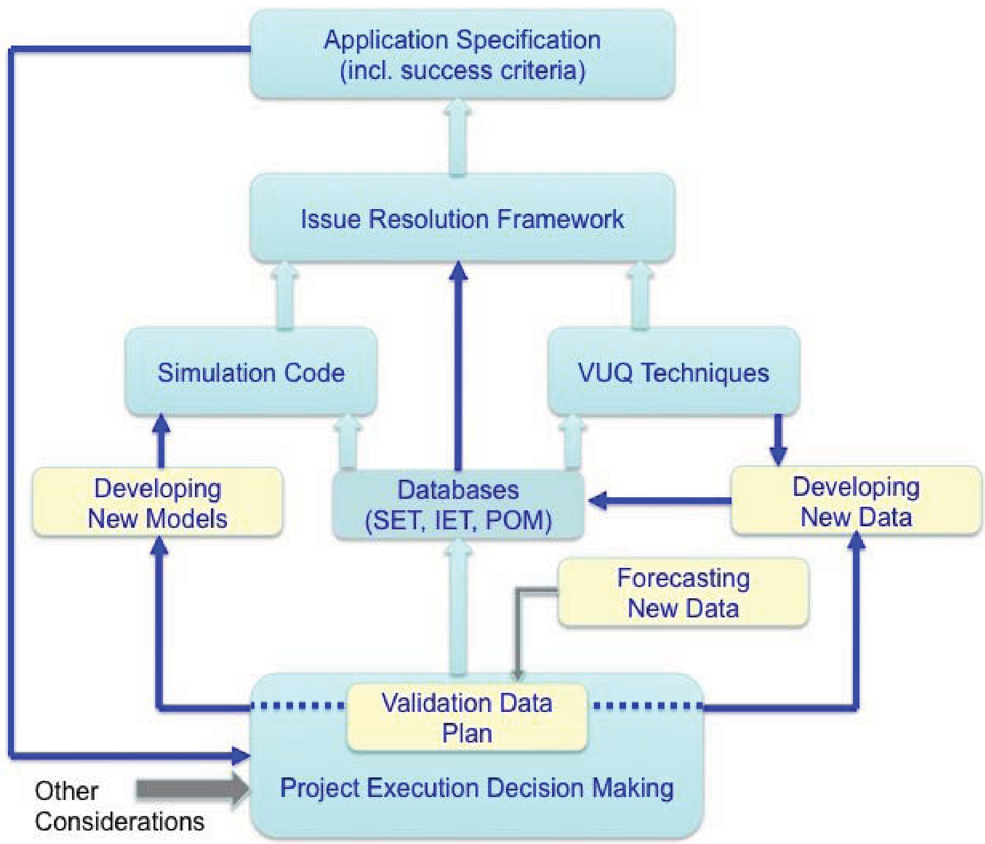

Figure 2.1. The project implementation chart for a specified application (challenge problem) involves an iterative cycle (in the figure, green arrows show a second round that my require development, validation, and implementation of nw models, methods, and experimental data. Validation data plan is part of the CASL project decision-making, which includes (and therefore must balance) several challenge problems (e.g., CRUD, GTRF, PCI, DNB) concurrently pursued in CASL.

[6] The current draft for "CASL Challenge Problem Technical specification (Z. Karoutas, 2010) provides an excellent starting point. Further refinement is expected and it would be highly beneficial to outline how information generated by desired codes be used in (design, analysis, licensing) applications and to have quantitative success criteria.

> Remark: Often a research program (with finite resource) includes several challenge problems and for one challenge problem, there might be more than one solution approaches (e.g., using two different sets of codes). Therefore, VDP for a program (e.g., CASL VDP) should integrate VDPs from selected challenge problems, weighted by potential impact, priority and resources allocated for the challenge problems.

Relative to (ii) [solution framework], VDP is specific to hypothesis(es) and framework for integrated treatment of different (physics, system) components involved in the problem solution[7]. However conceptual or approximate, such framework is central to the decision model [item (vii)] and decision-making on VDP. In a hypothetical extreme case when the goal can be achieved by the available and appropriately validated capabilities (tools), no further VDP action is required.

Relative to (iii) [codes], simulation capabilities evolve and presumably improve in time, although such assumption is subject to qualification through the validation process. In particular, as separate tools are integrated, the system may experience a “bathtub” curve with “infancy mortality” phase (larger uncertainties and errors) when new capability is not yet verified and calibrated. This is where a VUQ method (like PCMM) applies [item (iv)].

> Remark: VDP should reflect the choice of analysis tools (a set of simulation codes). This requirement is parallel to prerequisites of application of the US NRC CSAU methodology for licensing analysis (see discussion in Appendix A.1), although in the case of CASL, the tools are being developed and integrated, so the simulation codes in question are not “frozen”, but evolving through implementation, testing, application and refinement.

Relative to (iv) [VUQ], the VUQ process must be defined for the challenge problem, solution framework and simulation codes used. This means involving coupling to VUQ techniques (e.g., sensitivity analysis, QPIRT, data assimilation), effective utilization of each technique requires certain data format and characteristics. Also required here is a model for assessment of predictive capability maturity (PCM). The PCM model can and should be used to estimate the value of data sets (e.g., through reduction of uncertainty in challenge problem’s figure of merit). The Q-PIRT and PCM model are instrumental in

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[7] Examples for such integrated framework are Risk-Oriented Accident Analysis Methodology (ROAAM) pioneered by Professor T.G. Theofanous; see [Theofanous 1996]. A more recent ROAAM treatment for a LWR (ESBWR) using advanced simulation codes can be found in [Theofanous and Dinh, 2008]. Another example is the Risk-Informed Safety Margin Characterization (RISMC) framework developed in the LWR Sustainability program; see e.g., Dinh et al., 2009; Youngblood et al., 2010.

identifying data gaps, i.e., the types and quality of data that would significantly reduce uncertainty in simulation.

Relative to (vii) [decision model], in near term VDP decision-making is heuristic and ad-hoc, since both desirable elements such as solution framework and PCMM are yet to emerge for the selected challenge problem, and information is yet to be gathered and processed for items (v) and (vi). It is recommended to invest into development and application of techniques like Q-PIRT and PCMM to CASL challenge problems, so that the VDP process can be put on a more rigor foundation. It is also instructive to note that the VDP decision-making is a subset of the project execution decision-making, where the VDP priorities are integrated and harmonized with other project's priorities and constraints; Figure 2.1.

2.3. Outline of a Validation Data Plan (VDP)

In light of the above discussion, it is noted that as a project execution instrument VDP evolves in time and under influence of a number of factors. Figure 2.2 (upper half) outlines three main activity thrusts in a validation data plan. Let's take a CRUD problem to illustrate content of validation data plan.

The "database" activity would require collection, analysis, and qualification of existing and available data for supporting validation of neutronics, thermal-hydraulics (e.g., subcooled boiling), fuel cladding physico-chemical behavior, system materials and coolant chemistry (corrosion products generation and transport). The "qualification" part is expected to bring the data to the format compatible with VUQ techniques.

> The "database" activity has not been planned within CASL. While MNM/MPO and VUQ experts can and should participate in this activity (e.g., formulating requirements, providing guidance, developing special techniques), there is much technical work to be done. For the first challenge problem, this "database" activity requires substantial effort (est. 3 FTE/year, or $1M/year; this estimates does not include the cost needed for securing CASL access to relevant data sets, such as SCIP, Halden).

The "gap analysis" activity identifies data needs at all levels and from all known and possible sources (e.g., SETs, IETs, PMOs). For the CRUD problem, we expect a major "gap" in data for validation of multi-physics coupled models and codes. Also, quality of measurement (data) in integral-effect tests and plant data is likely to surface as inadequate for validation of high-fidelity models in VERA.

For each challenge problem, the "gap analysis" activity is most intense in the early phase. This should be part of AMA work with support from VUQ.

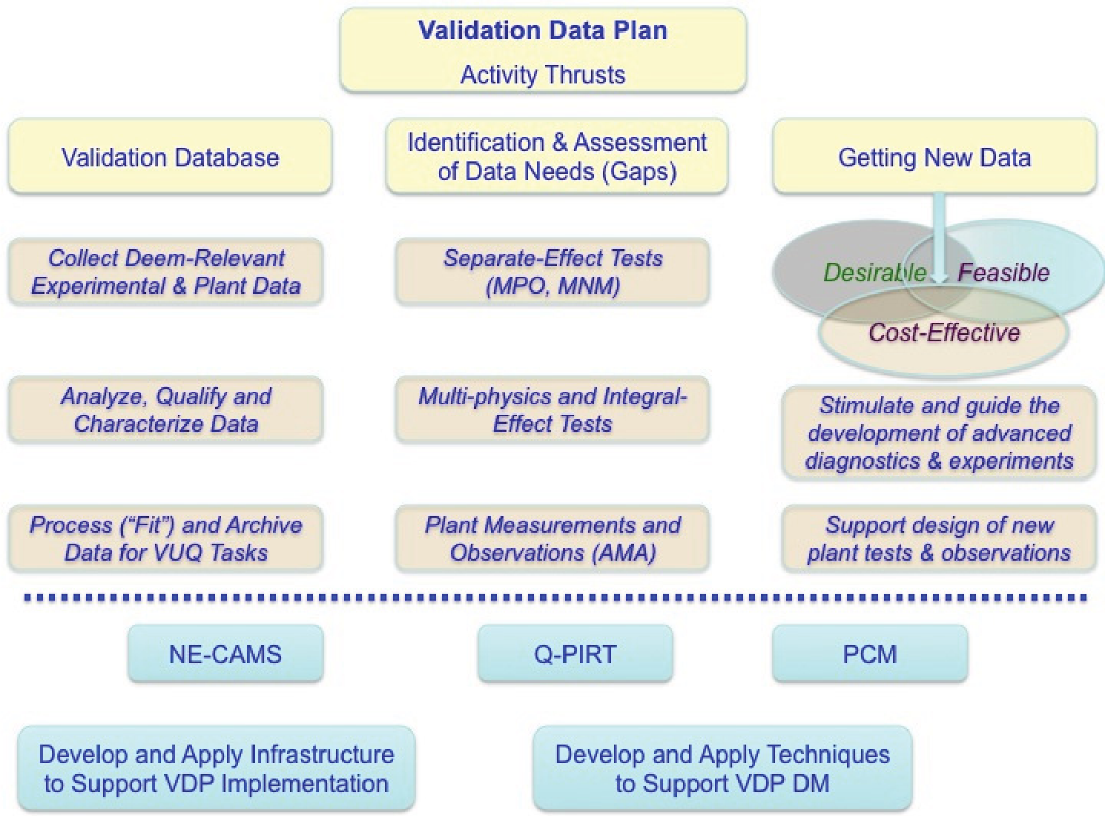

Figure 2.2. Validation data plan includes three thrusts of activity, (a) "database" – to maximize value of existing and available data for VUQ needs, (b) "gap analysis" – to identify missing information and cost-effective way to acquire it; and (c)"new experiments" – to develop plan and secure resources to develop necessary new experiments and plant tests.

<u>The "new experiments" activity</u> should build on the "gap analysis" outcome, taking into account capability, timeline and cost of experimentation needed to produce the data with required quality and quantity. For the CRUD problem, (as discussed in the next Chapter), relevant and sufficiently scalable experiments or plant tests on phenomena of importance to CRUD can take a decade-long period for preparation, experimentation, and post-test examination, thus unfit for CASL schedule and VERA validation purposes. While it is important to retain option for "new experiments", particularly for CASL Phase 2 (2015-2020), it is more cost-effective to acquire CASL access to data generated by past relevant experiments and plant tests (including those belonging to a CASL partner but yet to be released for CASL use, and by non-

CASL venues, e.g., SCIP, Halden reactor project) and to secure CASL rights for participating and guiding experiments and tests which are already under planning in international, national, and industry programs.

> CASL has not planned resources (either within CASL or other means) for securing non-CASL data sets. It is estimated that an initial installment of $1M and annual fee of $500K in subsequent years may be needed for CASL acquisition of several datasets (e.g., SCIP, Halden) and participation in future CRUD-related experiments.

Figure 2.2. (lower half) shows components/activities that – although not part of VDP itself - would beneficially support the development and implementation of CASL VDP. In fact, NE-CAMS, QPIRT, and PCM correspondingly support the three activity thrusts in VDP. In particular, the VDP decision-making will require balance between using resources for SETs, IETs, and PMOs, and consistency between development of models, methods, and data.

It is noted that as "by-products" outcome from VDP thrusts and VDP supporting activities (e.g., NE-CAMS, Q-PIRT, PCM)[8] can and will be useful for work on validation of models and codes developed in MPO and MNM Focus Areas. These FA investigate separate-effect processes. However, the driving objective of the CASL's integrated VDP is to support the VERA simulation capability to meet the challenge problem's specified objective.

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[8] A PCM model – yet to be investigated and developed for each of the CASL challenge problems – is central to the project implementation, including validation data plan. The VDP will also help identify and rank required capabilities and database content of CASL portion in NE-CAMS (Nuclear Energy – Computational Applications Management System). More discussion on QPIRT, NE-CAMS, and PCM is provided elsewhere in this report, its appendix, and cited references.

Chapter 3. Validation Data Review Framework

The preceding chapters provide a system application view and a decision-oriented framework for reviewing validation data for CASL challenge problems. In this Chapter, selected problems and data sets are reviewed. As several important VUQ instruments (i.e., PCM, QPIRT) for supporting the decision-oriented framework are yet to be developed in CASL (VUQ FA), their heuristic surrogates are used in this initial ("analytical") phase (see Appendix A.3).

3.1. Task objective and scope

The near-term objective of this task is to perform a [scoping] review of ***VUQ fitness*** of available and prospective experimental data and plant observations identified as relevant to, and of potential use for VUQ of, the CASL Challenge Problems (CP).

In a longer term, the data review task will also be concerned with

- Strength/weakness of VUQ plan/methods/tools (given the data reality)
- Recommendations for new experiments and plant measurements
- Feedback on plan for development of methods and tools in VUQ FA.

The scope of FY2011 initial review task is limited to two CASL Challenge Problems, namely Crud Induced Power Shift (CIPS) and Grid to Rod Fretting (GTRF).

Remark: In this initial stage, the Challenge Problem Technical Specification (CPTS) provided by AMA (Karoutas, 2010) and VERA development (integration) plan adopted in CASL Plan of Record are used as reference. As a result of the data review, suggestions may emerge on refining CPTS and VERA code development plan.

Remark: Information about a large number of data sets named and reviewed in this Chapter is gathered from sources the author has access to. Data sources, their limitations (in availability, accessibility) and assumptions made by the author about data characteristics are referenced and specified for each case.

3.2. A graded system for data characterization

This subsection discusses a system for characterizing data in nuclear engineering applications. The focus of this system is *VUQ fitness*. Such a characteristic is expected to be more stable over the phases of problem solution development, whereas information value of data sets can vary greatly over phases of the SAMAP process (Appendix A.3).

As a matter of fact, evaluation of VUQ fitness (at least initially) is ***subjective***, for expert opinion plays a critical role in determining relevance and scalability of a given data set to the problem. Nonetheless, a graded system for data characterization can provide a foundation for systematically representing expert opinion and streamlining their debate/disagreement as appropriate. As QPIRT and PCM are developed and applied for challenge problems, the VUQ fitness characterization can become more formalized, quantitative, and hence objective.

A data set (including observations, trend data) can be in three categories under five grades. The three categories (Relevance, Scaling, and Uncertainty, or R, S, and U) are not independent; in fact, a data set must first be assessed by relevance (and pass at least level 1), then by scaling (and pass level 1), and uncertainty.

For the purpose of ranking influence / importance of date sets, one may approximately evaluate the data set's numerical "worth" [W] as a multiplication product of R, S and U, i.e., [W] = [R] x [S] x [U].

Table 3.1. Grading of experimental or plant test data by their VUQ quality.

VUQ Quality	Grade				
	4	**3**	**2**	**1**	**0**
Relevance [R]	Very High (direct)	High	Medium	Low	N/A
Scaling [S]	Prototypic (full-scale)	Adequately scaled	Medium	Inadequately scaled (large distortions)	N/A
Uncertainty [U]	Well-Character-ized	Character-ized	Medium	Poorly-Characterized	N/A

Concepts and techniques developed for VUQ of CFD simulations (e.g., [AIAA, 1998], [Oberkampf et al., 2002]) are applicable to the "uncertainty" step in CASL challenge problems. One can follow "Seven Pillars" approach; see [Lee, 2010]. Notably, six out of the seven pillars are related to data, namely

(i) Experimental measurement uncertainties
(ii) Test unit geometric uncertainties (as-built geometry)
(iii) Test unit surface roughness uncertainties
(iv) Test condition uncertainties
(v) Fluid and material property uncertainties

(vi) Experimental data uncertainties, including initial and boundary condition data and propagation of uncertainty for derived engineering data and parameters.

It is noted that although the "uncertainty" step in-principle is more quantitative than the "relevance" and "scaling" steps, experiments performed in the past do not have the validation-level quality [e.g., deficient information and documentation about (i), (iii), (iv), and (vi)]. Hence, implementation of UQ necessarily involves subjective arguments.

For three main sources of data, i.e., SET, IET, and PMO, the grading for Relevance, Scaling, and Uncertainty covers a wide possible range; Table 3.2.

Table 3.2. Range of grades applied to three data sources.

	Relevance	Scaling	Uncertainty	Worth range [R]x[S]x[U]	CASL Data
SET	2-4	1-4 [[9]]	1-4	2…64	2…18
IET	1-4	1-3	1-2	1…24	1...12
PMO	3-4	3-4	**0-1**	0…16	0…16

Thee following remarks can be made with respect to Table 3.2:

- SETs are selected only when they meet or exceed "Relevance" Grade 2;

- IETs are expensive and relatively few, so even test of Grade 1 in "Relevance" is often included for analysis and model calibration;

- Large cost (if even possible) and long time are required to develop in-core diagnostics that help improve "Uncertainty" grade for PMO. This is why the maximum grade for PMO Uncertainty is 1.

- To a less extent, the above remark applies to IETs, explaining why the IET Uncertainty maximum grade is to 2.

- It is possible, and the trend confirms, that a high quality can be achieved in specially-designed, VUQ-guided SETs. This explains the maximum Uncertainty grade for SET being 4.

- In practice (for CASL data as discussed in the subsequent subsections), the Relevance grades for SETs and IETs are 2-3 and 1-3, respectively; the Scaling grades for SETs and IETs are 1-3 and 1-2, respectively; and the Uncertainty grades SETs and IETs are 1-2.

[9] Scaling for separate effect represented by a select set of dimensionless groups.

3.3. Solution Framework for CIPS Challenge Problem

Due to its role in causing Axial Offset Anomaly (AOA) in PWR cores, Crud-Induced Power Shift (CIPS) has been a subject of intense interest for commercial nuclear power industry and studied both experimentally and analytically over the past two decades. There is a substantial body of literature about AOA, CIPS, crud, and related phenomena (RBHT, SFB)[10].

Despite a long history and industry's effort on CIPS, an improved capability for predicting CIPS can have a positive impact on performance of PWRs, including enlarging potential for power uprate. For this reason, CIPS is selected as the top-priority application for CASL. Interested readers are referred to (Karoutas, 2010) for a comprehensive description of the CIPS challenge problem.

Interpretation of CIPS mission success, R&D path and other aspects are discussed below, serving as a framework for identification of validation data needs and review of data VUQ-fitness.

3.3.1. Intended Capability

In its Phase 1, CASL program adopted an approach for integrating into LIME-based VERA panoply of relatively mature (as stand-alone) capabilities developed and used by CASL partners. This includes Westinghouse's ANC code for core neutronics, EPRI/Westinghouse code VIPRE for core / bundle thermal-hydraulics, and EPRI's code BOA for calculating boron-induced offset anomaly. CASL considers integrating other codes in order to provide capabilities for system thermal-hydraulics (EPRI's RETRAN or INL's RELAP5)[11], fine-grain CFD (Star-CCM+)[12], and fuel analysis (EPRI's FALCON). Representing industry's standard in their defined mission, each of the above-listed codes has a long history of development, and its own V&V base.

Notably, with the exception of BOA code, other capabilities (ANC/VIPRE/RETRAN/RELAP5/Star/FALCON) were conceived, designed, developed, assessed and used for other applications than PWR/AOA/CIPS. Nonetheless, it appears that in combination these codes present a state-of-the-art workhorse. The

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[10] See references included in Chapter 4.

[11] RETRAN and RELAP5 code were developed for plant system transient and accident analysis. The computational engine of RETRAN and RELAP5 is based on solving two-phase flow models. They include no scalar transport model for chemicals and corrosion products.

[12] CFD Star-CCM+ code is a commercial software package with demonstrated capability for single-phase turbulent flow simulation. It also includes a RPI model for subcooled flow boiling. The model focused on heat removal mechanisms, and not designed to provide characteristics of potential interest to crud deposition modeling.

question is what one can and should expect from using VERA-integrated capability for addressing CIPS challenge problem.

The author's answer to the above question is three-pronged:

In long term, VERA-based "virtual reactor" serves as the simulation engine for an on-line monitor of plant operation and safety margins, including CIPS-related margins[13]. As such, VERA continuously interacts with plant measurements, using a data assimilation technique to calibrate models and enable margin forecast with high confidence. Having VERA-generated insights, plant operators can optimize reactor core loading pattern, maintenance, operating procedures (including emergency operating procedures, EOP), and operating conditions for achieving minimal / acceptable CIPS even under extended power uprate regime. [14]

In medium term, VERA-based capability serves as the simulation engine for "off-line" analysis of plant operation and safety margins, including CIPS-related margins. Using PMO from a selected PWR plant (including reactor operation and diagnostics data, e.g., flux traces, coolant chemical content, temperature and pressure, and data obtained from fuel/cladding/crud post-irradiation examinations), VERA models are recalibrated to enable reconstruction of reactor conditions over the past fuel reload cycle and forecast evolution of reactor /core / fuel/ cladding / crud over the next cycle.

In near term, the objective is to bring VERA-based integrated code capability for simulation of CIPS (referred to as VERA-CIPS) into a state sufficient for demonstrating that

(i) VERA-CIPS can reliably reproduce capability of component codes;

(ii) VERA-CIPS provides capability to perform integrated simulation of CIPS scenarios; [complete as a framework]

(iii) VERA-CIPS provides acceptable results for key validation experiments; [adequate as simulation engine]

(iv) VERA-CIPS is equivalent or superior over that of component codes (when coupled by an ad-hoc/non-VERA platform) with respect to simulation of multi-physics processes of importance for CIPS;

[13] Dinh et al. "RISMC Software Requirements Specification", 2010, Working Document.

[14] For example, simulations can help suppressing or preventing creation of "hot channel" / "hot spots" during a secondary-side event that caused asymmetric flow or overcooling in one loop. Plant operators are given guidance to use a group of control rods (relative to loop asymmetry) that minimizes the local power-flow disbalance. Simulations also help identify CIPS-prone fuel assemblies and organize effective cleansing of crud during maintenance.

(v) VERA-CIPS applications (including benchmarks and plant analyses) generate new significant insights into physics that govern processes in CIPS; and

(vi) further development of VERA-CIPS software (and supporting methods, models, data) within CASL (resources, timeline) has a reasonable likelihood that VERA will evolve and meet expectation set for it in medium- and long term goals.

Unless success is demonstrated for step (ii) and step (iii), the CASL approach and plan for VERA development and assessment should be revised. In such cases, considerations must be given (top-down) on whether or not improvements/ changes are required for

- integrating framework (is LIME too "lightweight"? or some codes are found to be - by their design - not amenable for integration/coupling)

- set of codes integrated for VERA-CIPS (other codes may be necessary; missing physics? Inherent global limitations of code(s) for CIPS analysis?)

- modeling approach, numerics of component codes.

Table 3.3. Technical Requirements (Karoutas, 2010) – Comments

	Comments
Uncertainty on total AO prediction is less than 3%	Quantifiable goal (success criteria)
3D pin power prediction with TH and Chemistry (boron) feedback	ANC/VIPRE/BOA
Model at least ¼ core	Asymmetric scenarios may lead to "hot spot"
Need full depletion including boron in the crud	
Account for subcooled boiling	Not only as heat transfer model, but condition for boron and corrosion product deposition
Model grid spacer effects on crud deposition	Lacking data for calibrating this model
Minimize calibration for individual plants	Over-optimistic expectation of codes and models. Due to large model and model parameter uncertainties, plant data assimilation is necessary and recommended.
Predict in-core instrument response	Assimilating rather predicting these data.

Technical requirements for VERA-CIPS (an initial set in draft dated December 2010) were outlined in Karoutas (2010); Table 3.3, left column. For the CIPS problem's figure of merit (AOA), the tool development's success criteria are clearly defined ("uncertainty less than 3%). However, the remaining technical requirements (Table 3.3) are vague. Relative to the simulation goal, some of these requirements don't appear necessary, while together the requirements set is not seen as sufficient for the success. In order to define a complete and consistent set of technical requirements, the later should be formulated for a case study, with a specific analysis approach (see Appendix A.3) along with an "issue resolution framework", basically a decision model.

Also, it is important to make clear whether success criteria for tool development ("uncertainty in AO less than 3%") make room for input data uncertainty. Of interest here are uncertainty contributions by processes associated with crud but are not mechanistically modeled in VERA-CIPS. For example, while AOA is significantly controlled by boron in crud, crud characteristics (thickness, composition) are in turn affected by a number of operation/ maintenance factors (e.g., effectiveness of cladding cleansing during fuel reloading campaign). These factors often are captured simply by coarse estimates.

"Key parameters for prediction" for VERA-CIPS (an initial set in draft dated December 2010) were also listed in Karoutas (2010), Table 3.4. While the parameters listed are relevant and important, their prediction does not ensure meeting the CIPS success criteria (which would require prediction of several other parameters).

Table 3.4. Key parameters for prediction (Karoutas, 2010) – Comments

Parameter	***Comments***
Boron deposition in crud	BOA models used to predict this parameter are largely empirical. Moreover, lack of VUQ-quality experiments to assess if the parameter can be reasonably predicted by VERA-CIPS.
Sub-cooled boiling rates and distribution	VIPRE can provide estimates of these parameters. Sound prediction would require "system thermal-hydraulics", especially under transient conditions.
Core boiling surface area	VIPRE models are largely empirical, particularly when it comes to nucleation characteristics, effect of heater materials, and surface chemistry/activation/nanomorphology. These models do not take into account presence/micro-structure/chemistry of crud layer. Boiling models in other codes (RELAP5, Star-CCM+) suffer the same issues.
Crud thickness	No well-controlled, prototypical experiments for calibration of models that govern crud buildup

3.3.2. Decomposition

CASL develops VERA-CIPS as capability for driving solution of CIPS as an industry's challenge problem. The solution framework is hierarchical.

Table 3.5 depicts the top level, where VERA-CIPS is integrated with plant operation data [POD], plant management options [P⇔MO], and operation and safety margin analysis [MA], to provide a R&D strategy [R&DS]. The later

Table 3.5. Four quadrants of the PWR/AOA/CIPS problem solution framework.

← ↓	**[R&DS]** **R&D Strategy** Application Success: *Removing AOA/CIPS as Reactor Performance Constraint* AOA Simulation: Success Criteria ↓ ⇑	⇐ Decision Model ⇑
[POD] **Plant Operation/ Maintenance /Testing Data** Data Assimilation ⇒	**[VERA-CIPS]** **Simulation Engine** ⇑ Neutronics, Fuels, Crud, T-H, Materials, Corrosion,	*R7* ⇒ **[OSMA]** **Operation and Safety Margins, affected by CIPS** RIA, LOCA, ATWS, etc. Safety Regulations
↓ *Suggest PMO, including adding in-core diagnostics and other PIE tests* →	⇑ **[PMO]** **Plant Management Options** *for AOA* *Define scenarios/ configurations to be investigated /simulated by VERA-CIPS*	*RISMC/R7* *Capability to Perform Analysis for a Range of Risk-Significant Scenarios*

It can be seen from Table 3.5 that simulation capability is needed not only for predicting AOA, but also for computing a range of operation and safety margins affected by CIPS and plant management options introduced to help manage AOA. This area (capability for [OSMA]) is not currently pursued in CASL, but can leverage on development in the LWR Sustainability Program RISMC/R7 project.

Table 3.6. Phenomenological decomposition

AOA Prediction: Time- and Space Resolved Core Power over a Fuel Reload Cycle				
FA/Fuels/ Rod/Clad	***T-H***	***Neutronics***	***Crud***	***Coolant Chemistry / Material Corrosion***
FALCON	RETRAN/ VIPRE	ANC	BOA	
Support for T-H, and Neutronics	Core-wide T-H coupled with Neutronics	Core power over long operation period	Initial inventory of crud after fuel reloading (e.g., effect of ultra-sound cleansing)	Material corrosion on RCS and heat transfer surfaces
	Plant / Reactor System T-H			Crud detachment in steady-state & transient conditions
Fuel Burnups	Nominal Operation	Core power during transients	Inventory of crud materials in RCS structural and heat-transfer (SG) surfaces	Inventory, transport and distribution of RCS chemicals and corrosion products (incl. particulate materials)
	Operation Transients	T-H feedback		
	Abnormal Transients			
PCI	Rod Bundle T-H (RBHT/RBTH)	Boron effect	Boron distribution (incl. its depletion)	System-level (incl. coolant chemistry regulation sub-system/filters)
	Inlet Flow incl. Temp. & Velocity Fluctuations			
Fuel Rod and Spacer Defor-mation		Hot channel Identified	Effect of grid spacer mixing/ vibration on crud deposition/detach	Core-level (Regional)
	Subchannel Mixing incl. Spacer Effect			Distribution between Rod Bundles
	Turbulence Flow	Pin-by-pin power (heat flux)	Crud character-ristics (thickness, micro-structure, chemical composition)	Within Rod Bundle (Pin Level)
	Subcooled Flow Nucleate Boiling (heat transfer)			Boundary layer concentration profile of different species
Multiphase micro-hydrodynamics that govern crud deposition		Hot spot identified	Physico-chemistry that govern crud characteristics	
Wall bubble layer configuration			Concentration of chemicals (boron, etc.) and particulates at the triple contact line	
Interfacial Instability				
Turbulence-Interface Interactions			Agglomeration, reactions, precipitation in supersaturated solution	
Condensation on bubble dome				
Bubble dynamics in SFB (sliding, coalescence, oscillations)		Fluence	Dry-spot synthesis &growth of micro-porous layer (area for further deposition)	
Meniscus / microlayer dynamics		Irradiation "aging" effect on cladding and crud stability	Crud insulation effect on boiling / heat transfer, local temperature, meniscus	
Dynamics of Evaporating Triple Contact Line (Recoil Effect)			Effect (e.g., Maragoni, disjoint pressure) of chemicals and particulates present in coolant on microhydrodynamics of evaporating liquid layer and vapor bubble nucleation	
Effect of surface/crud nano-morphology on micro-hydrodyn.				
Nucleation (energy barrier)				

Focusing on VERA-CIPS, the next level of problem decomposition is given in term of physical processes distinguished by their characteristic time/length scales (Table 3.6). It will be useful to perform a preliminary PIRT. Eventually, the integrated framework and a PCM model can be used to facilitate Q-PIRT of this complex challenge problem.

3.3.3. Integration

Table 3.7 provides a tentative ranking of uncertainty sources by their impact (H, M, L for High, Medium, Low).

Table 3.7. Physics and effects in CIPS: uncertainty impact ranking.

	Uncertainty Ranking by Impact	Potential for Reducing Uncertainty Impact by AMS	
Crud	**H**	L	
Initial inventory on cladding	H	L	
Physico-chemical (microscale)	H	L	HR-AOA
Effect of grid on crud	H	M	
Thermal-Hydraulics	**H**	M	
System T-H	L (for CIPS)	M	APEX
RBHT	M	H	[4.4.2]
Subcooled Boiling	H	M	[4.4.3]
Turbulence (mixing)	H	M	[4.4.2]
Condensation on bubble dome	H	M	TBI
Meniscus micro-hydro	H	L	[4.5]
Nucleation	H	L	[4.5]
Coolant Chemistry/ Materials Corrosion	**H**	M	
Inventory on RCS/SG surface	H	L	
Transport (all scales, incl. detachment)	H	M	TBI
Corrosion (sources)	H	M	Data base
Core Neutronics	M	L	HR-AOA
Boron/crud effect	M	L	
Fuel (FA, spacers)	L	M	
PCI	L	M	SCIP

TBI – To Be Identified

Also included are relevant reference experiments and an assessment of potential to use advanced modeling and simulation to reduce uncertainty (changing its impact to a lower rank). As it can be seen in Table 3.7, and in more detail in Chapter 4 (Assessment of Databases and Experiments), there are only few datasets that can be used to support VUQ of "high-impact" models of meso- and micro-scale processes. Understandably, "data existence" situation is markedly better for macroscale (e.g., subcooled flow nucleate boiling) and engineering-scale processes (e.g., rod bundle thermal hydraulics). Even then, data quality is deficient for use in calibration of models, particularly multi-physics models.

However, within the domain of engineering applications, a bottom-up integration of all (and more) phenomena/effects listed in Table 3.6 (in order to predict AOA/CIPS) is not feasible, and not necessary. The approach taken for CASL stems from recognition of its mission in supporting engineering decision-making. In engineering practice, all relevant evidences, both of experimental and computational origin, are "melted in" in order to arrive at solution. Datasets available from separate-effect tests (SET), integral-effect tests (IET) and plant measurements and observations (PMO) are evaluated (for their VUQ fitness) and used (with weight on dataset's VUQ quality) in a data assimilation procedure for model calibration. Key models used in such an integrated treatment should be designed to be consistent with reference/leading experiments, i.e., governing parameters in the key models correspond to directly measurable or robustly inferable data. Consistency between Modeling, Experimentation, and Validation (MeV) is a critical requirement for the "melting" approach to be effective.[15]

Along the same line, integration of models toward the problem's figure of merit melts-in variety of uncertainties present in detailed / individual description of participating processes. This leads to another requirement that errors (uncertainties) in numerical treatment of component models be removed from solution, or brought to the level that does not interfere with model uncertainties (e.g., eliminating concern about effect of numerical grid size used in experiments-scale solution vs. plant-scale solution)[16]. As a result, discrepancy between SET/IET/PMO data and simulation is fully attributed to uncertainty in model (due to modeling assumptions) and model parameters.

In a nutshell, VERA-CIPS success requires a balanced integration between VRI and data efforts. The data, however, have been the weak link in this balance.

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[15] Once validation data base is established, computer codes integrated in VERA should be reviewed against the data base in light of the required "MeV-consistency". Itn some cases, it will be necessary to design a new code, which meets the MeV requirements, but also brings in knowledge base from legacy, industry and state-of-the-art codes.

[16] This "zero-numerical-error" requirement presents a challenge in using many of the legacy (particularly, thermal-hydraulics) codes, which employ first-order-accurate scheme and suffer from excessive numerical diffusion (in some cases, due to ill-posed equations).

3.4. Solution Framework for CILC Challenge Problem

Crud-Induced Localized Corrosion (CILC)-related fuel failures have occurred in PWR cores but it presently constitutes only a minor contribution (1.6%) to the total number of fuel failures in the U.S. PWR plants (over past two decades, only 4 fuel failures are attributed to CILC) [17]. This is to be contrasted with GTRF, which contributes a major fraction (over 70%) of fuel failures in PWR cores. Notably, while CILC had occurred in the past [18], R&D on reactor material corrosion in 70's and 80's has led to innovations in primary system's structural and heat-transfer (steam generator) materials and coolant chemistry that largely suppress the threat of CILC failures.

While currently a minor contributor to PWR fuel failures, CILC is expected to present additional risk to fuels in PWR cores with extended power uprate. It has been argued that CILC failures are more likely to occur in thicker crud layers. It is also possible that "hot spots" (including local burnout) caused excessive stresses that accelerate corrosion and failures. Beside thermal-hydraulic factors that govern crud buildup, there are some other microscale interactions and physico-chemical processes in crud / coolant / cladding that accelerate cladding corrosion under certain conditions (crud porosity, composition, water pH, temperature).

A review of open literature on fuel failures suggests a more limited interest in CILC than GTRF. CILC-related information is primarily observations of fuel assemblies (e.g., failed cladding) from plant, where severe CILC occurred (although not necessarily resulted in fuel failures). No experimental programs on physico-chemistry of CILC and associated failure mechanism are found presently active. The limited knowledge/capability base makes it harder to develop and validate fine-grain models of physico-chemical processes in CILC.

Given the above arguments, within CASL effort to use advanced simulations to develop strategy to effectively reduce fuel failures in PWR cores, it is more cost-effective to direct resources on GTRF than on CILC. Nonetheless, interest to CILC in CASL can be explained by a strong overlap between CILC and CIPS, whose underpinning mechanism in both cases is CRUD.

In summary, it is recommended that CASL contribution to CILC challenge problem is limited to effort already planned in CIPS task, namely development and demonstration of capability for fine-grain simulations of Rod Bundle Thermal-Hydraulics and Corrosion Materials Transport, including subcooled flow boiling and crud layer growth.

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[17] Interested readers are referred to (Karoutas, 2010, CASL Challenge Problem Technical Specification) for a comprehensive description of the CASL's CILC challenge problem.

[18] During the 1970's, CILC was a major mechanism for fuel failures in BWRs. The issue is managed by introducing changes in reactor coolant chemistry and structural materials (Zn-injection, reduction of Co).

3.5. Solution Framework for GTRF Challenge Problem

Interested readers are referred to (Karoutas, 2010) for a comprehensive description of the CASL's Grid-To-Rod Fretting (GTRF) challenge problem. Interpretation of GTRF mission success, R&D path and other aspects are discussed below, serving as a framework for identification of validation data needs and review of data VUQ-fitness.

3.5.1. Intended Capability

The success of R&D effort in developing "Virtual Reactor" capability for GTRF may be expected in two main areas of applications:

(a) VERA enables coupled-code simulations that can be used by researchers and engineers to effectively test hypotheses about mechanisms that govern GTRF, thus developing insights that help improve design, operating procedure, and GTRF-related safety margins;

(b) VERA is a computational engine "fed" with data from on-line reactor diagnostics (data assimilation) for forecasting GTRF margins in support of plant operation optimization.

For CASL Phase 1, area (a) is the primary focus. Simulation capability that is available for integration into VERA for supporting analysis of GTRF includes a whole range of methods (with their respective capability and limitations) in core neutronics (diffusion, transport), thermal-hydraulics (assembly-based, subchannel, CFD-RANS; CFD-LES), and structural mechanics (including fluid-structure interactions)[19]. Selection of specific capability (tools) and evaluation of their maturity can only be made effectively for a technical hypothesis, preferably with a quantifiable figure of merit (FOM) and success criteria. Given the so-defined hypothesis as "challenge problem application", one can formulate an "issue resolution framework" and implement the project (see Figure 2.1).

The following subsections describe "decomposition" and "integration" steps needed to build "issue resolution framework" under a working hypothesis[20] that there exists a **"PWR fret map"** (similar to "BWR stability map") that the VERA capability is developed to predict this "fret boundary" that identifies fret-prone conditions ("fret" zone in the "fret map"). Thus, the GTRF problem can naturally be cast into a margin analysis task, with margin being a distance from operating conditions to the "fret boundary".

[19] Capability includes Sierra's Salinas/ABQUS, Adagio/ABAQUS, Salinas/Aria, Salinas/FUEGO, Star-CCM+ (Sham, 2010/CASL-only-info); VITRAN code (Lu, 2010/CASL-only-info).

[20] It is noted that this hypothesis is promoted by the present author, and used here as example for analysis of data. It is and not necessarily the industry-wide most accepted or go-after hypothesis about GTRF.

This hypothesis[21] assumes that, from utility point of view, it is desirable that the VERA capability be used to establish this “fret map” and determine the “fret boundary” with high confidence. This information can then be used to guide plant to operate alongside (but not crossing) the fret boundary. This outcome would also deemphasize the need to accurately predict the degree of wear that might occur when the plant operation conditions crossed the “fret” boundary.

3.5.2. Decomposition

The “fret boundary” hypothesis – while not eliminating the need for a sound understanding and assessment of the fretting wear (mechanism, rate) – places the focus on fluid-structure interactions.

(1) Fluid flow

[1.a] Plant system transient thermal-hydraulics; affecting [1.b]…[1.f]

[1.b] Large-scale unsteady (e.g., pump frequency; pump transient) fluid motion [and flow impingement on core structures] from cold leg inflow

[1.c] Large-scale unsteady fluid motion and mixing in downcomer, lower plenum [high-energy fluctuations that induce core structure oscillations], and upper plenum

[1.d] Core-wide flow distribution, including bypass flow, parallel channel flow communication

[1.e] Rod Bundle Thermal Hydraulics – Turbulent flow in fuel assemblies [including effect of grid spacers/ mixing vanes on fluid mixing, subcooled flow boiling]

[1.f] Fluid response (typically, loop-asymmetric) to plant operational and abnormal transient scenarios (e.g., due to an event in secondary side of a steam generator), [causing inertial fluid motion and FSI /residual oscillations over a prolonged period]

(2) Core neutronics

[2.a] [short time scale] Core power that affect in-core thermal-hydraulics, in-core thermo-structural mechanics, and fuel behavior, and any feedback mechanisms introduced by FSI (e.g., control rod oscillations, fluid temperature and void fraction variations)

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[21] As a rule, knowledge gained from R&D may lead to formulation of a better hypothesis, with correspondingly new FOM and success criteria. Consequently, this necessitates a new decomposition/integration, and “issue resolution framework”. However, implementation of the new framework can largely make use of knowledge and capability base developed for the previous hypotheses.

[2.b] [long time scale] Fluence on structural materials that cause irradiated material (properties) degradation

(3) Structural mechanics (tightly coupled with [1.c]…[1.e])

[3.a] Full-core structural dynamics including all mechanical coupling (e.g., contact friction, relocation) of structures e.g., fuel assemblies, core plates, core barrel, and coupling with fluid pressure.

[3.b] Fuel assembly structural dynamics, including effect of grid spacers (grid-to-rod gap), grid growth, cladding swelling (due to burnups and PCI), coupling with fluid turbulence [1.d]

[3.c] Contact friction and wear dynamics (accounting for structural vibration / turbulence excitation, rod and grid growth/relocation, i.e., results from [1.e], [3.b], [4.a])

(4) Fuel performance (tightly coupled with (2), to generate results for [3.b])

[4.a] Fuel behavior (e.g., PCI, hydriding) under burnups (including cycle length), causing degradation in cladding material properties, axial and radial rod growth

Apparently, whereabouts of a core condition in the "fret map" is affected by many factors, among them are reactor/core/fuel/spacer geometries, their materials, plant operating conditions and history. For example, couple "bad" transients during a fuel reload cycle have potential to bring an operating plant closer to the "fret boundary". Thus, a "fret mapping" is plant-specific and dynamic.

3.5.3. Integration

"Decomposition" step outlined above depicts a high degree of complexity of the GTRF challenge problem, involving multiple physics over a broad range of length and time scales. Validation of models and codes used to simulate these phenomena would require a vast amount of data whose acquisition would take well beyond timeline and resources available for CASL.

Enter the "PWR fret map" hypothesis. The "fret map" focuses simulation capabilities into an integral, "risk-informed" goal, namely the core's "fret-ability"; Table 3.5. The "fret boundary" effectively serves as the problem's FOM that is instrumental for sensitivity/uncertainty (QPIRT/PCM) analysis.

It is recommended that CASL-AMA effort in GTRF area be focused on devising, implementing, and demonstrating the "fret-ability" framework that integrates physical processes, their epistemic and aleatory uncertainty toward the FOM; see e.g., (ROAAM study, Theofanous, 1996; Theofanous & Dinh, 2008).

Table 3.5. Integration of component process models in GTRF problem.

"Fret Map": GTRF-prone domain boundaries				
GTRF wearing rate (at sensitive locations)				
Forcing at GTR Contact			Wear Rate	
Rod-Grid Vibration Analysis			Tribology	
Pressure/stress field	GTR Gap	Spring Relaxation Spacer Expansion		
Flow Turbulence Power Spectral Density (PSD)	Spring Dynamics Rod bending	Irradiation-Induced Grid Spacer Expansion	Cladding Properties	Grid Spacer Properties
Fuel Rod-Grid System ***Identify sensitive FRGS***		***Aging Effect***	**Materials Properties (Degradation)**	
Subcooled Boiling	FA Bowing	FA shuffling / Contact Reset	Contact area relocation	Fluence
Sub-channel Mixing	Friction Forces	Power transients,	Cladding Deformation	Pin-by-pin Power
Fuel Assembly ***Identify sensitive FAs***		Secondary side transients	Pellet-Cladding Interactions	Effect of Control Rod FSI
In-vessel flow mixing in downcomer & lower plenum	FA-to-structures couplings (incl. loose, float) FA-to-FA couplings	Pump transients, Pump asymmetry		Structural Feedback on Neutronics
System Thermal-Hydraulics	Core barrel Core support plates	Effect of Heat Axial Distribution on Subcooled boiling		Thermal-hydraulic Feedback on Power
Core-wide Structural Dynamics[22]		Plant Operation & Abnormal Transient	**Core-Wide Thermal-Hydraulics**	
Stresses	Mechanics	Heat Flux	Fuel Burnups	Core Power
Fluid Flow	**Structures**	**Thermal**	**Fuels**	**Neutronics**

[22] The present framework is more inclusive than methods currently used for GTRF analysis, that are limited to fuel assembly domain. Large-scale in-vessel fluid motion and small-scale thermo-fluid fluctuations (in-mixing) might introduce low- and high- frequency oscillations of the core system and fuel assembly, respectively.

Chapter 4. Assessment of Databases and Experiments

4.1. Databases on Nuclear Fuel Performance

4.1.1. Overview

There have been several international efforts (supported by IAEA, NEA and others) in developing and maintaining databases on nuclear fuel performance that include both plant data and experiments.

Most notably and relevantly is the Joint OECD/NEA-IAEA International Fuel Performance Experiment (IPFE) Database, which is established in collaboration with the OECD Halden Reactor Project. The IPFE Database's goal is excellently aligned with CASL interest, namely "to provide in the public domain, a comprehensive and well-qualified database on Zr clad UO_2 fuel for model development and code validation. The data encompasses both normal and off-normal operation and include prototypic commercial irradiations as well as experiments performed in Material Testing Reactors." (OECD-NEA, IFPE 2010).

In addition, IAEA performed a review of fuel failures in water cooled reactors and published a comprehensive report that covers statistical data on fuel failure as well as descriptions of failure modes, failure detection and mitigation techniques (Killeen, 2010; IAEA, 2010).

4.1.2. Status

The IFPE database is designed to include "well-qualified data that illustrate specific aspects of fuel performance. Of particular interest to fuel modellers are data on: fuel temperatures, fission gas release (FGR), fuel swelling, clad deformation (e.g. creep-down, ridging) and mechanical interactions." (OECD-NEA, IFPE, 2010). In addition to direct in-pile measurement, the data include PIE information on clad diameters, oxide thickness, hydrogen content, fuel grain size, porosity, and other parameters. According to the IFPE web statement (OECD-NEA, 2010), to date datasets about 1445 rods/samples from various sources encompassing BWR, CAGR, PHWR, PWR, and VVER reactor systems have been included.

4.1.3. Assessment

While providing useful insights on global mechanisms and causes of failure, the IAEA fuel failure review is highly qualitative and judged not fit for use in modern VUQ of models and codes developed in CASL.

The scoping review of the IFPE database content indicates that it has not yet included experiments of direct relevance to the CASL leading challenge problems, CRUD and GTRF. The IFPE datasets are rich on "classical" topics in fuel performance, including PCI and cladding performance under high burnups. Additionally, a significant portion of the IFPE data is related to fuel performance under transient and accident conditions, which are of interest to other challenge problems; see Table 4.1.1.

It is noted that analysis, modeling and simulation of each experiment in the IFPE Database characteristically require substantial, multi-year, multi-FTE effort, especially when the experiment is used for validation of a model or code. This is because the fuel performance experiments (even in world-class facilities like ATR and Halden Reactor) have many operational constraints, very limited control, and large-uncertainty diagnostics. The later (e.g., thermocouples) often degrade rapidly (and in unquantifiable manner) under the harsh irradiation and thermal-hydraulic (temperature, pressure) and chemical conditions of in-pile reactor testing. Other measured data such as from PIE are time-accumulative, hence not conducive for use in VUQ of time- and space-resolved models.

Thus a careful screening of experiments is a must before making commitment for including a selected dataset into the VUQ portfolio.

Table 4.1.1. Assessment of IFPE data VUQ quality relative to CASL interests.

	Problems	***Grade***	***Comments***
Relevance	CIPS	2	Corresponding to the extent cladding material degradation (in part due to pellet-cladding interactions) influences processes in CRUD and GTRF
	CILC	2	
	GTRF	2	
	PCI	3	
Scaling	CIPS	1	Conditions in a large fraction of tests are RIA and LOCA, not (near) nominal operation of interest to CRUD and GTRF
	CILC	1	
	GTRF	1	
	PCI	3	
Uncertainty	CIPS	0	[no detailed review and analysis on data uncertainty was performed]. It is judged that the tests were instrumented with standard diagnostics, and test conditions were not controlled and documented to a high degree required for CASL VUQ.
	CILC	0	
	GTRF	0	
	PCI	2	

4.1.4. Recommendations

Since the U.S. Department of Energy (along with EPRI) is (listed as) a member of the OECD-NEA IFPE Database project, it should be relatively easy and advisable to arrange access of CASL (MPO) researchers to the IFPE Database, to facilitate a critical in-depth review of IFPE data and – if justified – to encourage CASL experts to participate in developing data selection, screening, processing and archiving in IFPE that increase data value for both CASL and broader community. In a longer term, it is recommended that the IFPE be integrated within the NE-CAMS Database.

At this time, no experiments from the IFPE Database appear sufficiently relevant and adequate for CASL VERA VUQ.

Effort to work with IFPE is to be treated as exploratory and **low-to-medium-priority activity** for CASL.

4.1.5. References (for Nuclear Fuel Performance Databases)

IAEA, Review of fuel failures in water cooled reactors. — Vienna : International Atomic Energy Agency, 191p., 2010.

J. Killeen, "IAEA Program on Nuclear Fuel Performance and Technology", 2010.

OECD-NEA, International Fuel Performance Experiments (IFPE) Database (2010) http://www.oecd-nea.org/science/fuel/ifpelst.html

J.A. Turnbull, Review of Nuclear Fuel Experimental Data – Fuel Behaviour Data Available from IFE-OECD Halden Project for Development and Validation of Computer Codes, NEA, 67p. 1995.

4.2. Plant Measurement and Observation

4.2.1. Overview

Participation of several nuclear industry companies in CASL presents unique opportunity for researchers to access and utilize information from an actual plant for guiding the development of simulation codes and for assessment of predictive capability in addressing specific challenge problems [CASL, 2009].

Carefully selected, plant-based benchmarks are superior in their "Relevance" and "Scaling" categories. In the past, plant benchmarks (e.g., BWR stability) have proven indispensable for evaluation of multi-physics simulation capability (couple code system).

Past experience (e.g., with BWR stability benchmark) suggests that plant benchmark is a resource-intensive project that requires collaboration from multiple parties, particularly from plant/fuel vendor and utility personnel. This is because plant benchmarks require detail technical information about

(i) design of plant / reactor / core / fuel (to be obtained from respective plant and fuel vendors, possibly via arrangement with utility);

(ii) operational history of plant / reactor / core / fuel in the selected plant and cycle (to be obtained from utility)

(iii) physico-chemical/ structural/neutronic/thermodynamic / etc. properties of materials, coolants, fuels used, including their degradation under irradiation, chemical, mechanical, and thermal stressors;

(iv) testing results of plant design-specific equipment, and sub-systems (i.e. aggregate behavior not given in (iii) above)

(v) data from plant / core / fuel diagnostics and on-line condition monitoring

(vi) shutdown / maintenance observations and data, including post irradiation test results.

Release of such information can be cumbersome, both technically and organizationally, due to their commercial, legal, and regulatory implications.

Time-wise, CRUD- and GTRF-related physical processes of importance (i.e., those having a significant contribution to uncertainty in prediction of the problem's figure of merits) have their characteristic time scale spanning over a wide range. Space-wise, these physical processes include both system-scale phenomena (e.g., production and transport of chemicals and corrosion products in the primary reactor circuit), to local interactions (e.g., deposition of chemicals at the bubble meniscus' triple contact line; grid-to-rod contact wear). This dictates the need for multi-scale and multi-physics treatment, requiring data at respective scales and phenomena.

4.2.2. Status

For CRUD-related (CIPS, CILC) problems, it has been proposed that plant data from Watts Bar 1 and Seabrook be considered for test problem and validation activity [Karoutas et al., 2010].

For the GTRF challenge problem, options exist for Westinghouse (W), Babcock &Wilcox (B&W), and Combustion Engineering (CE) plants, but specific plant has yet to be identified.

4.2.3. Assessment

Table 4.2.1. Assessment of plant data VUQ quality relative to CASL interests.

	Problems	***Grade***	***Comments***
Relevance	CIPS	4	
	CILC	4	
	GTRF	-	Plant data is yet to be identified
Scaling	CIPS	4	
	CILC	4	
	GTRF	-	
Uncertainty	CIPS	[0-2]	Conservative expectation of quality (coverage, completeness) plant data
	CILC	[0-2]	
	GTRF	[0-1]	In-core diagnostics is practically non-existent for GTRF phenomena's time and length scales

The initial assessment of VUQ quality of plant data (Table 4.2.1) is based on expectation that a the following data types will be made available to CASL for VERA VUQ integrated benchmarks:

- reactor /core / fuel assembly design geometry
    - o difficulty exists in obtaining design features (e.g., spacers; mixing vanes) of commercial value

- nuclear fuel design and characteristics (core loading pattern, operating history) enough to computer time- and space-resolved core neutronics and core power
- in-core diagnostics e.g., flux traces, temperature measurements
    - low resolution in time and space, especially not located in areas of interest

- in-plant coolant chemistry monitoring
    - measurements, if any, are aggregative (e.g., pH, total concentration of corrosion products) rather than differential (i.e., by chemicals and by types of corrosion products)

- visual, structural and chemical characterization of crud layer or cladding material wear (e.g., observed and measured during fuel reloading).
    - "data" are end-of-cycle measurements, not reflecting dynamics of crud/wear development and any correlation between crud growth (or cladding wear) and dynamics of reactor operating parameters.

4.2.4.Recommendations

It is recognized that organizational steps should now be taken in CASL in order to facilitate establishing a data transfer agreement and building a (secure) data management system before any actual data from plants can be released to CASL researchers.

Independent of timeline in securing the actual plant data release (and hence, access of VUQ researchers to the plant data for in-depth data review), it is of **high priority** for the project progress that CASL organization and partners collectively address the following questions:

- what types of data are actually available from the plant and cycles identified for benchmark purpose;

- even preliminarily, which quantity (coverage) and quality (completeness) may be expected for the available data types;

    - answer to this question helps identify sources / types of uncertainty and establish a tentative range of uncertainty in measured data, local / boundary conditions

- estimated cost and timeline required to gather additional data (e.g., by modifying diagnostic system or by processing of archival data) for the types identified as critical for the plant benchmarks but not readily measured or documented by the vendor/utility;

- what are conditions for eventual release and usability of each class of data and datasets identified as relevant for plant benchmarks;

    - This information must be accounted for in developing a CASL validation data plan, e.g., by factoring in certain data which exist or can be measured but are not available for CASL-wide use in data assimilation and model calibration, due to e.g., legal, commercial or cost reason.

4.2.5. References (for PMO)

Z. E. Karoutas, “Challenge problem technical specification”, CASL-AMA, [Working Document], December 2010.

4.3. Integral-Effect Test Programs

4.3.1. Studsvik Cladding Integrity Project

4.3.1.a. Overview

Initiated in 2002, Studsvik Cladding Integrity Project (SCIP) is an OECD/NEA program with over 35 participating organizations (utilities, vendors, research institutes, and regulators) from 11 countries. Two CASL partners (EPRI and Westinghouse) are members of the SCIP program.

The SCIP project focus is knowledge and data on nuclear fuel evolution, particularly on response of cladding integrity at high and very high burnups, during steady state and transient operation, and design basis accidents. The experimental program is designed to support code validation exercises, and be complementary to other fuel testing projects (e.g., the Japanese ALPS and French CABRI programs).

The SCIP research approach combines in-pile (ramp) testing, post-irradiation examination, mechanical testing for characterization of Pellet-Cladding Mechanical Interactions (PCMI), primarily in ramp tests. The tests were performed originally in the Studsvik's R2 reactor and then in the Halden reactor through collaborative arrangement.

4.3.1.b. Status

Over the past seven years, the SCIP project has produced a wealth of data from out-of-pile and in-pile tests for LWR fuels with Zr-2, Zr-4, ZIRLO, and M5 cladding materials. An overview of tests and findings obtained in the SCIP-I (2004-2009) program is given in Alvarez (2007, 2009). Notably, at high burnup levels, the pellet-cladding interaction failures result from a combined effect of locally high stresses (due to pellet swelling) and aggressive fission products (mainly iodine, leading to iodine induced stress corrosion cracking).

In the SCIP-II (2009-2014) program, the study of the nuclear fuel failure mechanisms continues to focus on PCI (fuel rod failures where the cladding fails by stress corrosion cracking) and hydrogen induced failures [classical hydride embrittlement and delayed hydrogen cracking].

4.3.1.c. Assessment

Access to data obtained in SCIP tests is restricted to the SCIP project members, and as such they are not yet available to the broad partnership of CASL. Dissemination of the SCIP data to a broader community of researchers outside the SCIP project is being considered through OECD/NEA collaborative agreement and possible SCIP-CASL bilateral arrangement. Meanwhile, important findings from the experiments, analyses and code benchmark activities in the SCIP project have been made available through public presentations (Alvarez, 2009) and papers published in conferences (Herranz et al., 2009; Anghel et al., 2009; Holston et al., 2010).

Based on information about test program, measurement methods, and data collected for code validation from available references, the present author assesses the SCIP data fitness for VUQ for CRUD and GTRF challenge problems. The judgment is highly subjective at this point. *Notably, to the extent cladding material degradation (in part due to pellet-cladding interactions) influences processes in CRUD and GTRF, SCIP data are relevant to CRUD and GTRF challenge problems*. The assessment is also provided for SCIP data relative to PCI and DNB as separate challenge problems; see Table 4.3.1.

Table 4.3.1. Assessment of SCIP data VUQ quality relative to CASL interests.

<table>
<tr><th></th><th>Problems</th><th>Grade</th><th>Comments</th></tr>
<tr><td rowspan="5">Relevance</td><td>CIPS</td><td>2</td><td>Cladding mechanical state has a minor effect on crud</td></tr>
<tr><td>CILC</td><td>3</td><td>Cladding stress; hydrogen-induced embrittlement affect localized failure</td></tr>
<tr><td>GTRF</td><td>3</td><td>Cladding stress and properties affect wear and failure</td></tr>
<tr><td>PCI</td><td>4</td><td></td></tr>
<tr><td>DNB</td><td>0</td><td></td></tr>
<tr><td rowspan="5">Scaling</td><td>CIPS</td><td>2</td><td rowspan="3">Although the experiments are scaled for PCI-oriented testing, the use of real fuel and reactor conditions make then reasonably applicable for validation of fuel and cladding modeling under CRUD and GTRF scenarios</td></tr>
<tr><td>CILC</td><td>2</td></tr>
<tr><td>GTRF</td><td>2</td></tr>
<tr><td>PCI</td><td>4</td><td>Test conditions are reactor prototypic</td></tr>
<tr><td>DNB</td><td>0</td><td></td></tr>
<tr><td rowspan="5">Uncertainty</td><td>CIPS</td><td>0</td><td rowspan="3">Large uncertainty in characterizing fuel and cladding’s initial conditions and measured data, but adequate for second-rank mechanisms (in CRUD and GTRF)</td></tr>
<tr><td>CILC</td><td>0</td></tr>
<tr><td>GTRF</td><td>0</td></tr>
<tr><td>PCI</td><td>2</td><td>Special measurements (PIE) are informative, but need quantification and documentation of experimental data uncertainties</td></tr>
<tr><td>DNB</td><td>0</td><td></td></tr>
</table>

4.3.1.d. Recommendations

The SCIP data can help calibrate models in computer codes for simulating fuel/cladding behaviors. It is judged that solution of CRUD and GTRF challenge problems can significantly benefit from capability for predicting evolution of fuel cladding geometry, cladding material properties, cladding stresses, failure mechanisms and integrity under normal and abnormal operation conditions.

Therefore, it is recommended that SCIP data be a **high-priority acquisition** for CASL database. Provided DOE (CASL) membership in the SCIP-II project, CASL experts can use simulations for providing insights and developing guidance that make SCIP tests fit for VUQ of VERA codes.

4.3.1.e. References (for SCIP)

A.-M. Alvarez, Studsvik Cladding Integrity Programme, Touch Briefings [Nuclear Energy Review], 2007. Presentation, 2009.

C. Anghel, A.-M. Alvarez Holston, G. Lysell, et al., "An Out-of-Pile Method to Investigate Iodine-induced SCC of Irradiated Cladding", LWR Fuel Performance Meeting, September 6-9, 2009, Paris, France.

L.E. Herranz, I. Vallejo, G. Khvostov, J. Sercombe, G. Zhou, "Fuel performance during ramps: main results from a SCIP-based benchmark", 35 Reunión Anual de la SNE Sevilla, October 2009. Also "Insights into Fuel Rod Performance Codes during Ramps: Results of a Code Benchmark Based on the SCIP Project", LWR Fuel Performance Meeting, September 6-10, 2009, Paris, France.

A.M. A. Holston, V. Grigoriev, G. Lysell, et al., "A Combined Approach to Predict the Sensitivity of Fuel Cladding to Hydrogen-Induced Failures during Power Ramps", LWR Fuel Performance Meeting, September 26-29, 2010, Orlando, Florida.

M. Karlson, "Post Irradiation Examinations: Cooperation and Worldwide Utilization of Facilities", Studsvik, 2008.

J. Sercombe, M. Agard, C. Struzik, et al., "1D and 3D Analyses of the ZY2 SCIP BWR ramp test with the fuel codes METEOR and ALCYONE", Nuclear Engineering and Technology, V.41. N.2, March 2009, pp.187-198.

Herranz et al (2009) analyzed results of a SCIP-based benchmark by several leading nuclear fuel performance codes (including FALCON and FRAPCON codes[23]

[23] Y. R. RASHID, R. S. DUNHAM, R.O. MONTGOMERY. *FALCON MOD01: Fuel Analysis and Licensing Code – New*, Technical Report ANA-04-0666 Vol. 1, ANATECH Corp. (2004).

D.D. LANNING, C.E. BEYER, K.J. GELHOOD. *FRAPCON-3: Updates, Including Mixed-Oxide Fuel Properties.* NUREG/CR-6534, Vol.4, PNNL-11513 (2005).

of interest to CASL) and identified a range of needs for further experimentation to support both modeling (items a-b) and validation (items c-d).

a) "*Concerning advanced claddings, material properties, particularly creep/plasticity laws and corrosion rates, should be more extensively characterized under steady state and power transients would be valuable. Stress relaxation tests as well as "lift-off" experiments could provide significant information on creep/plasticity laws.*
b) *Regarding fuel, gas swelling has been identified as a key phenomenon for fuel response to transients. Further data on its effect and kinetics would be of high interest.*
c) *Extensive instrumentation of test specimens is highly interesting to achieve a global view of the scenario. Measurements of variables like fuel temperature, internal pressure and on-line cladding elongation would be desirable.*
d) *Data uncertainties should be clearly assessed and reported. This is of a vital relevance in any validation process." (Herranz et al, 2009)*

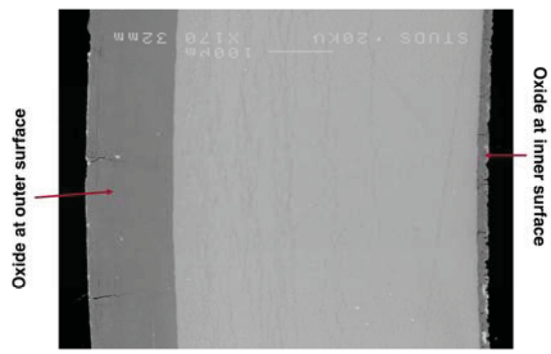


Figure 4.3.1. SCIP results: oxidation of outer/inner cladding surfaces (Alvarez, 2009).

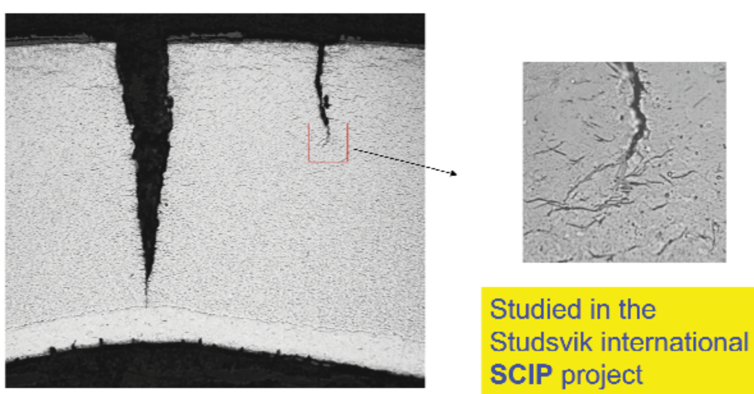


Figure 4.3.2. PIE local cladding hydrating (Karlson, 2008).

4.3.2. Halden Reactor Axial Offset Anomaly (Crud) Tests

4.3.2.a. Overview

Generally speaking, the Halden Project is referred to as a jointly financed research programme under the auspices of the OECD - Nuclear Energy Agency.

> The Halden Boiling Water Reactor (HBWR) is a test reactor (maximum power of 20 MW) cooled and moderated by boiling heavy water (normal operating temperature 235°C and pressure 34 bar). For tests requiring representative light water reactor (LWR) conditions, test rigs are housed in pressure flasks that are positioned in fuel channels in the reactor and connected to dedicated water loops. The reactor operates for two ~100 day reactor cycles each year.

In the present data review, the Halden Reactor (AOA/crud) tests refer to a set of experiments carried out in the Halden Reactor (in part funded by the U.S DoE Nuclear Enery Plant Optimization Program and EPRI Fuel Reliability Program) to investigate the Axial Offset Anomaly (AOA) in PWRs by

> "entraining boron within fuel crud deposits and measuring the resulting flux depression under prototypical PWR conditions" (Bennett et al., 2004).

4.3.2.b. Status

A test program (in three cycles) sponsored by the US DOE and EPRI is described in detail in Bennet et al (2004) and summarized in Bennett et al. (2007).

> A bundle of eight tests rods (active fuel length 60 cm) was irradiated in the Halden reactor for 349 full power days (three reactor cycles) under PWR water chemistry and thermal-hydraulic conditions.
>
> One of the test requirements was that no boiling should occur long the lower section of the fuel rods and that sub-cooled nucleate boiling was required along the upper section. Hence, the lower (20 cm) and upper (40 cm) sections of the test rods were fuelled with UO_2 with different enrichments.
>
> On-line, in-core instrumentation included a diameter gauge to detect crud deposition, and neutron detectors and coolant thermocouples to detect flux/power depressions. An Fe-Ni-EDTA solution was added to the loop coolant to accelerate crud deposition. After irradiation, crud samples were collected for post irradiation exposure (PIE) to investigate their composition and morphology (Bennett et al., 2004).

Bennett (2009) provides discussion of results of five other tests designed to study the effects of coolant thermal-hydraulics and water chemistry on crud formation and composition; see Table 4.3.2.

> A typical experiment contains from one to six test fuel rods, with an active fuel length of up to 60 cm. PWR water chemistry is simulated by additions of LiOH, B(OH)3 and dissolved hydrogen, together with any required additives, for example zinc. Although the

coolant flowrate through the test section (1 to 1.8 m/s) is a factor of three lower than that in a commercial PWR, a representative degree of sub-cooled nucleate boiling (SNB) can be achieved by adjustment of the coolant inlet temperature and fuel rod power (Bennett, 2009).

Table 4.3.2. Test thermal-hydraulics and water chemistry conditions (Bennett, 2009).

Parameter	Test 1	Test 2	Test 3, Phase 1	Test 3, Phase 2	Test 4	Test 5
Time at power, days	1000	160	160	120	267	500
Void fraction	0 – 0.05	0.13	0.012	0.01 – 0.022	0.05	0.12 - 0.19
Inlet temperature (°C)	305 -310	322	290	294	317	310
Temperature rise (°C)	6 -10	7	24	30 - 35	13	10
ALHR (kW/m)	15 - 34	30 - 40	16 - 34	30	26 - 34	40 (mean)
Heat flux (kW/m^2)	500 - 1140	890 - 1180	455 - 855	980	870 - 1180	1180 (mean)
LiOH, ppm	3.0	3.2 / 2.2*	3.15	3.15	2.3	2.3
B, ppm	1000	992 / 290*	1400	1400	1170	1170
pH_{300}	7.1	7.1 / 7.4	7.0	7.0	6.93	6.93
Soluble Fe, ppb	5	0.1 - 27	3.5	15	3 – 15	3 – 15
Soluble Ni, ppb	0.15	0 - 1.4	0.3	2	< 0.5	< 0.5
Soluble Zn, ppb	< 1	< 1	< 1	< 1	50	50
Max crud thickness, µm*	0	20	0	500	(2)**	65***

* Measured during PIE
** Crud formed in localised regions, not full surface coverage
*** Measured in-core, at power

4.3.2.c. Assessment

The Halden Reactor AOA (crud) tests are highly relevant to the CASL CRUD (CIPS, CILC) challenge problems. The tests provide conditions for crud deposition on fuel rods and then the crud is characterized. The Axial Offset Anomaly was also observed in some cases.

Microscopically, the Halden Reactor crud test data are expected to be useful for calibration and validation of crud deposition models, as they are developed and applied for simulation of AOA in PWRs. However, ***scalability*** of the Halden Reactor AOA/crud tests for the PWR conditions remain an open question. According to Bennett (2009) the crud test is designed under assumption that subcooled boiling is the primary mechanism that governs the crud deposition. While subcooled boiling is necessary, it may not be sufficient to reproduce the physico-chemical (e.g., concentration profile, local conditions) and thermal-hydraulic environment (e.g., bubble size and bubble dynamics) and complex interactions between physico-chemistry and micro-hydrodynamics (of bubble meniscus) that control crud formation, growth and detachment.

Macroscopically, the Halden Reactor test data are expected to be useful for calibration and validation of Axial Offset Anomaly models. However, it is noted that core neutronics and thermal-hydraulic conditions (outside the test section) in the Halden Reactor are not PWR-prototypical. Also open is question about to-be-determined ***uncertainty*** in measurement of reactor/core-scale parameters and calculation of local test conditions; see Table 4.3.3.

Table 4.3.3. Assessment of the Halden AOA/crud data VUQ quality relative to CASL interests.

	Problems	***Grade***	***Comments***
Relevance	CIPS	3	A majority of tests is designed to study crud as underlying factor for AOA, but not the AOA itself.
	CILC	3	
	GTRF	0	
	PCI	2	Sensitive to cladding material / chemical and thermal conditions
	DNB	2	Sensitive to cladding surface conditions
Scaling	CIPS	2	Neither scaling nor mechanistic models were provided. Subcooled boiling conditions are reproduced under non-prototypical local flow/power conditions.
	CILC	2	
	GTRF	0	
	PCI	1	Not scaled for PCI-limiting conditions
	DNB	1	T-H conditions not scaled for CHF study
Uncertainty	CIPS	2	Qualitative observations. Data (i.e., crud elemental compositions) are limited to accumulative (end-of-cycle) measurements
	CILC	2	
	GTRF	0	
	PCI	1	Limited information of PIE type
	DNB	1	Lack information required for accurate reconstruction of local power and heat transfer conditions

4.3.2.d. Recommendations

Questions about scaling and uncertainty notwithstanding, the Halden Reactor crud tests are one-of-a-kind with a high potential to help calibrate models for simulating crud deposition in VERA computer codes. It would be extremely beneficial for CASL mission that the VERA code demonstrates its capability to analyze the Halden crud tests and capture results of relevant tests, both qualitatively and quantitatively. In this process, caution is necessary for not misrepresenting the value of the benchmark until issues in test scaling and uncertainty in experimental data and test conditions are satisfactorily addressed.

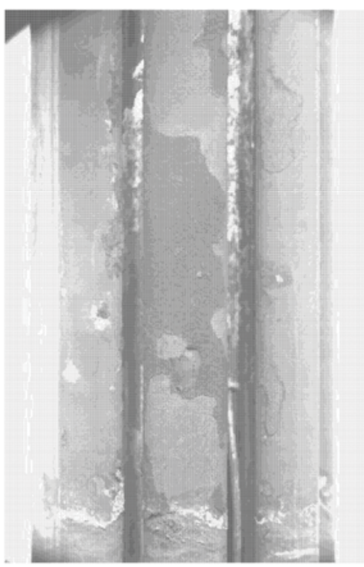
Based on the above discussion, it is recommended that the Halden crud test data be a CASL immediate and **high-priority acquisition** item. As a first step, this will require overcoming legalistic and commercial obstacles in providing CASL researchers with access to the Halden crud data. The next step is to cultivate a strong collaboration with the Halden team; this can help obtain additional insights and information that increase the VUQ fitness of the Halden data. Uncertainty reduction should be pursued through a more resolved characterization of experimental (neutronics, power, thermal, hydraulic, and chemical) conditions, and a more complete examination of the resulting crud on fuel rods. The former may require reconstruction of the reactor operation history over the test cycles, disclosure of reactor core content (outside the LWR test rig/pressure flask) and other measured data in the test rig, while the later may require access to detailed reports and additional measurements.

4.3.2.e. References (for HR-AOA)

P. Bennett, B. Beverskog, and R. Suther (J. Deshon). "Halden In-Reactor Test to Exhibit PWR Axial Offset Anomaly", EPRI-1008106, 120p., December 2004

P. Bennett, B. Beverskog, and R. Suther (J. Deshon). "Demonstration of the PWR AOA in the Halden Reactor", IFE, Norway, 2007,

P. Bennett, , "Effects of water chemistry and thermal-hydraulic conditions on crud formation on PWR fuel in the Halden reactor", IFE, Norway, 2009.



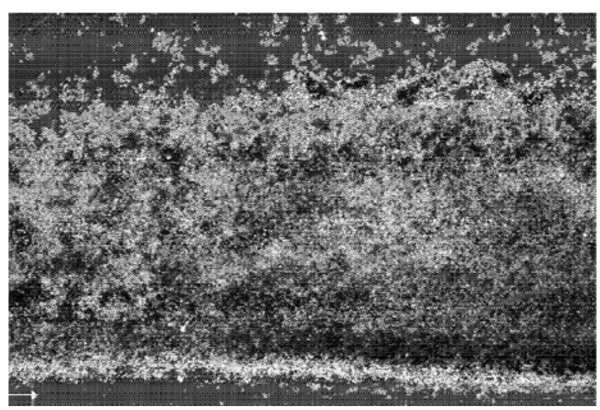


Figure 4.3.3. Left: Crud deposits on upper section of fuel bundle; Right: Crud morphology analysis by optical microscope (Fig.9.1 and 9-3 in Bennett et al., 2004). [Q: How this information is to be used in VUQ of crud process model and codes?]

4.3.3. Industry Out-of-Pile Integral-Effect Test Programs

4.3.3.a. Overview

Nuclear industry and particularly nuclear reactor fuel vendors have in-house capability for performing experiments that support fuel assembly design and testing program. Of relevance to CASL are test programs (and data) generated and/or owned by Westinghouse and Electric Power Research Institute (EPRI), both CASL partners.

WALT and NESTOR programs were identified in Karoutas (2010) as component of validation of VERA for CILC challenge problem. Wang et al (2008) provides an update information on WALT (Westinghouse Advanced Loop Tester) facility

> In order to understand crud formation on the fuel rod cladding surfaces of pressurized water reactors (PWRs), a crud Thermal-Hydraulic test facility referred to as the Westinghouse Advanced Loop Tester (WALT) was built at the Westinghouse Science and Technology Department Laboratories in October 2005.
>
> In this test loop, crud can be deposited on the heater rod surface and the character of the crud is similar to what has been observed in the PWRs. In addition, chemistry in the WALT loop can be varied to study its impact on crud morphology and associated parameters. The WALT loop has been successful in generating crud and measuring its thermal impact as a function of crud thickness.

NESTOR (New Experimental Studies of Thermal-hydraulics of Rod Bundles" is a project jointly supported by EPRI, EdF and CEA, "aimed at elucidating thermal-hydraulics unknowns pertaining to axial offset anomaly (AOA) of PWR cores" [EPRI, 2006, 2009].

> The primary motivation of NESTOR is to develop improved single-phase heat transfer correlations and to estimate/assess the ONB criterion for supporting detailed thermal-hydraulic analyses in AOA cores.
>
> The onset of nucleate boiling (ONB) tests will provide data to compare predictions of ONB boundaries based on thermal-hydraulic (T/H) codes. If the comparison is not satisfactory, it may be necessary to modify ONB correlations.
>
> The success of the actual NESTOR measurement campaigns will depend on the ability to measure the rod surface 2-D temperature maps with sufficient accuracy and reliability on the nine central rods of the heated rod bundle.

Beside study of crud, fuel-related experiments were also conducted in other Westinghouse test facilities or Westinghouse-sponsoring test programs, both in the U.S. and abroad; e.g., the TF-2 facility in Windsor, Connecticut for testing vibration-induced fuel failures [Haslinger et al., 2001], V5H fuel assembly tests [Karoutas, 2010]. These and other industry-sponsored test programs too may have data that are useful for CASL work on VERA VUQ. However, at the time of this report, no information about status of these programs and quality of their data is available for review.

4.3.3.b. Status

According to an update of WALT program provided by Wang et al (2008):

> Currently, this test facility is supporting an Electric Power Research Institute (EPRI) program to assess the impact of zinc addition to PWR reactor coolant.

According to a 2010 technical report (EPRI, 2010),

> The NESTOR program has generated complete sets of data from extensive testing on a 5x5 rod bundle in the OMEGA and MANIVEL loops in two separate rod bundle configurations: 1) simple support grids (SSG) and 2) alternating SSGs and mixing vane grids (MVG). These data sets were published, respectively, in EPRI reports 1016618 (in 2008) and 1019423 (2009).

Both WALT and NESTOR test programs and data are not accessible in the public domain, and not available to this author for the purpose of this initial data review.

4.3.3.c. Assessment

From limited information (Wang et al., 2008) about the Westinghouse's WALT program, it appears that WALT test data are highly relevant and can be very useful for VUQ efforts that support both CIPS and CILC challenge problems.

Table 4.3.1. Assessment of the WALT data VUQ quality relative to CASL challenge problems.

	Problems	***Grade***	***Comments***
Relevance	CIPS	4	The program is designed to study crud phenomena
	CILC	4	
	DNB	[3-4]	WALT facility is also used for burnout and dryout tests
Scaling	CIPS	[2]	Preliminary evaluation. The irradiation effect and microscale / near-wall process (species transport, deposition, synthesis) rate can complicate scaling
	CILC	[2]	
	DNB	[3]	Expect that conditions are nearly prototypical, except that effect of coolant chemistry, heater/cladding materials and irradiation are not representative
Uncertainty	CIPS	-	Information about test procedure and diagnostics is to be obtained
	CILC	-	
	DNB	-	

It should be noted that the WALT tests are conducted in out-of-pile facility. Thus, the experiments are designed under assumption that certain reactor conditions have insignificant influence over processes being studied. It remains to be evaluated whether irradiation environment and hydraulic (e.g., vibration) setting may have influence on surface (e.g., activation) conditions, and subsequently on physico-chemistry and micro-hydrodynamics that govern crud formation, growth, and detachment; Table 4.3.1.

The NESTOR tests are relevant to ONB, and hence CRUD (CIPS, CILC) challenge problems. Being out-of-pile, NESTOR tests too suffer the same scaling issues as WALT tests, namely cladding materials, coolant chemistry, and irradiation conditions (which are not prototypic in NESTOR tests) may have influence on delicate microscale processes that govern nucleation of vapor bubbles (ONB); Table 4.3.2.

Table 4.3.2. Assessment of the NESTOR data VUQ quality relative to CASL challenge problems.

	Problems	***Grade***	***Comments***
Relevance	CIPS	3	The program is designed to support analysis of AOA in PWR cores
	CILC	3	
	DNB	[3]	Common microscale phenomena associated with ONB and DNB
Scaling	CIPS	[2]	Although macroscopic conditions are nearly prototypical, microscopic behaviors may be influence by effect of coolant chemistry, heater/cladding materials and irradiation are not representative in NESTOR test section
	CILC	[2]	
	DNB	[2]	
Uncertainty	CIPS	-	Information about test procedure and diagnostics techniques used (in particular, thermometry) is to be obtained
	CILC	-	
	DNB	-	

4.3.3.d. Recommendations

It is a high-priority action item to finalize an arrangement within CASL that makes information about the WALT and NESTOR test programs (including description of test facility, experimental procedure and control, characteristics of measurement and diagnostics techniques employed, data form, process and results of measurement and data uncertainty analysis) available to CASL researchers for assessment of the fitness and value of the data for VERA VUQ purposes.

4.3.3.e. References (for Industry IETs)

EPRI, "New Experimental Studies of Thermal-hydraulics of Rod Bundles (NESTOR)", Technical Report 1013424, December 2006.

EPRI, "New Experimental Studies of Thermal-hydraulics of Rod Bundles (NESTOR)", Technical Report 1019423, August 2009.

EPRI, "New Experimental Studies of Thermal-hydraulics of Rod Bundles: Generic Analysis of OMEGA Data", Technical Report 1021039, October 2010.

K. H. Haslinger, P. F. Joffre, L. Nordstrom, S. Andersson, "Flow Induced Vibration Testing of a PWR Fuel Assembly", SMiRT-16, 16th International Conference on Structural Mechanics in Reactor Technology, Washington DC, August 2001.

Z. E. Karoutas, Challenge problem technical specification, CASL-AMA, [Working Document], December 2010.

G. Wang, W. A. Byers, M. Y. Young, and Z.E. Karoutas, "Westinghouse Advanced Loop Tester (WALT) Update", Paper no. ICONE16-48480, 16th International Conference on Nuclear Engineering (ICONE16), May 11–15, 2008 , Orlando, Florida, USA.

4.4. Separate-Effect Test Programs

4.4.1. Overview

Characteristically, a nuclear reactor engineering application (e.g., CIPS, GTRF) involves a large number of phenomena and processes, as discussed for respective challenge problems in Subsections 3.3-3.5. In turn, each phenomenon or group of phenomena can be modeled and simulated in a variety of ways. For phenomena identified and ranked as important (influential on figure of merit), their models (and codes) must be assessed against a set of relevant experiments. These experiments, generalized under category "separate-effect tests" (SET), in turn can be further classified by their level of complexity and sub-divided by their characteristic time and length scales [24].

For instance, subcooled boiling is singled out as a basic "separate-effect" phenomenon, which plays an important in CRUD challenge problems. In turn, subcooled boiling prediction requires integration of phenomena and effects at three (conditional) scales, microscale, mesoscale and macroscale [25]; see Table 4.4.1. In this Table, "macroscale" processes are coupled with other physics (e.g., neutronics/power) or physical domain (e.g., through inlet /fluid or boundary / thermal conditions) and characteristically "integral-effect", subsuming microscale and mesoscale phenomena.[26]

In practice, when one is faced with a new engineering issue, it is natural to bring to the new task available simulation tools, which appear to provide close-enough capabilities in investigating the new issue, thus minimizing or eliminating the need for developing new tools. Simultaneously, the brought-in capability carries with it constraints/assumptions and relations/arrangements that are not applicable to the new issue but not easily decoupled.

[24] A fuzzy zone exists between IETs and SETs, as some experimental facilities can be used to support testing both separate-effect phenomena and more complex, multi-physics integral-effect processes The WALT and NESTOR programs (discussed in previous subsections) include relatively large-scale experiments and tests where separate effects are studied. Experimental studies on RBHT (such as tests conducted in Columbia Heat Transfer Facility) discussed shortly below in this subsection can arguably be considered "integral" as its result (ONB, DNB, etc.) integrates a myriad of phenomena and effects (turbulence, phase change, friction losses, surface treatment, etc.).

[25] Definition of "micro" and "macro" scales are relative to the subcooled boiling only; the "microscale" effect in subcooled boiling (e.g., surface nanomorphology) is "macro" for a material-science process that studies crud deposition.

[26] It is recommended that Tables like 4.4.1 be generated for all "basic phenomena" identified in "issue resolution framework" for each challenge problem.

Example are CFD codes' solution algorithms and associated turbulence models that are developed for incompressible fluid flow processes, making them not friendly for compressible water/steam phase-change simulation. Another example is legacy STH codes, which are based on ill-posed two-fluid models, requiring significant numerical diffusion in solution, making them not friendly for "hot spot" detection, and scalar transport modeling.

Table 4.4.1 Phenomena and effects considered in a subcooled flow boiling model. [27]

Macroscale	**Mesoscale**	**Microscale**
Inlet conditions (including flow distribution, velocity and temperature fluctuations resulted from lower plenum mixing)	Bubble dynamics (shape, growth, motion, detachment)	Cladding /crud materials / physico-chemistry/ nano-morphology
	Bubble-bubble interactions (coalescence, breakup)	Surface deposit, crud layer microstructures/ composition
Complex geometry flow turbulence, subchannel mixing (cross-flows)	Fluid turbulence (production), incl. thermal and compressible effect	Nucleation of vapor bubble (nucleation energy barrier; nucleation site density)
Grid space, mixing vanes effect on subchannel flow	Interfacial instability	Disjoint pressure; intermolecular forces at triple contact line
Thermal/power transient	Turbulence-interface interactions	Dynamic wettability, incl. effect of evaporation/ recoil pressure
Space-dependent heat flux	Local effects of grid spacer / mixing vanes on turbulence, boiling	
"Soft" wall (condensing bubble dome) effect on turbulence	Turbulence effect on bubble dome condensation in subcooled fluid	Meniscus micro-hydrodynamics
Void fraction distribution along and across the channel (fuel assembly)		Coolant chemistry effect on thin film rupture
	Nucleation pattern	

Thus, SET classification can be approached from phenomenology point of view or from code point of view.

[27] The table content is tentative and to be updated to reflect evolution of understanding of participating physics in SFB and changes in modeling program.

From "phenomenology" (PIRT) point of view, for an unresolved (relatively new) engineering issue, a number of relevant experiments are few (and even less are experiments, which have validation quality). This lack of relevant data often prompts investigators to include less relevant or arguably relevant experiments into model/code assessment portfolio. Without a system for evaluating, "labeling" and appropriate weighting the role of such experiments, the effort on model / code validation against such low-relevancy experiments can rapidly become a goal in itself, whose result can ***dangerously misguide model calibration for the application of original interest***.

From software (VRI) standpoint, a VERA system (configured respectively for solving a challenge problem) includes a number of computer codes, which communicate through LIME. Each computer code simulates a physical process (e.g., neutronic, fluid dynamics, structural mechanics) using a model at appropriate resolution (e.g., CFD STAR-CCM vs. subchannel VIPRE vs. system thermal-hydraulics RETRAN; VITRAN vs. Sierra).

> On the one hand, each such computer code has its own developmental assessment / V&V base, which includes a set of SETs and in some case (e.g., VIPRE, RETEAN) also IETs and PMOs.
>
> On the other hand, validation/application domain of some codes employed in VERA (especially, general-purpose, commercial software) includes numerous models and covers parameter ranges not relevant to the challenge problems studied in CASL. At the same time, the code validation coverage can be notably deficient for models and parameter ranges directly relevant to CASL.

CASL has identified several computer codes (for physical process simulation) for integration into LIME/VERA. Code manuals, and particularly validation references, for industry-owned codes and industry-owned databases have been subject of restricted access. There are several studies where SET data of relevance to the CRUD and GTRF problems were accessed.

4.4.2. Rod Bundle Heat Transfer (RBHT)

4.4.2.a. Status

Data review was documented in EPRI Technical Reports (2000, 2010). The EPRI (2000) study concludes that

> "This literature review has shown that there is no high fidelity data on which to base new heat transfer models for rod bundles. The only realistic way to improve the knowledge of heat transfer in PWR open lattice rod arrays is through prototypical testing. Performing a comprehensive test with top quality instrumentation can provide improved information, which will allow the design and operation of fuel cycles with minimal economic impact from concerns of developing an adverse axial offset or deposits that may cause fuel failures.

> Acquiring such information through prototypical testing at the desired PWR operating conditions may present significant challenges to the researcher."
>
> "Some important results of the literature and model reviews included:
>
> The data on which the major correlation for the single-phase liquid heat transfer coefficient in rod bundles is based are significantly deficient relative to the bundle length, other geometric parameters, fluid conditions, and operating states.
>
> There are no heat transfer data in the open literature, either single-phase or boiling, available for the rod array geometry at typical PWR fluid conditions and chemical species.
>
> Application of standard engineering models of turbulent flow fields to the rod array geometry cannot be justified.
>
> No systematic experimental investigations of heat transfer in rod arrays at PWR steady state operating conditions have been reported in the open literature in about four decades."

The EPRI (2010) study updated the EPRI (2000) report, analyzed experimental data available from literature, prepared a databank for both single-phase and two-phase data for rod bundle geometries, and made recommendations for data use in a single-phase CFD benchmark exercise. It concludes (EPRI, 2010) that

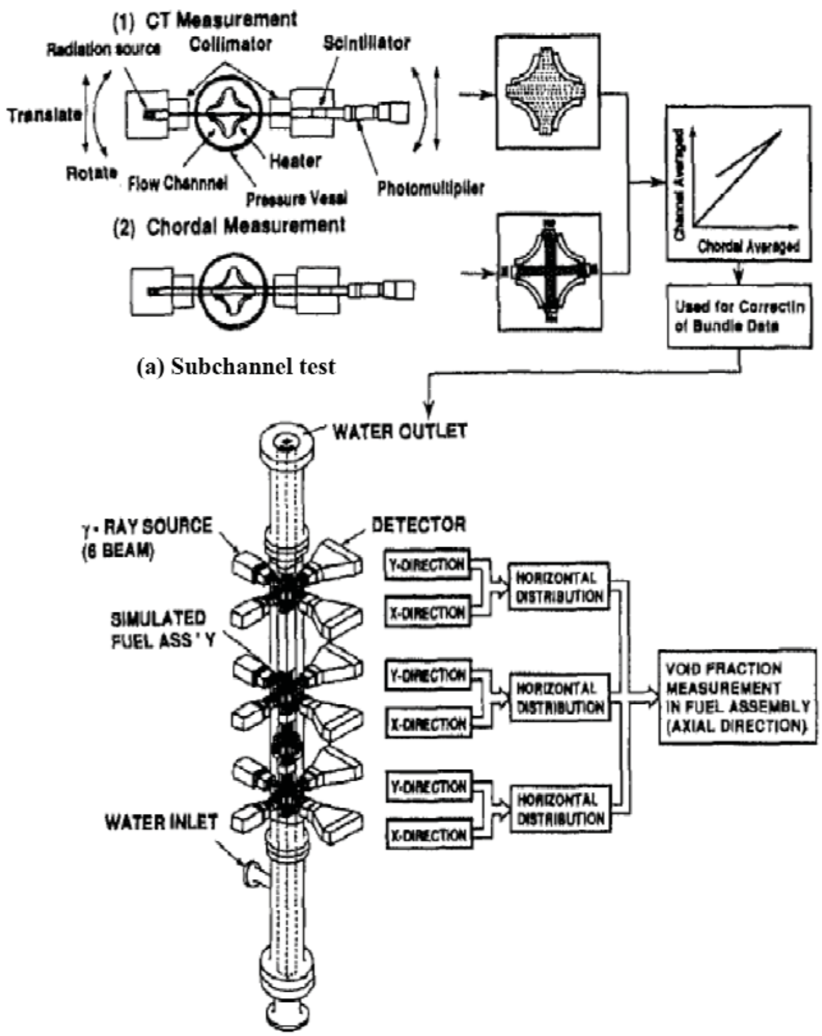
> A good amount of experimental data on PWR rod bundle-related flow and heat transfer is available for detailed understanding of the local behavior of flow at the microscale level. There are few (local) data sets with high spatial resolution that can be used to validate CFD models. Several studies (cited in this report) with good high-fidelity experimental data sets provided the detailed local flow properties such as temperature, velocity, and turbulent intensity distributions.

For subcooled boiling, EPRI (2002) / Karoutas et al (2004) study analyzed data from two 5x5 tests performed at the Columbia University Heat Transfer Research Facility by VIPRE model and shows that

> "… current heat transfer models used in thermal-hydraulic codes are adequate for average steaming rate calculations supporting AOA evaluations as long as the appropriate grid enhancement factor is used for spacer grids in the analysis. However, further testing and modeling are needed to simulate local grid effects and hot spots downstream of spacer grids. Currently available heat transfer data are not sufficiently resolved to develop accurate correlations to incorporate into today's aggressive core design thermal-hydraulic modeling needs. For example, local heat transfer effects in peripheral rods of fuel assemblies and those downstream of mixing vanes are not well understood.

This results in uncertainties in core thermal design and may lead to excessive clad corrosion, abnormal crud deposition, and even fuel failures. It is well recognized that subcooled nucleate boiling plays a significant role feeding the axial offset anomaly (AOA), where requisite thermal-hydraulic knowledge for proper coupling of local and chemical processes may be lacking for detailed modeling of the phenomenon.

The only viable way to improve heat transfer knowledge in open lattice rod bundles is through additional prototypical testing. Comprehensive testing with state-of-the-art instrumentation in modern fuel assembly designs is necessary to provide the data for optimal core thermal design and reliable operation of reactor cycles."



(b) Rod bundlel test

Figure 4.4.1. Void fraction measurement procedure in PSBT. The transmission method of gamma-ray is adopted in this study to measure the density and converted to the void fraction of the gas-liquid two-phase flow.

Other two datasets are the BFBT and PSBT benchmarks based on NUPEC BWR and PWR sub-channel bundle tests (OECD-NEA, 2007; OECD/NRC, 2010). Most notably, these experiments are equipped with void fraction measurements using Computer Tomography (CT) technique.

The PSBT tests for PWR fuel assemblies have been performed since 1987 to 1993. This test contains the subchannel experiments and the rod bundle experiments. The void fraction in each experiment is measured by the gamma-ray transmission method (Figure 4.4.1).

The subchannel test section, simulates one of subchannels of a PWR fuel assembly. The effective heated length is 1500 mm where the void measuring section is set near the top end at 1400 mm from the bottom of the heated section.

The rod bundle test section is fabricated simulating partial section and full length of the 17×17 type PWR fuel assembly. These are arranged in 5×5 square array. The effective heated length is 3658 mm where the void measuring sections are set 2216 mm (Lower), 2669 mm (Middle) and 3177 mm (Upper) each from a bottom of the heated length.

4.4.2.b. Assessment

Table 4.4.2. Assessment of the BFBT and PSBT data VUQ quality relative to CASL interests.

	Problems	***Grade***		***Comments***
		BFBT	***PSBT***	
Relevance	CIPS	1	3	The BFBT benchmark features flow regimes not directly relevant to PWR operational regime
	CILC	1	3	
	GTRF	1	3	
	DNB	1	4	
Scaling	CIPS	2	3	Although both BFBT and PSBT are full-scale rod bundles, cladding materials and coolant chemistry are non-prototypical
	CILC	2	3	
	GTRF	2	3	
	DNB	2	3	
Uncertainty	CIPS	3	3	These are highly instrumented tests using CT scan for measuring void fraction distribution. Quantification of CT data uncertainty remains a challenge.
	CILC	3	3	
	GRTF	3	3	
	DNB	3	3	

4.4.2.c. Recommendation

For RBHT single-phase flow modeling, there exist limited body of data (e.g., PIV) that can be used for model VUQ. However, no similar VUQ-fit high-resolution data exist that can be used for VUQ of CFD-grade model of two-phase flow in rod bundle geometries and reactor prototypic conditions. With its high "worth" (27), the PSBT benchmark (OECD/NRC, 2010) presents a unique dataset for RBHT VU, particularly when one is interested in predicting void fraction and hot spot location. It is proposed that this PSBT benchmark be planned as a key cornerstone in AMA and MNM FAs.

VUQ of the VERA CFD-grade two-phase flow model will necessarily be relying on a combination of carefully selected datasets for validation of RBHT's component model(s). One of such model is Subcooled Flow Boiling considered in subsection 4.4.4 below.

4.4.2.d. References on RBHT (for RBHT)

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EPRI, "Subcooled Boiling Data from Rod Bundles", Technical Report 1003383, Sep 2002 (also Karoutas et al, 2004)

Z.E. Karoutas, Y. Sung, Y.R. Chang, G.A. Kogan, P.F. Joffre, "Subcooled Boiling Data From Rod Bundles", Paper no. ICONE12-49492 pp. 775-794, 12th International Conference on Nuclear Engineering (ICONE12) April, 2004 , Arlington, Virginia, USA).

4.4.3. **Subcooled Flow Boiling**,

4.4.3.a. Status

Different approaches to modelling have been developed for Subcooled Flow Boiling (SFB), which is a component model with Rod Bundle Heat Transfer; see e.g., Krepper et al (2007); Yeoh & Tu (2004); Yeoh et al (2005b); Basu et al (2005a). It is noted that previous studies of subcooled flow boiling were motivated by the role of SFB in rod bundle thermal-hydraulics, including fluid flow, void fraction (quantity and spatial distribution), and heat transfer partitioning.

For CRUD challenge problems, subcooled flow boiling modelling paves way for providing more accurate evaluation of fluid flow configurations and conditions that consequently determine influx and concentration of chemicals and corrosion products in the near-wall layer and their subsequent deposition on the cladding surface (forming crud). The fact that chemicals (not limited to boric acid) and particulates (corrosion products) reach to the triple contact line of the liquid meniscus beneath the bubbles highlights the importance of characterizing mesoscale and microscale processes of subcooled flow boiling.

Due to decades-long interest in subcooled flow boiling (and related topics in bubble dynamics, nucleation), deem-relevant experiments exist for a number of composite phenomena and effects listed in Tables 4.4.3-4.4.6. Many of such experiments were performed under conditions (working fluid, pressure, temperature, surface, geometry) not reactor prototypical for CASL challenge problems. Those few experiments included in the list are selected for apparent relevance. A more in-depth analysis is a must when the experiments are scrutinize, modelled and analyzed. Insights derived must then be weighted when an integrated model becomes available and allowing for sensitivity/uncertainty analysis.

4.4.3.b. Assessment

A substantial body of measurement[28] data of air-water flow (and to a lesser extent, in steam-water flow) exists and can be useful for validation of two-phase turbulent flow models. However, the data are typically measured in bubbly flow regime, corresponding to fully-developed nucleate boiling, and not addressing the subcooled boiling flow pattern.

[28] Diagnostic techniques used include void conductivity probe (developed by Professor M. Ishii's school), wire-mesh sensor (developed by Professor H.-M. Prasser's school), X-ray tomograph, electrode-mesh tomography, and other methods.

Table 4.4.3. Potential sources of data for assessment of macroscale components in subcooled flow boiling model.

Macroscale Effects	References	Comments/ Refs to Consider
Inlet conditions (incl. flow distribution, velocity and temperature fluctuations resulted from lower plenum mixing)		Use SA to study the effect
Complex geometry flow turbulence, subchannel mixing (cross-flows)	PSBT (OECD/NRC, 2010) RBHT (EPRI, 2010)	Sadatomi et al (2004) FRIGG facility DESIREE facility
Grid space, mixing vanes effect on subchannel flow		Important effect; need industry data
Thermal/power transient		Data exist for simple-geometry channel, but not in subcooled boiling regime
Space-dependent heat flux		
“Soft” wall (condensing bubble dome) effect on turbulence	Roy (1992, 1997, 2002) Situ et al (2004) Maurus & Sattelmayer (2006)	
Void fraction distribution along and across the channel (fuel assembly)	Bartolomei & Chanturiya (1967) Bertel et al (2001) Garnier et al (2001) Kang & Roy (2002) Yeoh & Tu (2004, 2005a, 2005b) Tu et al (2005)	Thorncroft et al (1998) Basu et al (2005a, 2005b) Kumar et al (2003) Hibiki et al (2003)

Table 4.4.4. Potential sources of data for assessment of mesoscale components in subcooled flow boiling model.

Mesoscale Effects	**References**	**Comments / Refs to Consider**
Bubble dynamics (shape, growth, motion, detachment)	Unal (1976) Chang et al (2002) Situ et al (2004b) Okawa et al (2005a, 2005b)	Luke & Chang (2006) Myers et al (2005)
Bubble-bubble interactions (coalescence, breakup)	Chen & Chung (2003)	Chatpun et al (2004) Bonjiour et al (2000)
Fluid turbulence, incl. thermal and compressible effect	[substantial body of data exist - CFD Database]	
Interfacial instability		Critical to predicting condensation rate, but hard to measure, especially in narrow heated channels
Turbulence-interface interactions		
Local effects of grid spacer / mixing vanes on turbulence, boiling		
Turbulence effect on bubble dome condensation in subcooled fluid	Warrier et al (2002)	DEBORA facility TOPFLOW facility
Nucleation pattern	Basu et al (2002) Dinh et al (2004)	

Typically, parameters representing a "mesoscale" effect cannot be directly measured in a boiling or flow boiling experiments, especially under narrow-channel, high-pressure, high-temperature conditions characteristic of a PWR core. Thus such "mesoscale" data are derived from measurable (macroscale) information using a model. As a result, data become dependent on assumptions of the model used for extracting the data, hence introducing biases and uncertainty that are not quantifiable.

It is also noted that data on bubble dynamics are obtained in experiments in saturated pool boiling in which bubble configuration and bubble-fluid interactions differ significantly from a wall bubble in subcooled flow boiling.

Table 4.4.5. Potential sources of data for assessment of microscale components in subcooled flow boiling model.

Microscale Effects	References	Comments/ Refs to Consider
Cladding /crud materials / physico-chemistry/ nano-morphology		Ohtake et al (2003)
Surface deposit, crud layer microstructures/ composition		
Nucleation of vapor bubble (nucleation energy barrier; nucleation site density)		Hibiki & Ishii (2003) Dinh et al (2004) Dinh and Theofanous (2006)
Disjoint pressure; intermolecular forces at triple contact line		
Dynamic wettability, incl. effect of evaporation/ recoil pressure		Theofanous and Dinh (2006)
Meniscus micro-hydrodynamics		Dinh and Tu (2007) Gong, Ma, Dinh (2010)
Coolant chemistry effect on thin film rupture		Tu et al (2004)

Data for microscale processes and effects of potential importance for subcooled flow boiling in the context of CRUD problems are largely absent. If any, they are obtained through reconstruction, via post-processing of data measured in macroscale. One way or another, "data" representing microscale effect are both hard to acquire and carry with them large uncertainty. This lack of data at microscales constitutes the weakest link in modeling of subcooled flow boiling, and, most likely, a weaker link in the CRUD challenge problem "issue resolution framework".

A scoping review of sources (references) of data for their VUQ fitness is summarized in Table 4.4.6. Although scoping in nature, the effort leads to the following observations and findings.

The amount of potentially-useful data decrease rapidly from "macroscale" to "mesoscale", and to "microscale", due to limitations in two-phase flow diagnostics at lower length scales. Along this "scale-miniaturization" line, data uncertainty increases dramatically. This trend is observed for subcooled flow boiling, but expected to be valid for all other "composite" multi-scale phenomenon.

In light of the severe lack of data needed for calibration of models for micro- and meso-scale processes (which are building blocks in a high-fidelity subcooled flow boiling model), care must be exercised in planning developments of models (e.g., dynamic wettability) and methods (e.g., interface tracking) that involve micro-/meso-scale description.

Table 4.4.6. VUQ fitness of selected datasets for subcooled flow boiling in CASL challenge problems (CIPS, CILC, GTRF, and DNB).

	Relevance	***Scaling***	***Uncertainty***
PSBT (OECD/NRC, 2010)	4	3	2.5
Bartolomei & Chanturiya (1967)	3	3	2
Bertel et al (2001)	2	1 (1 atm)	[2]
Garnier et al (2001)	2	1 (R12)	[2]
Kang & Roy (2002)	3	1 (R113)	3
Yeoh & Tu (2004, 2005a, 2005b); Tu et al (2005)	2	1 (1-2 atm)	1
Roy (1992, 1997, 2002)	3	1 (R133)	3
Situ et al (2004)	3	1 (1 atm)	2
Maurus & Sattelmayer (2006)	3	1 (horiz.)	1
Unal (1976)	3	3 (full P)	1 (aged)
Chang et al (2002)	2	1 (R134a)	2
Chen & Chung (2003)	2	1 (1 atm)	1
Bang et al (2004)	3	1 (R134a)	2
Situ et al (2004b)	3	1 (1 atm)	2
Okawa et al (2005a, 2005b)	3	1 (1 atm)	2
Warrier et al (2002)	3	1 (low P)	1
Basu et al (2002)	3	1 (low P)	1
Hibiki & Ishii (2003)	2	1 (1 am)	3
Dinh et al (2004)	2	1 (1 atm)	2
Dinh & Tu (2007)	2	1 (1 atm)	2

4.4.3.c. Recommendations

The effort reported in this subsection (for Rod Bundle Heat Transfer and Subcooled Flow Boiling) suggests that even without having a well-defined model, a scoping assessment of data sources, types, and quality can provide insights into status of data that can prove very useful for developing a consistent modelling-experimentation-validation strategy. It is recommended that scoping review of data be undertaken by respective domain experts (i.e., in MPO and MNM FAs) for other "basic phenomena" in challenge problems.

The next step of this SET data review should be carried out by a joint task force of VUQ, VRI, MPO/MNM experts. It is critical to establish an arrangement in order provide the task force with access to industry-owned code manuals, validation references, and to the extent possible, information about characteristics and content of supporting databases.

CASL has also identified several areas where additional separate-effect tests deem desirable (i.e., intuitive and subjective rather than based on a systematic evaluation of uncertainty and sensitivity) and seemingly feasible (i.e., without a rigor assessment of the maturity of experimental design and scaling, experimental and diagnostic capability, measurement uncertainty, resources and timeline). This includes experiments planned at TAMU, CCNY, and MIT for obtaining data for validation of CFD codes in single and two-phase flow. It is recommended that these efforts be carefully planned in light of the forthcoming Validation Data Plan and resources be directed to areas identified (through PCMM and QPIRT) as most "data-deficient".

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***4.4.4.* Fuel Rod Vibration**,

Fuel rod vibration experiments have been performed by nuclear fuel vendors as part of their study of fuel structural behavior, including the effect of Grid-To-Rod Fretting Wear.

4.4.3.a. Status

IAEA (2005) on Structural Behavior of Fuel Assembly in Water Cooled Reactors reports:

> "Hydraulic test systems at Westinghouse Columbia (USA) are comprised of various loops to optimize design features of the fuel assembly by investigating the phenomena associated with fuel rod failures due to fretting and debris. The primary test loops are the VISTA loop for high frequency vibration, FACTS loop for single assembly hydraulic studies, VIPER loop for long term wear tests, and a small scale debris loop to study debris mitigation designs.
>
> **The VISTA (Vibration Investigation of Small-scale Test Assemblies)** loop is a closed-loop, isothermal, room temperature, hydraulic test loop designed for vibration testing of small-scale test assemblies. The actual rod diameter, rod pitch, and grid strap designs are tested, but a smaller array (typically 5x5) and shorter bundle (2 m) are used relative to the fuel assembly design.
>
> A unique high frequency vibration (above 1600 Hz) has been discovered in certain performance in that it may be a contributor to fuel rod fretting. Under flow conditions, the interaction of the HFV and the low frequency rod/assembly vibration is a complicated phenomenon. Therefore, a separate effects test, using the VISTA loop was devised to study HFV.
>
> Measurements of HFV are taken with a laser vibrometer (to measure grid strap vibration) and with a bi-axial accelerometer placed within a test rod (to measure the force vibration in the rod). By varying the flow rate (axial flow) in a VISTA HFV test, relationships between flow velocity, HFV frequency, and HFV magnitude can be established.
>
> **The FACTS (Fuel Assembly Compatibility Test System)** can test a single full-scale fuel assembly. The FACTS test loop consists of a closed hydraulic loop with a test vessel, pump, heat exchanger, "make-up" water tank, and pressure regulators, as shown in Figure 4.4.2.
>
> Since a fuel assembly is a long, slender structure and is susceptible to some distortion, the test flow housing surrounding the test fuel assembly is slightly larger than the in-core pitch size to avoid contact between the fuel assembly and flow housing walls. This contact may dampen and mask a fuel assembly vibration problem and produce an invalid test. It is normal for a fuel assembly to have low

and random vibration under operational flow conditions in a reactor. However, some fuel assembly designs experience high resonant fuel assembly vibration under normal axial flow conditions. This anomalous fuel assembly vibration is defined as the fuel assembly self-excitation vibration, as the assembly vibrates resonantly without external periodic excitation forces. Westinghouse currently uses this full-scale hydraulic test loop, FACTS for fuel assembly vibration testing." (Aulo and Rabenstein, in IAEA, 2005)

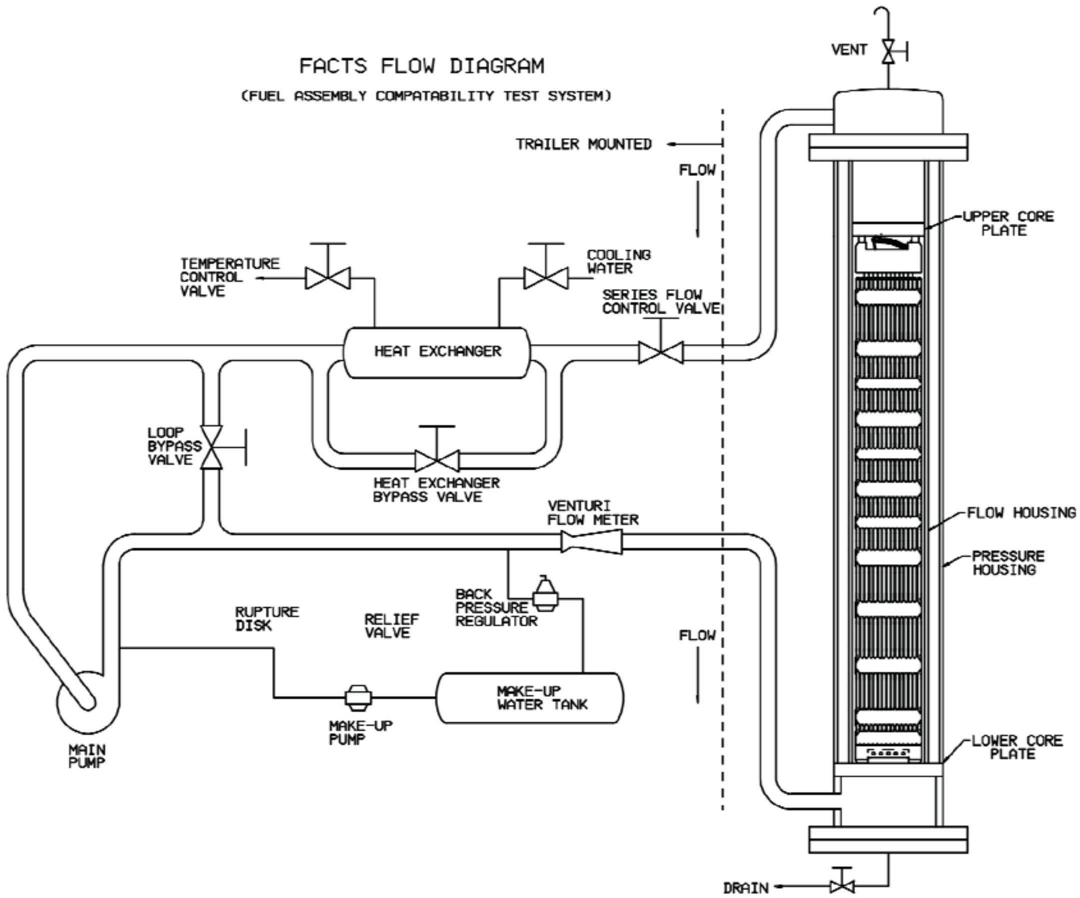

Figure 4.4.2. The FACTS hydraulic test loop.

Additional but largely incomplete information about GTRF-related experimental programs can be found in open literature (Kim et al., 1995, 1997, Conner et al., 2001, Lu et al, 2004). With few exceptions (e.g., Kim, 2009, 2010), the data are design-specific and proprietary. Even in case the experiments are used and presented in an open publication, the detail information about the design, diagnostics and data is not provided.

4.4.3.b. Assessment

A scoping review of open-literature information suggests that vendor-based Fuel Rod Vibration tests are highly relevant (Relevance grade 4), well-scaled (including full-scale test in FACTS, thus giving Scaling grade 3-4), and instrumented with advanced diagnostics. However, at the time of this review, sample datasets and details of test program, including data uncertainty, are not available for review.

4.4.3.c. Recommendations

Arrangement be made to allow for CASL VUQ to perform an in-depth review of VUQ quality of data obtained in Fuel Rod Vibration tests.

4.4.3.d. References (for GTRF)

M.E. Conner, R.Y. Lu, M.L. Boone, C.L. Wilbur, and R. Marshall, 2001, "Nuclear Fuel Assembly Flow-Induced Vibration and Endurance Testing", Proceedings of ASME-PVP Symposium on Flow-Induced Vibration, July 22–26, Atlanta, Georgia, USA.

IAEA, "Structural behaviour of fuel assemblies for water cooled reactors", Proceedings of a technical meeting, Cadarache, France, 22–26 November 2004, IAEA-TECDOC-1454, July 2005. 324p.

K.T. Kim, "A study on the grid-to-rod fretting wear-induced fuel failure observed in the 16×16KOFA fuel", Nuclear Engineering and Design 240 (2010) 756–762.

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Y.H. Kim, S.Y. Jeon, J.W. Kim, "Fretting wear of *fuel* rods due to flow-induce**d** vibration", SMiRT-14, Lyon France, 1997 (Also referenced Y. H. Kim, S. Y. Ieon, "*FACTS* Loop *Vibration* Test for *PWR Fuel* Assembly", Korea, 1995.)

R.Y. Lu, K.D. Broach, J.J. McEvoy, 2004, "Fuel Assembly Self Excited Vibration and Test Methodology", Proceedings of ICAPP'04, June 13–17, Pittsburgh, Pa, USA.

4.5. Advanced Diagnostics and Experimentation

In an early study on "VU-assed code development effort" (Nourgaliev and Dinh, 2010), within a limited scope of "System Thermal-Hydraulics" (STH), development of the STH VU plan has revealed a number of VU issues that are generic in nature, requiring attention and further research. Issues were grouped in three classes: methodological, programmatic and technical. It was noted that the technical issues identified present opportunity and challenge for a broader (experimental) R&D community. In particularly, it is noted that

"… technical issues can and must be addressed by developing advanced diagnostic techniques and instruments that capture spatio-temporal behaviors [29] and provide uncertainty information on measured data.

Also needed are new experimental procedures (e.g., with reproducibility variability assessment, sensitivity probing) that allow quantifying uncertainty of closure relations (obtained in SET) when they are used in simulations of system dynamics and transient conditions."

For single-phase flow, techniques for Particle Image Velocimetry (PIV) have been developed and demonstrated widely over the past two decades as a main tool for obtaining validation-quality data on velocity field that can be used for benchmarking and validation of turbulence models in CFD codes. It is instructive to note that despite its potential role and value, no methods were developed for providing realistic experimental uncertainty quantification for a huge amount of data generated by PIV-diagnosed experiments.

> "The uncertainty of PIV measurements is an estimate of the predicted error range between the image-based computed velocity and the true velocity. Depending on the processing parameters and size of interrogation region used, the number of computed velocity vectors from PIV can range from hundreds to thousands. The error for each vector can vary substantially from its neighbors and its variation depends on many factors. Because of this, it is crucial to define individual vector uncertainties rather than try to quantify an uncertainty estimate for the entire velocity field." [30]

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[29] The EPRI/EdF/CEA NESTOR program on onset of nucleate boiling in rod bundles emphatically links the project success to capability for resolved measurement of fuel rod surface temperature pattern. This is not an unreasonable expectation, given success in development and application of high-resolution infrared imaging thermometry for the study of boiling in (Theofanous et al, 2002; see below).

[30] B. Smith, Report for INL, Utah State University, 2010. Also in:

B. H. Timmins, B. L. Smith, and P. P. Vlachos, "Automatic Particle Image Velocimetry Uncertainty Quantification," ASME Fluids Engineering Conference, August, 2010, Paper number 2010- 30724.

> Like any measurement, the uncertainty of PIV consists of bias and precision uncertainties. Our work concerns the bias and precision uncertainty generated by the PIV algorithm itself.

In fact, the work on PIV experimental UQ is just in its infancy phase [31]. This suggests that while digital-based diagnostic methods provide a large quantity of "high-fidelity measurements" data (intended for use for validation and uncertainty quantification of advanced computational models), the data themselves suffer from lacking a sound method for data uncertainty quantification. This implies severe limitations in using modern techniques for VUQ. The situation (deficient UQ baseline) is not unique for PIV, which is a "gold standard" in providing "validation-quality" data for single-phase flow CFD, as it applies to many (all) other state-of-the-art techniques for generating "high-fidelity" experimental data for VUQ of advanced models and codes.

Table 4.5.1. Comparison of optical techniques for the liquid film thickness measurement (Gong, Ma, and Dinh, 2010).

> [Dynamics of evaporating liquid film beneath bubbles in subcooled nucleate boiling is central to modeling and simulation of micro-hydrodynamic processes that arguably affect crud deposition].

Technique	Measured range	Accuracy	Operability	Measurement principle
Interface detection (Gstoehl et al. 2004)	20 μm–1.3 mm	Low	Good	Light intensity gradient at interface
Light attenuation (Tibiriçá et al. 2009)	1.5–3 mm	Low	Good	Fluid absorptivity
Scanning ellipsometry (Liu et al. 1994)	10 nm–1 μm	High	Hard	Dynamic imaging ellipsometry
Interferometry (Lan et al. 2008)	10 μm–1 mm	High	Hard	Interference of light waves
Beam laser shadow (Zhang et al. 2000)	0.4–0.9 mm	Medium	–	Refraction and reflection
Fluorescence imaging (Jones et al. 2001)	5 μm–1.5 mm	Medium	Dye needed	Induced fluorescence
Focus displacement (Takamasa and Kobayashi 2000; Hazuku et al. 2005; Han and Shikazono 2009a, b; Kavehpour et al. 2002; Rullière et al. 2007; Zhou et al. 2009)	2 μm–2.8 mm	High	Good	Position displacement

For two-phase flow, there are digital imaging and other technologies (based on X-ray, infrared, optics) developed for various defense and industry applications that can and have been adopted for measurement of thermal hydraulic processes of interest to CASL challenge problems. For instance, Figure 3.4 shows images from infrared thermometry of boiling surface; Table 3.10 lists panoply of techniques developed over the past decade for think film diagnostics.

[31] Research on PIV UQ is carried out within the INL LDRD NE-156 (PI: N. Dinh).

Experience (including that of the present author [32]) suggests that a cycle of development, demonstration, and broad use of high-fidelity (time- and space-resolved) diagnostic methods for two-phase flow and heat transfer can take between one to two decades.

For effects and low-length-scale processes associated with physico-chemistry and micro-hydrodynamics, such as microstructural / compositional evolution of crud layer, diagnostic techniques are limited to methods developed for material science and nanotechnology; see e.g. Figure 3.5. These techniques, while very powerful and sophisticated, are not readily usable for generating the types and quality of data needed for challenge problems, like CRUD and GTRF.

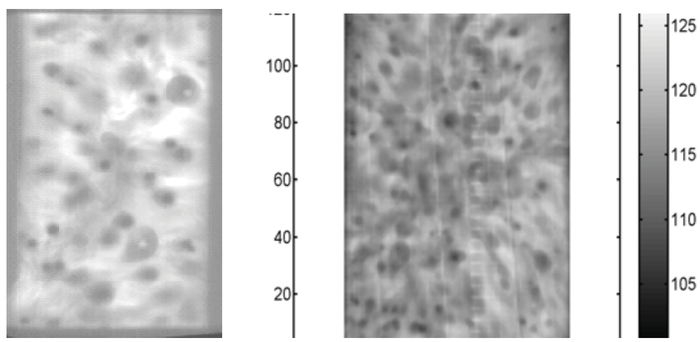

Figure 4.5.1. Patterns of vapor bubble nucleation on a heater surface, imaged by (high-speed, high-resolution) infrared thermometry camera for clean water and water with nano-particles. (from Dinh et al., 2003, 2004, 2007; Tu et al., 2003, 2004) [33]

[32] Examples of recent advances include work by the author (T.-N. Dinh) and collaborators:

S. Gong, W. Ma, and T.N. Dinh, "Diagnostic techniques for the dynamics of a thin liquid film under forced flow and evaporating conditions "*J. Microfluidics and Nanofludics*, Vol.9, N.6, 1077-1089, 2010.

R.C. Hansson, H.S. Park and T. N. Dinh, "Simultaneous High Speed Digital Cinematographic and X-ray Radiographic Imaging of a Intense Multi-Fluid Interaction with Rapid Phase Changes", *Experimental Thermal Fluid Science*, Vol.33, N.4, pp.754-763, 2009.

T.G. Theofanous, J.P. Tu, A.T. Dinh and T.N. Dinh, "The Boiling Crisis Phenomenon – Part 1: Nucleation and Nucleate Boiling Heat Transfer", *J. Experimental Thermal and Fluid Science*, pp.775-792, V.26 (6-7);– Part 2: Dryout Dynamics and Burnout", *J.* pp.793-810, V.26 (6-7), August 2002.

[33] T.N. Dinh, J.P. Tu, A.T. Dinh, T.G. Theofanous, "Nucleation Phenomena in Boiling on Nanoscopically Smooth Surfaces", 41st Aerospace Sciences Meeting, Reno, NV, Jan 2003. AIAA-2003-1035.

T.N. Dinh, J.P. Tu and T.G. Theofanous, "Hydrodynamic and Physico-Chemical Nature of Burnout in Pool Boiling", International Conference on Multiphase Flow, Yokohama, Japan, May 2004. Paper 296. 14p.

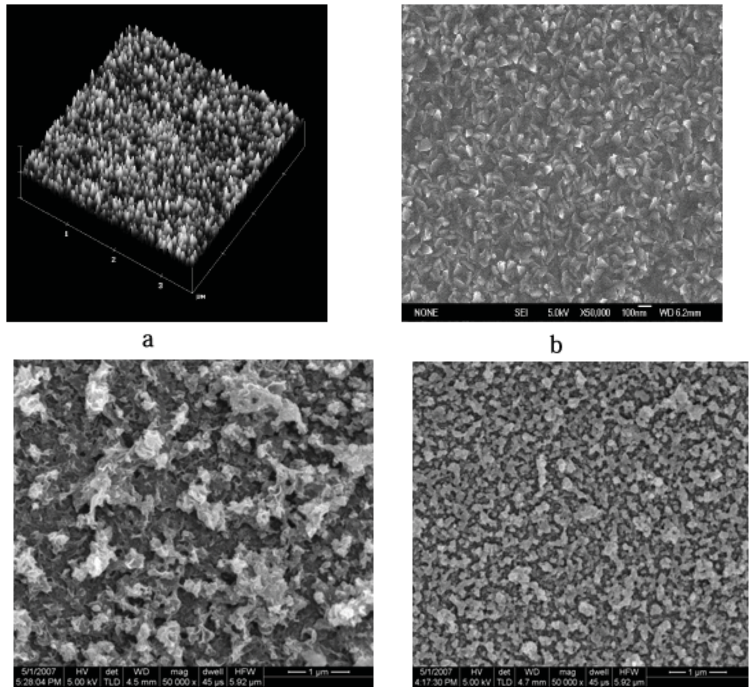

Figure 4.5.2. (Upper row) Atomic Force Microscopy and Scaling Electron Microscopy images of a fresh heater surface. (Bottom row): SEM images (50000x magnification) of “aged” heaters used in BETA-B tests (Dinh et al., 2004, 2007).

The above discussion suggests that a comprehensive review of advanced diagnostics and experimentation methods of potential relevance to CASL challenge problems is necessary for developing a sound Validation Data Plan. For a selected diagnostic/experimental technique, such a review should include:

- Assessment of the technique’s current capability and limitations; summarized in a grade [0-4] for their fitness in producing data of VUQ quality;
- Assessment of world-wide efforts and investment on the technique and projection of developmental pace (timeline);
- Identification and assessment of potential paths for synergistic use of the technique with other diagnostic and experimental methods for CASL problems.

T.N. Dinh and J.P. Tu, “The Micro-Hydrodynamics that Govern Critical Heat Flux in Pool Boiling”, International Conference on Multiphase Flow, Leipzig, Germany, July, 2007.

J.P., Tu, T.N. Dinh, T.G. Theofanous, “Enhancing Resistance to Burnout via Coolant Chemistry”, 10th International Topical Meeting on Nuclear Reactor Thermal Hydraulics NURETH-10, Seoul, Korea, 2003.

J.P. Tu, T.N. Dinh and T.G. Theofanous, “An Experimental Study of Boiling Heat Transfer with Nanoparticles”, 6th Intern. Symposium on Heat Transfer, Beijing, June 2004.

Table 4.5.2. Scoping assessment of diagnostic techniques of potential use in separate-effect experiments for CRUD / GTRF problems

	VUQ fitness [Grade 0…4]	Developmental Timeline / Resources Required	Synergistic Use Potential
Thermal-hydraulics			
PIV	3 (for single-phase flow (SPF) – need UQ of data	2-3 y to VUQ4 [est. ~$1M]	Opt, IR
	1: for two-phase and interfacial systems	3-5 y to VUQ3 [est. ~$3-6M]	OPT, IR
IR	2 for boiling heat transfer	3-5 y to VUQ3 [est. ~$2-3M]	PIV, Opt
Optical	1 for thin liquid film	3-5 y to VUQ2 [est. ~$2M]	IR, PIV
	2 for single bubble dynamics and simple interfaces	2-3 y to VUQ3 [est. ~$1M]	
X-ray	1 (for 2D phase distribution)	5-10 y to VUQ2 [est. ~$10M]	
Probes	3 (for local void (phase) fraction)	3-5 y to VUQ4 [est. ~$1M]	
Mesh	2 (for 2D phase distribution)	3-5 y to VUQ3 [est. ~$3M]	
	1 (for small channel)	3-5 y to VUQ2 [est. ~$3M]	
CT	1 (for 3D phase distribution)	5 y to VUQ2 [est. ~$10M]	
Physico-chemical (crud)			
Surface microscopy		5 y… 10 y	
TBI			
Fluid-Structure Interactions (fretting wear)			
TBI		5 y… 10 y	

TBI – to be identified

The tentative review indicates a large gap between advanced modeling and diagnostic capability (and hence data quality), and un-proportionally large resources required to bridge that gap. It suggests that for CASL mission, it is important to formulate "issue resolution framework" and identify critical experiments that leverages on state-of-the-art diagnostics for producing data within time frame needed to sustain industry interest's to the CASL-enabled framework to challenge problems.

Chapter 5. Recommendations for CASL Development and Validation Data Planning

Figure 5.1 depicts components of a VUQ-guided process and their relationship. In this process, PCM (predictive capability maturity) model helps quantify the level of maturity. Q-PIRT method helps identify and rank data "gaps", formulating an effective strategy to improve PCM. Thus, the data "gaps" are assessed in the context of engineering decision-making, i.e., what additional data are required to help calibrating the model and reduce uncertainty of simulations that brings PCM to a level acceptable for the decision of interest. Data "gap" is thus tightly related to predictive capability maturity, which in turn depends on the decision's acceptance criteria and the set of underlying models and simulation codes available for use in an "issue resolution framework"(see Figure 2.1).

In effect, the "gap" can be narrowed down by improving the [Simulation Code System], by adjusting the [Challenge Problem Application]'s acceptance criteria, and finally, by enhancing the [Supporting Databases]. Improvement of [Simulation Code System] can be achieved by improving models, algorithms, and solutions. Both better use of old data and assimilation of new data can improve the model.

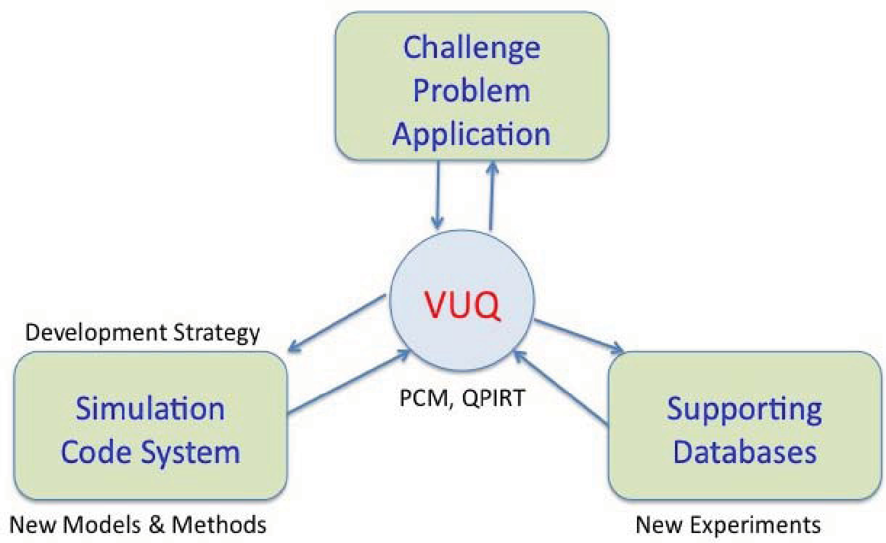

Figure 5.1. A VUQ-guided process and elements.

<u>Recommendation (for AMA):</u> Due to the complexity both of multiple physics involved in CASL challenge problems and of simulation codes developed and integrated in VERA, it is critical for the validation task that the challenge problems (nuclear engineering applications) are specified with a comprehensive

and quantifiable set of hypotheses[34], figures of merits, and success criteria[35]. This can be captured in refined technical specifications of challenge problems.

Recommendation (for VUQ, AMA): Although as a concept, the predictive capability maturity model (PCMM) has been established and successfully applied by researchers at Sandia National Laboratories (see e.g., Oberkampf et al., 2007; Pilch et al., 2010) for defense-related problems, it is suggested that CASL considers a VUQ case study that develops a PCMM for assessing VERA code maturity for a CASL challenge problem.

> Based on the initial data review and other considerations, CIPS problem can be an appropriate case study for PCMM.

Recommendation (for SLT/VUQ): It is suggested that CASL considers a VUQ case study that investigates, selects and implements a Q-PIRT algorithm (including the use of sensitivity/uncertainty analysis techniques) to VERA for a challenge problem.

> The main technical challenge for Q-PIRT is an integrated hierarchical treatment of multi-scale/multi-physics problem.

Recommendation (for SLT): Systematic assessment of data, and effective use of data for validation purpose require CASL to implement a coordinated, security-controlled, VUQ-enabled system for data management.

> Implementation of this recommendation is underway, having made use of CASL resources allocated for the present "data review" task for supporting the effort to formulate, build and demonstrate NE-CAMS (Nuclear Energy -- Computational Applications Management System) jointly sponsored by NEAMS, and CASL.

While the database effort (leveraged on NE-CAMS) is expected to be both time- and resource-consuming for the first challenge problem, the infrastructure developed (including algorithms for screening and preparing data into format consistent with VUQ techniques) will be useful for management of data in other challenge problems.

In the early phase of CASL implementation, a substantial effort is devoted to integration of existing capabilities in a Lightweight Integrating Multiphysics

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[34] Hypotheses are instrumental for problem decomposition, for narrowing down the scope of representation (modeling), and making possible formulation of an "issue resolution framework", through which uncertainty propagation can be realized toward qualifying or disqualifying the hypotheses.

[35] The current version of AMA-led "Challenge Problem Technical Specification" is heuristic, lacking quantitative definition of figure of merits and success criteria.

Environment (LIME). The project would greatly benefit from experimental data, which can be used to assess implementation accuracy (verification) and additional capability provided by the code coupling (validation). Presently, such multi-physics experimental data are the most significant gap in CASL/VERA/VUQ plan.

> Recommendation (for VUQ, MNM): Attention (and respectively resources) should be paid on R&D on developing methods and acquiring data for supporting validation of multi-physics capabilities.
>
> > Acquisition, critical review and dissemination of the Halden Reactor crud tests and Studsvik Cladding Integrity Project tests for VUQ are highly recommended.
> >
> > Access to and critical review of (Watts Bar 1 or another) plant data (types, VUQ fitness) must be arranged and performed as soon as possible, in order to provide technical basis for developing a sound and realistic Validation Data Plan.

Within CASL Phase 1, there are insufficient resources for supporting work on designing and conducting new experiments. To a limited extent, experiments (directly relevant to the validation needs in CRUD and GTRF problems) may be supported by and carried out within other DOE-NE programs (e.g., LWR-S, NEUP) but those activities too are subject to substantial programmatic and technical uncertainty.

Furthermore, “high-worth” separate-effect and integral-effect experiments designed with VUQ process in mind require substantial resources and long development time, while they pose significant risk of under-delivery (due to assumptions in diagnostics, process control, etc.).

> Recommendation (for VUQ, MNM, MPO): Long development time notwithstanding, it is critically important for CASL to identify and design such “high-worth” experiments, and motivate R&D community (to come up with creative solutions.
>
> > For CRUD problem, the “high-worth” experiments may include:
> >
> > - Study of turbulence in channel with “soft” wall (i.e., phase-change vapor-liquid interface)
> > - Visualization and characterization of subcooled boiling
> > - Rate and structure of chemicals deposition in high-pressure subcooled flow boiling regime

Recommendation (for SLT, MNM): A carefully selected set of such experiments designed and performed under CASL auspice and in close collaboration with CASL-VUQ experts is highly desirable, especially in testing limitations of advanced diagnostics, so to enable planning for CASL Phase 2.

For CRUD problem, the list of advanced diagnostics includes:

- Particle Image Velocimetry for diagnostics of turbulent flow in subcooled flow boiling;

- Confocal optical sensor, high-resolution video imaging, and infrared thermometry for diagnostics of evaporating thin liquid film, meniscus evaporation dynamics and heat transfer;

- Microscopic imaging, material structure and chemical characterization of heater surface crud morphology.

Recommendation (for SLT): Due to the cross-cutting nature of validation data, both planning and implementation, it is more effective that the CASL Validation Data Committee's activity be coordinated with, and (preferably) subsumed within, the activity of the CASL Cross-Cutting VUQ Working Group.

Formulate and provide resource for a high-priority task (joint between AMA and VUQ) for collection, review, and management of data from PMOs (plant measurement and observations) and IETs (including larger-scale multi-physics experiments).

Formulate and provide resource for a high-priority task (joint between MNM, MPO, and VUQ) for collection, review, and management of data from SETs.

Chapter 6. Concluding Remarks

Data is central to the development, assessment, and application of simulation codes. Role and requirements on data (types, quantity, quality) differ in these three different phases of a project (like CASL) that involves advanced modeling and simulation. This recognition can help discern a broad range of views (some time leading to contentious debate) about "validation data" and appropriately place efforts that have often been lumped under "data" umbrella.

There exist best practice guidelines for V&V of computer codes, most notably in AIAA (1998) and ASME (2006, 2009) communities. In nuclear reactor engineering, efforts have also been made in formulating and disseminating VUQ methodologies and multi-step / iterative processes (e.g., like CSAU/PIRT/BEPU, EMDAP, and more recently RISMC/SAMAP; see Appendices) for supporting the use of codes in licensing and engineering decision-making.

While it is instructive to consider data needs in light of a well-defined VUQ process, by and large, the underpinning of different VUQ processes is similar. The distinctive trend in state-of-the-art VUQ is to streamline VUQ steps, making them more formalized, objective, and efficient (e.g., using PCMM, Q-PIRT, and advanced sampling techniques, respectively).

In this report, we develop an application-oriented framework for data review (Chapter 1) and outline a proposal for systematic approach to validation data planning (Chapter 2). The scope of validation data review and decomposition of selected challenge problems are provided in Chapter 3, that prepares a basis for assessment of test programs whose data may be used for supporting validation of models / codes in CRUD and GTRF challenge problems. The review of databases and experiments is documented in Chapter 4. Along the way, we identify gaps in methods and data, and make recommendations for a CASL validation data plan, including proposals for further development and adaptation of VUQ process and CASL data management (Chapter 5).

The initial review of validation data confirms that CASL challenge problems (not limited to CRUD, GTRF) feature a common characteristic for unresolved issues in nuclear reactor engineering, namely:

- There is an appearance of severe lack of relevant experimental data, especially when it comes to validation of models for integral-effect, multi-physics and fine-grained processes;

- VUQ value of deem-relevant experiments performed in the past is severely hampered by issues in scaling distortion and data (un-quantified) uncertainty;

- Models that underpin modern simulation codes are [far] more fine-grained, sophisticated, and complex than data that can be used to support model calibration and validation;

- New experiments are time- and resources consuming (neither is available for engineering application at high stake).

While the present effort uses a set of "VUQ fitness" criteria (Relevance, Scaling, Uncertainty) for data review, their characterization is ad hoc and subjective. It is highly desirable to bring this effort to a next level, developing, demonstrating and applying a goal-oriented quantitative methodology for characterization of data "fitness-for-purpose" in nuclear engineering applications.

Due to the scaling effect, there is a substantial disconnection between (nuclear reactor) "reality" and <u>experimental</u> data obtained in out-of-pile and scaled-down test facilities. This situation in many nuclear reactor engineering applications[36] is be contrasted against other applications (e.g., weather prediction), where high-performance computational simulations and modern methods for VUQ (including assimilation of <u>field measurement</u> data) were developed and successfully applied.

Derivatively from above, it is important to recognize that CASL mission success is measured by enabling simulations for supporting engineering decision-making, as opposed to simulations for predicting (e.g., weather) processes or isolated physical phenomena. This recognition should lead to increased emphasis in development of a methodology (a PCM/Q-PIRT-based decision model) that integrates results of VUQ activities conducted on a broad range of test facilities / models into the nuclear reactor application.

[36] Exception is a potential application of the "virtual reactor" for supporting on-line plant decision-making, when plant measurement data are assimilated in the simulator for predicting un-measurable plant/core/fuel characteristics, monitoring and forecasting plant near-term safety margins.

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Appendix

A.1. US NRC Code Scaling, Applicability and Uncertainty Methodology (CSAU)

Development, evaluation, and application of simulation codes have a long history in nuclear reactor design and safety field. Leveraged on high-performance computing power, advanced simulation tools and VUQ techniques developed and applied today and tomorrow have the potential to revolutionize the field. Yet, methodologically, it is important to see these advances in the context of theory (wisdom) and practice (procedures, acceptance criteria) of nuclear reactor engineering that have evolved over the past several decades.

This section briefly discusses the Code Scaling, Applicability, and Uncertainty (CSAU) methodology developed by the US Nuclear Regulatory Commission (US NRC) in the late 1980's to support a systematic quantification of uncertainty in results calculated using reactor transient and accident simulation codes; see [Boyack et al., 1990] for basics and [Young et al., 1998] for the first CSAU demonstration in a licensed application. The CSAU method thus provides guidance for development and assessment of computer codes used to support nuclear reactor safety applications. For a specified scenario in a given nuclear power plant, the traetment focuses on important processes and/or phenomena, assesses the code capability to scale them up, and evaluates the accuracy with which the code calculates them. The CSAU evaluation methodology consists of three primary elements as shown in Figure A.1 below. Implicitly, data provides the foundation for step 3 (PIRT); see also [Wilson and and Boyack, 1998]. Data support is shown in SET and IET databases (step 8). Data are also central to steps 9 and 10, where measurement, experimentation, and scaling inaccuracies embedded in the experimental data are evaluated. However, such an evaluation (particularly scaling effect) and incorporation into the framework for systematic quantification of uncertainty remains a subject of debate and development [Zuber, 2001; Nutt and Wallis, 2004; Prosek and B. Mavko, 2007].

The Code Scaling Applicability and Uncertainty evaluation methodology (CSAU) is a comprehensive framework to guide quantification of uncertainty in safety parameters calculated by computer codes. The methodology includes three Elements, (1): Requirement and Capabilities, (2): Assessment and Ranking of Parameters, and (3): Sensitivity and Uncertainty Analysis; with 14 Steps; see Figure A.1. It can be seen that the CSAU method has considered a broad range of issues borne by the specificity of nuclear engineering applications and characteristics of data support for these applications. "Data" as a subject are implicitly present through out all steps in CSAU. Scaling, Applicability, and Uncertainty are all evaluated through data. However, the CSAU methodology leaves open to practitioners to use expert judgment and "best practice" to characterize data. This subjectivity (notably in PIRT and scaling) has been the main criticism of CSAU.

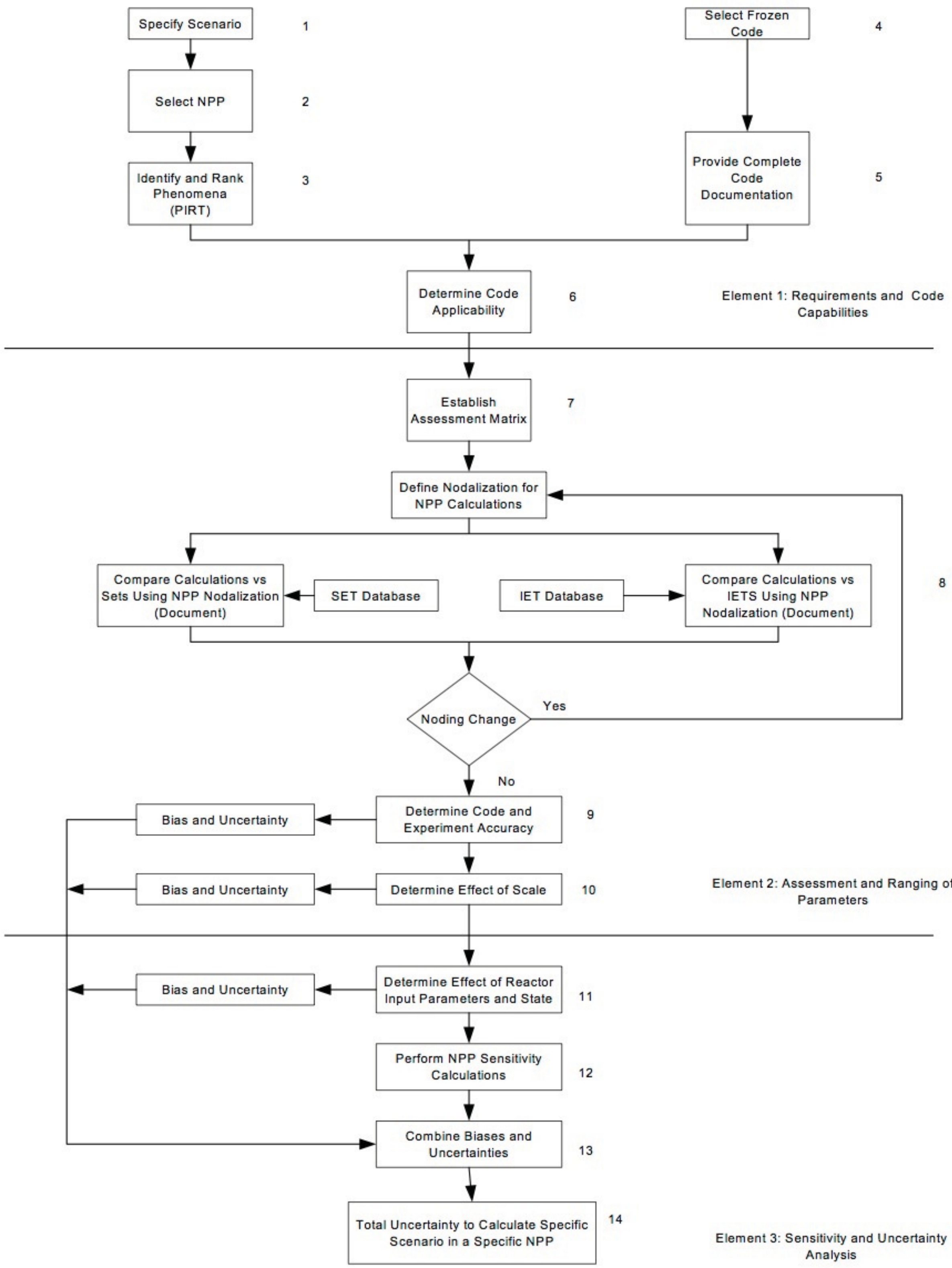

Figure A.1. CSAU evaluation methodology (3 Elements, 14 Steps).

It should be noted that advanced methods and tools in VUQ (e.g., sensitivity analysis, efficient sampling algorithms) developed and applied (largely in non-nuclear fields) over the past two decades can help realize, more comprehensively and effectively, the intent of the CSAU steps. Particularly, advanced techniques help bring CSAU from the realm of art (qualitative, expert-opinion-based) to the domain of science (quantitative, e.g., Q-PIRT). Consequently, implementation of the advanced VUQ techniques requires a more formalized approach to data.

PIRT: Phenomena Identification and Ranking Table

Phenomena Identification and Ranking Table (PIRT) is Step 3 in the CSAU or Step 4 in EMDAP. Given the complexity of engineered systems and phenomena under consideration, PIRT objective is to reduce a number of phenomena and components that require detailed analysis to a manageable set, thus making uncertainty quantification in a reactor safety analysis and decision-making practical and effective. Given figures of merit in a code application, the PIRT can be achieved using expert opinion, scoping analysis, and subjective decision-making methods, such as the Analytical Hierarchical Process (AHP). Sensitivity analysis is a powerful, and quantitative way, to identify and rank phenomena with respect to their influence on the figures of merit. Of importance for decision-making are phenomena, which have both a large impact on figures of merit (e.g. safety /risk measures) and a large uncertainty.

For reactor safety, a critical and intellectually demanding aspect of the PIRT is scaling. The US NRC developed - under the leadership of Dr. Novak Zuber - a so-called Hierarchical Two-Tiered Scaling (H2TS) method (Appendix D of NUREG/CR 5809). The H2TS analysis method includes four elements. The first element is ”System Breakdown”, subdividing the plant into a hierarchy of systems. The second step is ”Scale Identification”, that determine the scaling level at which the similarity criteria should be developed. The third element is Top-Down / System Scaling Analysis”, which uses the conservation equations to determine characteristic time ratios and scaling groups, and identified important processes for bottom-up scaling analysis. The fourth element is Bottom-Up / Process Scaling Analysis”. This analysis provides similarity criteria for important local processes identified by the PIRT.

It is noted that while PIRT was invented and applied to support development and assessment of computer codes to analyze safety of the existing plants, system simulation codes can nowadays be used as a scaling tool and to support the PIRT in the analysis of new reactor designs or addressing new challenges.

Q-PIRT: Quantified Phenomena Identification and Ranking Table

Q-PIRT is a concept to use advanced methods in sensitivity/uncertainty analysis to streamline and strengthen the traditional PIRT process, which relies heavily on expert opinion solicitation.

While the motivation for Q-PIRT and general idea are broadly recognized, development of techniques for supporting Q-PIRT is still in an early stage. There are several alternative approaches for Q-PIRT under development by researchers in national laboratories and universities (e.g., Ohio State University, MIT, Oregon State University). In one classification, Q-PIRT methods are classified by the level of entities subject to PIRT, ranging – in a “top-down” order, from “scenario”, to “physical processes/mechanism” (i.e., sub-set of a scenario, super-set / aggregate of parameters), to “model parameter”. It is expected that for engineering applications, the Q-PIRT techniques developed will be used in a complementary fashion.

More detailed discussion of status of development of different Q-PIRT methods will be included in a revised edition.

BEPU: Best Estimate Plus Uncertainty

Best Estimate Plus Uncertainty (BEPU) refers to an approach that applies state-of-the-art, best available (hence, best-estimate) tools and codes to compute safety margins in nuclear power plants, with the provision that the best-estimate code provides a more realistic prediction of plant physical behaviors. Computer codes used in BEPU must be subject to CSAU. To be meaningful, Best Estimate (BE) predictions of plant transient and accident scenarios must be supplemented by a comprehensive uncertainty quantification.

Today BEPU has been applied to analysis of yet a limited set of design-basis events. There have been efforts to use BEPU to support nuclear power plant design, modifications, safety analysis and licensing, including assessment of operational events, development and validation of emergency operating procedures (EOPs) and severe accident management guidelines (SAMGs), containment analysis, and periodic safety reviews. Notably, both human cost and computational expenses are still high, largely due to limitations of the current generation of best- estimate tools.

Efficacy of methods for propagating model input uncertainties through code calculation to obtain error bars in the models outputs is improved by using Wilks order statistics formula. Such a statistical framework has been formalized into a methodology proposed by GRS for analysis of uncertainty of system thermal-hydraulic codes (and more recently, also reactor physics codes). The GRS methodology considers as ”input parameters”: models coefficients, initial and boundary conditions, application-specific input data, and solution algorithm, in its quantification of the effect of input uncertainty on code output.

A.2. US NRC Evaluation Model Development and Assessment Process (EMDAP)

As part of the US NRC's Regulatory Guide 1.203 "Transient and Accident Analysis Methods," issued December, 2005, Evaluation Model Development and Assessment Process (EMDAP) is built on the principles developed and applied in a study on quantifying reactor safety margins, which applied the code scaling, applicability, and uncertainty (CSAU) evaluation methodology to a large-break LOCA). The EMDAP provides "guidance to the applicant in developing the evaluation models, i.e., practices and principles that the method developers would use in creating the models for analyzing transient and accident behavior that is within the ***design basis*** of a nuclear power plant".

An EMDAP includes four Elements (with 20 Steps), followed by a decision:

- Establish Requirements for Evaluation Model Capability
  - Specify Analysis Purpose, Transient Class, and Power Plant Class
  - Specify Figures of Merit – Identify Systems, Components, Phases, Geometries, Fields, and Processes That Must Be Modeled
  - Identify and Rank Key Phenomena and Processes

- Develop Assessment Base
  - Specify Objectives for Assessment Base
  - Perform Scaling Analysis and Identify Similarity Criteria
  - Identify Existing Data and/or Perform Integral Effects Tests (IETs) and Separate Effects Tests (SETs) To Complete the Database
  - Evaluate Effects of IET Distortions and SET Scaleup Capability
  - Determine Experimental Uncertainties as Appropriate

- Develop Evaluation Model
  - Establish an Evaluation Model Development Plan
  - Establish Evaluation Model Structure
  - Develop or Incorporate Closure Models

- Assess Evaluation Model Adequacy
  - Determine Model Pedigree and Applicability To Simulate Physical Processes
  - Prepare Input and Perform Calculations To Assess Model Fidelity or Accuracy
  - Assess Scalability of Models
  - Determine Capability of Field Equations To Represent Processes and Phenomena and the Ability of Numeric Solutions To Approximate Equation Set
  - Determine Applicability of Evaluation Model To Simulate System Components
  - Prepare Input and Perform Calculations To Assess System Interactions and

Global Capability
- Assess Scalability of Integrated Calculations and Data for Distortions
- Determine Evaluation Model Biases and Uncertainties

• Adequacy Decision.

A.3. Simulation-Aided Margin Analysis Process (SAMAP)[37]

A margin analysis process has two objectives. The ultimate goal is to build a formalized, robust, and traceable "analysis report" ("safety case"), that helps streamline the case review and subsequent decision making. The process' objective is to enable analysts to make the "safety case" in an effective and efficient manner.

The first part of the objective emphasizes effectiveness, i.e. the safety case's "end" structure and visualization, defining which analytical results are needed and how they best support each other, so to provide necessary and sufficient information for an expedient review, understanding and acceptance. In other words, "effectiveness" is to spend analytical effort on what matters for decision ("do the right thing").

The second part of the objective emphasizes efficiency, of the analysis process. Given (a) the time and resource constraints that analysts face, (b) characteristic uncertainty and cost associated with each simulation (mode and resolution), and (c) limited, and lack of data to support code calibration, maximum effect (on understanding and managing the risk) must be achieved by a "smart" combination of simulations. In other words, "efficiency" is to optimally execute the analysis process under time, resource, knowledge / data constraints ("do thing right").

Following the ROAAM's "phases of development" approach [Theofanous, 1996], the analysis process (e.g., for a challenge problem in CASL formulated as a "margin analysis" for supporting an application decision) can be structured into five phases:

I. Scoping,
II. Analytical,
III. Quantitative,
IV. Maturation, and,
V. Extension;

It can be seen (Figure A.2) that there is no sharp division between Phases, as technical components often span over several Phases. Each Phase is, however, recognized for its objective, and the Phase is completed when the objective is accomplished. Depending on application, availability of data, findings from the Scoping and Analytical Phases, the rigor required in Quantitative and Maturation Phases varies.

Phase I: Scoping

- (I.1). Use information, data and insights from plant operating experience,

[37] Text is adopted from Dinh, Nourgaliev, and Youngblood (2010) "Software Requirement Specification for RISMC", Idaho National Laboratory, "Working Document.

past experiments, existing methods/codes, and related analyses to sharpen the formulation of the application's objective and requirements.

- Document the problem formulation as starting point of the RISMC analysis; including rationale for definition of the problem's figure of merit;
- Document information, data and insights used; in particular, identify application-relevant experiments, which have not been used in the code's general-purpose calibration;
- Use state-of-the-practice methods, models and codes to perform scoping analysis; document the scoping analysis' findings, including perceived limitations of the state-of-the-practice tools.
- Perform and document a standard Phenomena Identification and Ranking Table (PIRT) by polling experts.

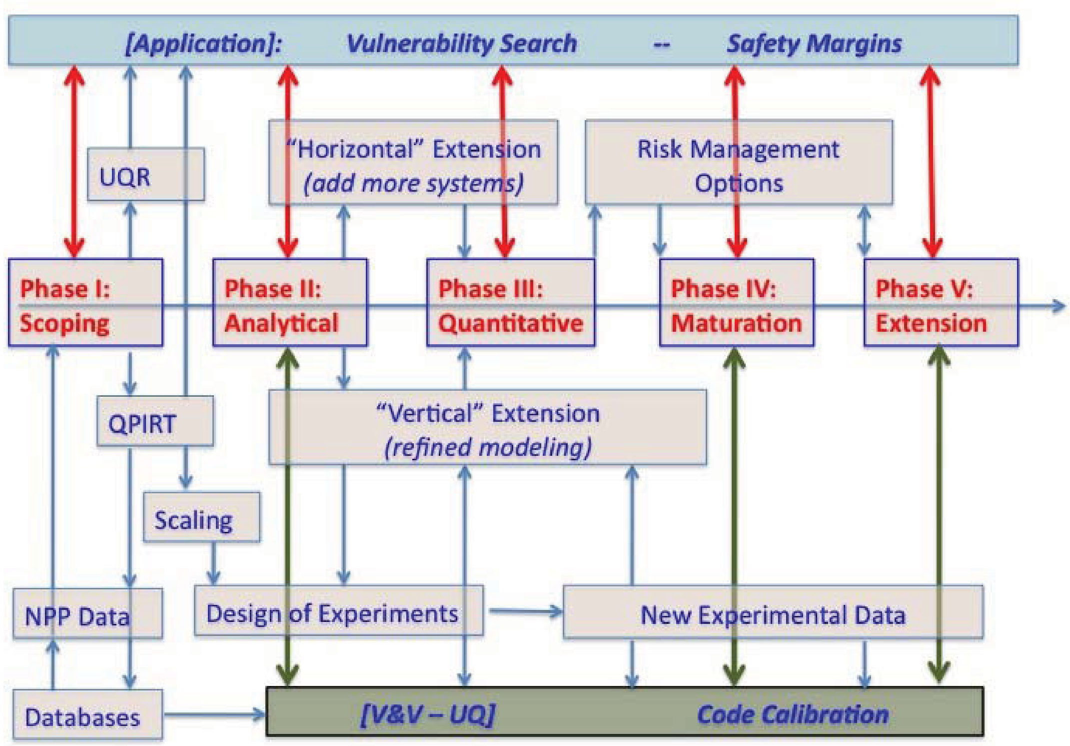

Figure A.2. Phased development.

• (I.2). Build a scoping model, using capability and functionality available in (VERA) software at the time of this Scoping Phase.

- Use experience to select models, their resolutions, and closure relations; Preference is given to both lower-resolution models and higher-resolution but computationally affordable models;

- Use expert opinions to assign PDF for parameters ranked as ”high importance” in the expert-based PIRT[38]
- Even when model parameters are specified with large uncertainty, their representation in the model allows for sensitivity analysis of the uncertainty impact on the problem’s figure of merit;
- Perform a basic assessment of the model, using available data (e.g. normal operation, past events) from the nuclear power plant under consideration;

• (I.3). Use the model created in Step (I.2) to perform scoping analysis.

- Perform simulations of a selected set of scenarios to develop a basic understanding of how different physical processes (or more precisely, their models) and plant systems (their operational characteristics) interact and contribute to the figure of merit
- Perform the Quantified Phenomena Identification and Ranking Table (QPIRT) e.g., using π-group method when applicable;
- Provide the model’s Uncertainty Quantification and Ranking (UQR), including the following
    - Scenario uncertainty
    - Model uncertainty
    - Numerical uncertainty
    - Model parameter uncertainty

  for both physical models and system operation models

• (I.4). Develop an application-specific realization of a ”predictive maturity” framework to enable a cost-benefit analysis of uncertainty reduction

- Use insights from Steps (I.2) and I.3) to perform a scoping assessment of the RISMC model’s predictive maturity

• (I.5). Identify experiments that may address major sources of uncertainty in the integrated model.

- Develop options for the experimental program
- Develop a scoping basis for scaling and establish threshold scale and minimal system complexity representation required for the experiment’s applicability

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[38] When epistemic uncertainty is large (lack of data), use a qualitative probability scale to characterize process likelihood (Theofanous, 1996), e.g.,
- 1/10 is for process characterized by behavior within known trends but obtainable only at the edge-of-spectrum parameters,
- 1/100 for process characterized by behavior that cannot be positively excluded, but it is outside the spectrum of reason,
- 1/1000 for process characterized by behavior that is physically unreasonable and violates well-known reality; its occurrence can be argued against positively.

to the issue
- Evaluate technological readiness and resource requirements for the experimental options (varied with scale and complexity).

Phase II: Analytical

• (II.1). Assess qualitative applicability of the models in the code version developed in Phase I. Provide refined models in selected areas identified by Phase I's UQR and QPRIT as a high priority.

• (II.2). Create an application-specific data base to support calibration of the code for the present application. This database collects application-relevant information (i.e. additional to the generic database already provided for the general-purpose code calibration).

• (II.3). Perform an initial calibration of the code for the present application.

- Update the QPIRT
- Update the uncertainty quantification and ranking (UQR).
- Provide uncertainty range (PDF) for a selected set of parameters, including, but not limited to, those identified in PIRT and QPIRT as ”high importance” for the present application.

• (II.4). Use the (II.3)-calibrated code to perform simulations of reactor scenarios of interest

• (II.5). Use the (II.3)-calibrated code to perform scaling analysis for different experimental objectives and experimental concepts.

- Scaling distortions (either due to the small scale of the experiment or by decomposition i.e. by assuming small effect of interfacing system dynamics) cause errors / uncertainty thus reducing the ”value of information” provided by an experiment;
- Use the ”predictive maturity” model (Step I.5) to qualitatively assess the ”value of information” of data to be provided by a new experiment. The same data (i.e., with a given level of uncertainty) is less valuable in a mature model.
- Use the ”value of information” measures to set requirements for experimental scale, design and diagnostics.

• (II.6). In light of results and insights gained in Steps (II.3), (II.4) and (II.5), update recommendations from Steps (I.4) and (I.5) to guide optimal design of the application-driven experiments to support Phase III and Phase IV objectives.

• (II.7). Provided an estimated pace of executing the experimental program and required timeline of the issue resolution, define a plan to execute Phase III and Phase IV. Rationale that leads to decisions in the plan must be transparent and well documented, allowing for review and update as new evidences and data become available; see Step (III.5).

Phase III: Quantitative

The objective of the Quantitative Phase is to improve confidence (via uncertainty reduction) and build a bulk of quantitative evidences, both experimental and computational, needed for the ”safety case”.

• (III.1). Improve models to address weaknesses in decomposition (”horizontal” refinement and extension) and scaling (”vertical” refinement). Priority is given to models, which are identified as large uncertainty contributor (in UQR); and for which there are (or will be timely) data to qualify the pro- posed model improvements as reducing uncertainty.

• (III.2). Perform extensive calibration of the code for use in under prototypic conditions of the application in question.

- Gather related and potentially applicable data from (other) experiments, plants and simulations, including numerical ”experiments”;
- Qualify the data and utilize them for code calibration;
- Qualify and utilize data from experiments (planned in PhaseII) as they become available.
- Properly-scaled and appropriately designed, these experiments should help to reveal model uncertainty (due to both system decomposition and scaling) and adjust the model parameters to reduce uncertainty
- Quantify and document whether and for which parameters the uncertainty range specified in Step (II.3) has changed (narrowed, enlarged).

• (III.3). Perform experiments designed and planned in Phase II.

- The experiments should be conducted in close collaboration with (III.1) and (III.2);
- This includes tests to identify and quantify experimental uncertainty and to characterize system sensitivity that provide high-order information to support code calibration.

• (III.4). Perform simulations and analyses to build the case-specific simulation database and establish key quantitative findings.

• (III.5). If the quantitative analysis reveals new areas that put uncertainty ranking, decomposition and scaling rationale established in Phase I under question, return to Phase II for re-evaluation, accounting for lessons learned from previous pass(es) of the Quantitative Phase.

• (III.6). Use the ”Visualize Safety Margins” function to present and interrogate the findings and demonstrate that a convergence (”predictive maturity”) is achieved or reachable with a finite amount of technology-ready confirmatory experiments and simulations.

It is noted that the Quantitative Phase is neither a ”single-run” treatment nor uses a single optimized model. There is significant room for code-user interactions, for user’s decision that takes into account the user’s own experience and input from the larger community who is interested in the issue resolution. Also, due to the complexity of issues in real-life applications (characterized by large un- certainty), the users should approach the subject matter from different angles and at different scales. Therefore, a set of ”combs” with different resolution is more effective in the search for vulnerability. Moreover, the users should be given the platform to build his/her own combs, based on what he/she sees as more effective for the application. This interactive and iterative nature of the Quantitative Phase requires a flexible, modular, and user-friendly modeling and simulation frame- work.

Phase IV: Maturation

The objective of the Maturation Phase is to solidify the ”safety case” (broadly defined) regarding the challenge analyzed by preparing and documenting a comprehensive and consistent set of arguments and a traceable and interrogate-able body of evidences. The latter include code simulation results and data and pedigrees of code calibration.

• (IV.1). Continue calibration the integrated code to increase confidence in the simulation

- Initially, additional experiments in this Phase are cost-effective, because they capitalize on infrastructure (facility and diagnostics) developed in the previous Phases to reduce uncertainty in the problem’s highest-priority area
- Using ”predictive maturity” and ”value of information” measures in code calibration to establish whether further experimentation on the same infrastructure is decision-effective (time) and cost-effective (re- source)
- Generate a traceable set of code calibration pedigrees for independent interrogation.

• (IV.2). Use the calibrated code to perform a large number of simulations to support (IV.4), including the following

- Computation of safety margins (probabilistic loading versus probabilistic capacity), with focus on ”tail” (when loading exceeding capacity)
- Analysis of the ”tail” structure and signature of ”tail” sequences (e.g. common cause)
- Analysis of the margins (”tail”) sensitivity to a group of parameters identified as governing the ”tail”
- Extended search for vulnerability, confirming the vulnerable scenarios set.

• (IV.3). Use the calibrated code to perform simulations that assess various management options by their effectiveness to suppress the ”tail”. This may include plant actions such as surveillance, maintenance, and replacement, or analysis actions e.g., reducing uncertainty in modeling of a physics.

• (IV.4). Synthesize a computerized ”safety case” document, using simulation results, code calibration evidences, and other data, non-statistical observations, and insights from related studies. Depending whether the synthesis produces a convincing case, it may require returning to Phase III and re-doing it and steps IV.1 and IV.2.

• (IV.5). Resource permitting, assess the robustness of the analysis’s findings. Use the integrated code (with updated calibration by new data)

- To analyze outcome’s sensitivity to assumed model parameter distributions
- To analyze outcome’s sensitivity to parameters of decomposition / coupling schemes
- To perform simulations with finer resolution in sampling
- To perform analysis for scenarios previously screened out based on qualitative judgment.

• (IV.6). Use the function ”Visualize Safety Margins” and data from the simulations to create a ”virtual engineering” environment that al- lows reviewers to interrogate the ”safety case”.

Phase V: Extension

The objective of the Extension Phase is to ensure ”defense-in-depth” through maintenance of the analysis status as reflecting ”state of the art” and ”best knowledge”. The idea is to ameliorate the impact of ”unknown unknowns”, through continuous improvement of the analysis scope and quality.

• (V.1). Update the analysis as new and refined modes of physical processes become available. This includes models developed by others and / or for other applications / issues but judged as potentially applicable for the analysis in question. Such updates may bring out new areas that require attention. If this happens, the applicability of the new models should be scrutinized before proceeding further.

• (V.2). Update the analysis as new data from experiments including “external” experiments, new measurements and operational evidences from plants (not limited to the analyst’s plant), and relevant insights (e.g., from other independent analyses) become available;

• (V.3). Use the so-calibrated code to perform analysis of other related scenarios, or other plants.

A.4. Issues in VUQ – Lessons Learned in a NEAMS Study[39]

Methodological Issues

The fundamental issue in VU of a nuclear reactor safety simulation is rooted in using the code well beyond the domain of supporting data. No full-scale directly-relevant data from in a nuclear power plant is available for use in code calibration, with the exception of certain plant measurements obtained under plant's normal operation and operational transients, but those are far from safety-significant transients and accidents. Even IET are scaled. Furthermore, the IET and SET are designed with a number of assumptions that lead to simplified geometric and functional representation of the plant systems, structures, and components. Therefore, the profound and generic (not limited to system thermal-hydraulics VU) question is: how to assess uncertainty of code calculations when used outside the calibration domain. The question boils down to the following considerations:

- Assessing the effect of system decomposition:

  SETs are made possible by modeling a plant component while isolating other parts. An example is fuel (cladding) performance experiments conduced in a test reactor under prototypic neutron irradiation, pressure and temperature conditions (in a test capsule), ignoring thermal and structural fluctuations in a reactor fuel assembly. Another example is reflooding experiments, forcing an equivalent, steady coolant flow into pre-heated channel, ignoring flow oscillatory behavior due to core-downcomer manometer-like interactions. In both cases, models calibrated on such SETs possess physical "model uncertainty", largely an unknown unknown until it is recognized, tested and quantified.

  IETs also require decomposing the plant system into a sub-system, which is modeled by the IET facility.

  - Evaluating the effect of interfacing sub-systems, structures, and components represented (explicitly or implicitly) by boundary conditions

  - SET and IET must be designed to suppress sensitivity to boundary conditions

- Assessing the effect of physics decomposition:

  By and large, IET and SET conducted in reactor safety area are single

[39] Text adopted from Nourgaliev and Dinh, "An Initial VU-Assessed Code Development Effort", INL/LTD-10-20668, 236 p.

physics, whereas nonlinearly coupled multi-physics dominates in many risk-significant transients

- Evaluating the effect of physics which has been isolated in experiments which produced data for code calibration

• Assessing the effect of scaling distortion:

System (geometric) scaling: both volume and linear scaling have been used; the scaling is conserved in some selected elements (e.g. down- comer), but distorted in others (e.g., lower plenum).

- Evaluating the effect caused by processes in components that are not geometrically scaled

- Evaluating uncertainty of simulation results calculated for full- scale (prototypic) systems by a code / model calibrated on scaled (say, a 1/10 and 1/4 scale) facilities

Physics (dimensionless group) scaling: when one presumably-leading group (e.g. convection) is maintained in relevant regimes, other deem- to-be-secondary-physics groups (e.g. conduction) are not prototypical

- Evaluating the effect caused by secondary physics on the presumably-leading physics.

Technical Issues

Technical issues are associated with uncertainty in data used for VU, i.e., deficient data quality relative to advanced models and solution methods. An even deeper issue is uncertainty about uncertainty of the ”legacy” data, which were obtained in pre-VU era. This diminishes the value of data generated in SET and IET and stored in historical databases for STH VU even under relevant conditions.

”Legacy” IET data are sparse in parameter space (very few experiments). New IET must supply information on uncertainty and sensitivity of the measurements to system perturbations

Both ”legacy” and many current SET experiments do not provide information on measured data’s sensitivity to physical modeling assumptions (i.e., boundary or interface conditions). This imposes unknown uncertainty when using such data for VU of models to be used under system (i.e. coupled to other components and / or other physics) and transient conditions. New SET experiments must assess sensitivity to decomposition and scaling assumptions

Instruments used (e.g., thermocouples and pressure transducers) provide characteristically local information, whereas models in a STH code deal with volume-averaged (STH mode) and space-dependent (CFD mode) quantities.

These technical issues can and must be addressed by developing advanced diagnostic techniques and instruments that capture spatio-temporal behaviors and provide uncertainty information on measured data.

Also needed are new experimental procedures (e.g., with reproducibility / variability assessment, sensitivity probing) that allow quantifying uncertainty of closure relations (obtained in SET) when they are used in simulations of system dynamics and transient conditions.