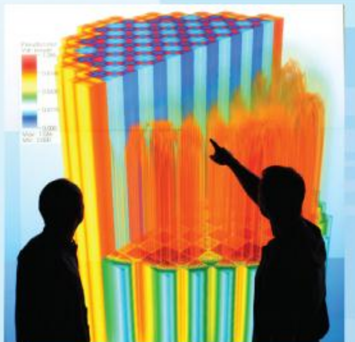
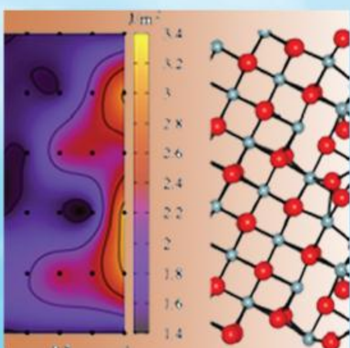
CASL-U-2011-0074-002

Power uprates
and plant life extension

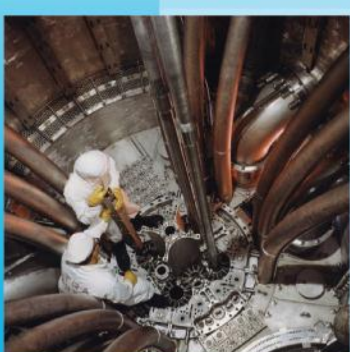


Engineering design
and analysis

Science-enabling
high performance
computing



Fundamental science



Plant operational data

Consortium for Advanced Simulation of LWRs

VERA Requirements Document (VRD) – Revision 1

Stephen M. Hess

AMA Focus Area

30 March 2012

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

REVISION LOG

Revision	Date	Affected Pages	Revision Description
0	2/25/2011	All	Original Version
1	3/31/2012		Revision 1
1A	4/19/2012	all	Revision 1A (Mario)

Document pages that are:

Export Controlled ________________None___________________________________

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CONTENTS

CASL VERA Requirements

Revision 1A

Approved for Use: TBD

INTRODUCTION

This document presents overall requirements for the Virtual Environment for Reactor Applications (VERA) software developed by the Consortium for Advanced Simulation of LWRs (CASL). In general, a requirement imposes conditions or capability needed to solve a problem or achieve an objective. The objective of the VERA software is to provide an integrated software platform employing advanced modeling and simulation capability and high performance computing resources making possible the addressing of problems of importance to light water reactor (LWR) performance with a particular emphasis on enabling extended nuclear plant operating lifetimes, power uprates and extended fuel cycles.

In general, requirements fall into one of the following four categories:

1) Business ("primary why") requirements reflect established goals and objectives of the CASL project. These goals and objectives are developed and approved by the CASL Senior Leadership Team (SLT) with direct input from key project stakeholders. CASL business requirements are described in the project charter, vision statement, strategic plans and goals and objectives.

2) Functional ("what") requirements dictate what the VERA product must do to achieve the approved business objectives. Sources for development of these requirements are the various VERA stakeholders including identified end users (such as industry, regulatory authorities, and research community users). Functional requirements can be found in use cases, specifications, interview notes, and models. Functional requirements typically can be identified by the use of verbs in their specification.

3) Quality ("how ") requirements define the properties that the VERA product must have. Examples include product look and feel, usability, performance, operational environment, maintainability, portability, security, etc. Sources for development of these requirements include product end users and applicable codes and standards. Quality requirements can be found in models, specifications, use cases, and product notes. Quality requirements typically can be identified by the use of adjectives in their specification.

4) Design ("secondary why") requirements depict design choices imposed by a binding authority or overriding business need. Sources include architectures, contracts, style guides, and standards. Design requirements can be found in models, specifications, and high-level design documentation.

This CASL VERA Requirements Document primarily addresses the Functional ("what") and Quality ("how ") overall requirements that will be imposed on the VERA software product. The business ("primary why") requirements are provided in other project level documents owned by the CASL SLT. Specific design ("secondary why") requirements for individual elements of VERA design, modeling, development and testing are controlled by lower level documents owned by individual CASL Focus Area (FA) leads.

For successful achievement of its intended objectives, a requirements process must follow three basic steps: planning, development, and management. The AMA FA Lead has ownership of the process of managing VERA requirements through the duration of the CASL project. This document provides guidance in the planning, development, and management of the requirements associated with the VERA software.

1. PURPOSE

The purpose of this document is to define overall functional and quality requirements for the Virtual Environment for Reactor Applications (VERA) modeling and applications software that is being developed by the Consortium for Advanced Simulation of LWRs (CASL). To achieve this objective, this document also specifies a process from which the VERA requirements are managed.

The primary objective of revision 1 of the VRD is intended to focus VERA development to achieve a foundational capability to function as a core simulator as defined in the foundational requirements (Appendix A) by a specified date (taken to be 31 December 2013). This revision will accomplish this by providing high priority requirements such that VERA will be able to perform analyses and simulations to address the benchmark problems identified in the detailed VERA Technical Requirements document. These specific technical requirements are specified in Appendix A. Thus, the main body of the VRD will continue to provide high level requirements that are intended to reflect the "end state" capabilities of VERA (i.e. at the end of the planned CASL research and development effort). It is the intent that as future capabilities and their associated projected needed dates are identified, these will be reflected in future VRD revisions. The second major objective of revision 1 of the VRD is to provide a more comprehensive specification of quality assurance requirements necessary to align with the CASL Quality Assurance Plan.

In addition, CASL currently is establishing Challenge Problem Integrators that will further define the specifications for the CASL Challenge Problems. As the Challenge Problem Integrators become engaged in the further specification of the CASL Challenge Problems, further needs and requirements are anticipated to emerge which will be reflected in future revisions to the VRD.

Because these requirements are driven by user needs (for both the foundational capabilities and to support execution of the challenge problems), specific activities and their prioritization will be performed via interactions between AMA and the other CASL Focus Areas in the execution of Step 2.4 below and the development of specific milestones for the CASL Plan of record (POR) planning process.

2. RESPONSIBILITIES

2.1 This Requirements Document shall be owned by the CASL Advanced Modeling Applications (AMA) Focus Area (FA) Lead. Change control will consist of, as a minimum, review by the AMA FA Lead and Approval by the CASL SLT and will be managed by the CASL document control and archival process. In addition, the management of the VERA requirements throughout the CASL project shall be performed in accordance with the processes specified in Section 8 of this document.

2.2 Respective CASL FA Leads are responsible for ensuring activities performed under their respective focus areas are conducted in accordance with the requirements specified in this Requirements Document.

2.2.1 Individual VERA development, testing (including unit, integral, regression, etc.), verification and validation activities shall be assigned to a responsible CASL FA Lead. This FA Lead shall have single point accountability to ensure compliance with the requirements specified in this Requirements Document.

2.2.2 The assigned CASL FA Lead shall evaluate each assigned activity for the need to obtain input / expertise from other CASL FAs. This requirement is intended to ensure each planned CASL activity / project associated with VERA development is integrated across the CASL FAs.

2.3 For development of models and methods to address specific issues associated with individual challenge problems, respective CASL Focus Area Leads are responsible for ensuring that development performed under their respective focus areas is conducted in accordance with the requirements specified in the applicable Challenge Problem Technical Specification documentation.

2.4 For each technical capability identified in this requirements document as critical to achieving VERA capability to function as a core simulator, the respective CASL Focus Area Leads are responsible for developing an integrated plan and schedule for achieving the required level of functionality in the required timeframe. This development will be done interactively with the AMA Focus Area to ensure consistency and that necessary capabilities are developed in a timely manner to support user needs and CASL objectives. The CASL SLT is responsible for ensuring appropriate projects and milestones are included in the approved CASL POR planning and scheduling process.

2.5 The CASL SLT is responsible for the approval of this Requirements Document and revisions thereto.

3. FUNCTIONAL REQUIREMENTS

The functional requirements described in this specification represent overarching high level requirements that shall be applicable for all physics based models, numerical solution methods and validation data included in VERA. In addition to these requirements, additional detailed technical requirements will be specified to address individual challenge problems. These specific technical requirements will be documented in the individual Challenge Problem Technical Specification documentation. Note that documentation of these requirements is described in Section 6.5.

3.1The following actions shall be conducted for each physics based model integrated into VERA. As a baseline these actions shall be performed for the following models:

- Core Physics Models
- Thermal Hydraulics Models (including computational fluid dynamics)
- Chemistry Models
- Materials Models (including modeling of material phase changes such as water, cladding and fuel)
- Thermo-Mechanical Models
- Structural Models (including incorporation of fluid – structural interactions (FSI))
- Fuel Performance Models

3.1.1 The theoretical bases for both physics-based and correlation-based models integrated into VERA shall be documented. As a minimum, this documentation shall include discussion of the following:

- theoretical models,
- mathematical formulations,
- identification and application of relevant validation data (including relevant experimental and plant operational data),
- specification of relevant test / verification problems.

These model bases shall be included in the VERA basis documentation. Comment: what is the basis(c?) documentation?

3.1.2 For each physics based model selected for integration into VERA, a verification and validation assessment shall be performed to evaluate the model's numerical accuracy and its fidelity against relevant experimental / operational data. This assessment and its results shall be documented in the VERA basis documentation.

3.1.3 VERA shall provide quantification of uncertainties for all physics-based models integrated into VERA for its defined range of applications. This assessment and its results shall be documented in the VERA basis documentation.

3.2 Interfaces and coupling between phenomenological models that address diverse physics (e.g. core neutron physics and thermal hydraulics models) shall be explicitly documented (including any associated accuracy requirements). Required boundary and initial conditions and feedback / interaction mechanisms shall be specified and documented in the VERA basis documentation. Moreover, Requirements 3.1.1, 3.1.2 and 3.1.3 shall be imposed on the integrated VERA model.

3.3 Workflow Environment

3.3.1 VERA workflow management (which may include multiple or different approaches depending upon the challenge problem being modeled) shall be owned and controlled by the Virtual Reactor Integration (VRI) Focus Area (FA) Lead. However for individual Challenge Problems, the workflow shall be developed by the assigned Challenge Problem Integrator with support from the Advanced Modeling Applications (AMA) FA. Typically, each challenge problem being addressed will require a unique analysis of the workflow. We also note that different organizations often will require modifications to the workflow that are unique to the organization. Examples of such workflows are provided in CASL Report CASL-U-2011-0236-001 "IC Workflow Project: Phase 1 Report" (Revision 1) in which CASL Industry Council members were surveyed (via questionnaires and on-site interviews) to develop sample workflows for the Crud Induced Power Shift (CIPS), Crud Induced Localized Corrosion (CILC) and Grid to Rod Fretting (GTRF) Challenge Problems.

3.3.2 The VERA simulation suite will consist of integration between the Workflow Environment (WFE), the Physics Simulation Suite (PSS), the VUQ tools and the capability to integrate external applications (e.g. systems analysis codes such as RELAP5, RETRAN, or R7). Shown in Figure 1 below is a simple depiction of the integrations that are required for initial VERA deployment.

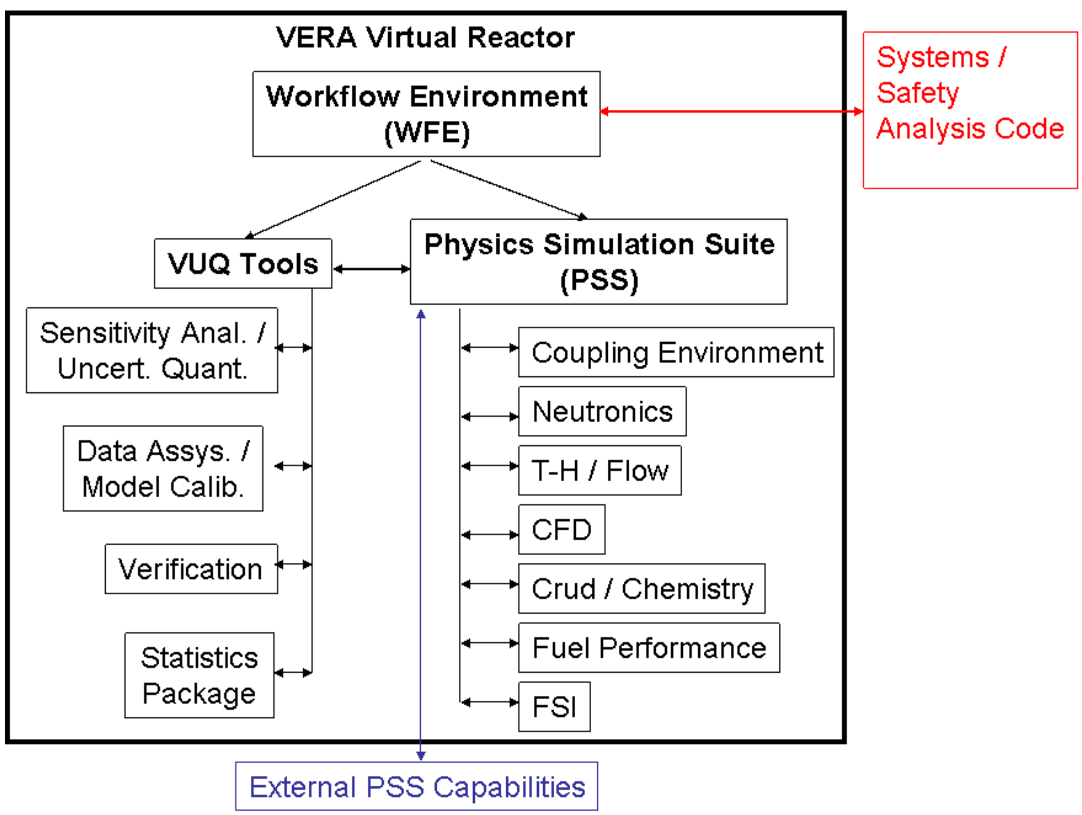

Figure 1: Simplified VERA Interfaces and Integrations

Note that Validation and Uncertainty Quantification (VUQ) Tools, when intrusive, would be incorporated into the Physics Simulation Suite. Comment: not clear, what is intrusive/, the figure shows VUQ tools at same level as WFE and PSS interacting with each other, now there are cases (which are they?) where the VUQ tools are incorporated Descriptions of the codes integrated into the VERA-PSS suite and modifications made during the course of VERA development shall be documented in the VERA basis documentation.

3.3.3 The VERA workflow environment shall address the following specific elements:

- Model Setup and Review
- Application Creation (development of specific VERA model integrators to couple the necessary VERA components to address the application)
- Simulation Execution
- Analysis of Simulation Results
- Data Management and Visualization

The VERA workflow management approach and instructions for its application by end users shall be documented in the VERA basis documentation.

3.4 Meshing Requirements

3.4.1 VERA shall provide sufficient meshing capabilities to address the physics being modeled as specified in the applicable technical documentation (e.g. Challenge Problem Technical Specification). In development of these capabilities, a fundamental objective is to provide automated mesh generation to the reduce user burden to the greatest extent practicable.

3.4.2 VERA shall provide capability for:

- performance of mesh sensitivity studies,
- demonstration of mesh convergence,
- mesh visualization,
- solution verification (including errors in mesh generation due to geometry errors, poorly shaped elements that lead to numerical problems, discretization errors, etc.).

3.4.3 Multi-physics applications are anticipated to require multiple meshes to represent diverse physical phenomena. VERA shall provide capability to map meshes used to model each of the diverse phenomena that are used to address the application being studied and assess the resulting contribution to uncertainty.

3.5 Modeling Capability Requirements

VERA is intended to provide advanced modeling capability applicable to a broad range of end users including:

- reactor vendors / nuclear fuel suppliers,
- nuclear utility owner operators,
- regulatory authorities,
- academic and research staff for R&D, education, and training.

Initial VERA development will focus on development activities intended to address challenge problems related to operation of Pressurized Water Reactor plants. However, VERA development will be performed, to the greatest extent practicable, to permit eventual expansion to support analysis of Boiling Water Reactor and Small Modular Reactor plants.

Specific technical requirements applicable to VERA will be provided to address the individual challenge problem requirements as described in the Challenge Problem Technical Specifications. The following provides a listing of general technical modeling requirements that have been identified as common to addressing the CASL objectives and challenge problems selected for VERA demonstration. As models are developed to address the individual challenge problems, it is anticipated that this listing of general requirements will change and be included in future revisions to this requirements document to incorporate additional features and capabilities.

3.5.1 VERA core simulator models shall include capability to model at least ¼ of reactor core (and eventual expansion to full core modeling when necessary, e.g. for modeling of reactivity insertion accident (RIA)). These models shall be capable of predicting:

- criticality (eigenvalue, critical soluble boron concentration, control bank position, coolant inlet temperature and core power level),
- 3D power distribution, total pin power and neutron fluence versus time,
- 3D exposure distribution and total pin exposure,
- 3D coolant / moderator density,
- 3D gamma energy deposition in fuel, water, and structural components,
- in-core and ex-core instrumentation response,
- radial and axial fuel rod growth versus time,
- lateral core support plate and grid growth versus time,
- reactor vessel, internals and coupons neutron fluence versus time,
- transient simulation capability spanning power maneuvering to accident scenarios. Comment: need to define which accidents, we are limited on level of accidents to be considered

Comment: can we tighten up the grouping?e.g. neutronics, TH, fuel,structures,transients and accidents and then for each one go to the details

3.5.2 Core neutronics modeling shall provide 3-dimensional power prediction with pin level resolution which is capable of addressing geometry changes such as due to thermal expansion (exclusive of fuel / reactor internal geometry changes due to fuel melting) and chemistry feedback (including CRUD, boron, and additives).

3.5.3 VERA shall have capability to provide 3D maps of coolant temperatures and velocities as well as evaluations of pressure drops, quality / void fraction / DNB margin.

3.5.4 VERA shall have the capability to provide fuel behavior and performance evaluations of the following as a function of operating conditions (power density, coolant thermal hydraulics, and chemistry) as it relates to history effects and transients:

- fuel and cladding geometry changes (including swelling),
- fuel rod and assembly distortion,
- pellet - clad interaction,
- fission gas pressures,
- crud deposition,
- clad oxidation and hydriding.

3.5.5 VERA shall be capable of providing nonlinearly consistent numerical solutions of coupled pin-by-pin neutronics, core thermal hydraulics (including modeling of localized subcooled boiling regimes), fuel rod heat generation and transfer and crud mass balance.

3.5.6 VERA shall provide capability to predict fuel rod corrosion and cladding failure.

3.5.7 VERA shall provide the capability to model thermal hydraulic fluid interactions with the fuel / core / vessel structures and structural materials.

3.5.8 VERA shall provide a library of materials models for fuel (including fuel rod and assembly components), vessel internals and reactor pressure vessel material properties and performance. These models shall be baselined / validated against appropriate experimental and operational data.

3.5.9 VERA shall provide capability to add additional models for fuel material properties and configurations to support modeling and analysis of advanced fuel prototypes (e.g. SiC cladding) as they become available.

3.5.10 VERA shall provide capability to provide 3D prediction of temperature, stress, fluence, cracking, and growth of reactor vessel and internal structures to predict fatigue, radiation damage, chemical interactions, and vessel internal component vibration.

3.5.11 VERA shall provide capability to integrate systems analysis codes (e.g. RETRAN, RELAP5, R7) to support performance of nuclear safety analyses and analysis of plant accidents and transients. These capabilities include:

- reactivity insertion accident (RIA) (ejected rod),
- loss of coolant accidents (LOCA) – including small / medium / large break,
- non-LOCA transients and accidents (including cold water injection, loss of flow (LOF), loss of pressure control, main steamline break, etc.),
- departure from nucleate boiling (DNB) condition (PWRs) or dryout (BWRs) conditions and events.

Note that these capabilities are anticipated to be added in stages as the challenge problems which address them are modeled.

3.6 VERA components shall be designed to support end user substitution of their own components / proprietary versions of generic components (e.g. clad material properties (e.g. M5 or Zirlo cladding)) and models to perform proprietary analyses.

3.7 VERA shall provide capability to incorporate modeling / simulation / prediction of integrated reactor operational performance via inclusion of items such as reactor internals / reactivity control components, burnable poison rods, control targets, and annular fuel pellet configurations.

4. CHALLENGE PROBLEM REQUIREMENTS

To accomplish the CASL vision, VERA development will focus on a set of challenge problems that encompass the key phenomena that limit the performance of LWRs. In particular, the challenge problems will address issues that impact the current performance of the existing LWR fleet or are anticipated to provide limitations to achieving improved performance (e.g. power uprates and extended fuel cycles) or long term plant operation. Initial VERA development will focus on PWR applications and challenge problems with the expectation that much of the capability developed will be applicable to other types of reactors. Comment: this could open up a can of worms. Right now we are limited to PWRs with extensions to BWRs and iPWRsTo ensure effective and efficient investigation of identified Challenge Problems, assuring their synergism and integration, CASL will assign a Challenge Problem Integrator to serve as the single point of contact to coordinate personnel across CASL Focus Areas working on aspects associated with the individual Challenge Problems. Comment: the first sentence sounds like the CPI oversees each CP. Actually the role of the CPI is to assure synergism and integration

4.1 For each challenge problem addressed during VERA development, a detailed technical specification shall be developed. This specification shall include the following:

- Discussion of problem and its impact on nuclear plant operation, safety, and economics (i.e. describe the problem's relevance to commercial nuclear power plant operation).
- Identification of physics features, critical processes and parameters that need to be addressed to model the problem including physical, chemical, thermal, material, and structural elements. This discussion shall be of sufficient depth to identify modeling, data and validation requirements.
- Identification of modeling assumptions, initial conditions, and boundary conditions applicable to the modeling of all phenomenological elements required to address the particular challenge problem.
- Identification of test problems and sources of experimental / operational data required to validate the VERA predictions and identify sources of and quantify uncertainties.
- Description of validation plan that will be used to perform model verification, validation and uncertainty quantification.

These specific technical requirements will be documented in the individual Challenge Problem Technical Specification documentation.

4.2 For each challenge problem addressed during VERA development, the capability and performance of the VERA software to address the challenge problem shall be performed and documented. This performance evaluation shall include the following attributes:

- The extent of coverage of physics features of the VERA verification test suite shall be identified, evaluated, and documented
- Technical results of VERA simulations shall be compared to experimental / operational data identified in 4.1.
- Technical results of VERA simulations shall be baselined against results obtained from other existing industry models / codes. Differences in results obtained shall be identified and analyzed.
- Uncertainties shall be identified and quantified.
- Computation capability shall be evaluated against a predefined set of performance attributes (such as computation accuracy, speed or reliability) as specified in the Challenge Problem Technical Specification documentation.

4.3 An appropriate plan for modeling, mesh mapping, and scale up will be developed for each challenge problem to provide a defined pathway to address the challenge problem and validate the solution. A suggested sequence for scale-up to demonstrate and validate challenge problem solution is the following:

- Reduced 3×3 pin geometry array (see Figure 2) standard test bench,
- Full 5×5 pin geometry array (for comparison to experimental test data such as Nestor, OECD / NEA, PSBT etc.),
- 17×17 pin fuel assembly,
- 3×3 fuel assembly array,
- ¼ core geometry,
- Full core geometry (which may include asymmetries).

For each level of development selected for challenge problem model development and coupling, modeling results (including uncertainty quantification) shall be documented.

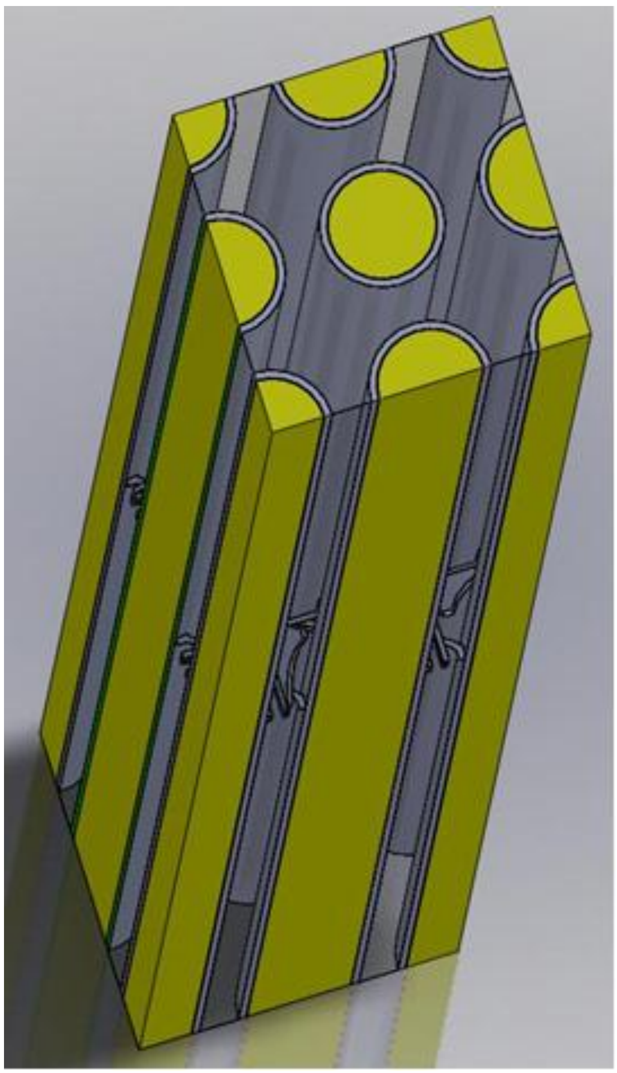

Figure 2: Reduced 3×3 Pin Geometry Test Bench Array

5. INSTRUCTIONS AND END USER CAPABILITY REQUIREMENTS

2.1 VERA documentation shall provide instructions and end user capability to select, setup, and modify physics models from predefined libraries for simulation of the application to be evaluated. As a minimum these libraries shall include capability to model the following phenomena.

- Core Physics
- Thermal Hydraulics
- Chemistry
- Materials
- Thermo-Mechanics
- Structural Elements (including Fluid – Structure Interaction)
- Fuel Performance

5.2 VERA shall provide instructions and end user capability to link the models applicable to the problem being investigated to create the simulation that will be used to model the phenomena of interest. This shall include providing instructions and end user capability to load the application onto VERA on the selected computational platform and test input and output files to confirm proper installation.

5.3 VERA shall provide instructions and end user capability to execute the application simulation on the selected computational platform. This end user capability shall include instructions to execute VERA on a range of platforms up to and including state of the art high performance computing capability.

5.4 Visualization

5.4.1VERA shall provide instructions and end user capability to visualize and analyze data and results obtained from executed simulations.

5.4.2VERA shall provide capabilities for end users to manipulate, edit, store, graph, print and transfer / export simulation output data in predefined user selected formats and provide traceability tags (e.g. execution date and time, codes and versions used, compiler used, computer platform used, etc).

5.4.3 VERA shall provide capabilities for end users to manipulate, edit, store and transfer visualizations of simulation outputs and provide traceability tags.

5.5 Data Management

5.5.1 VERA shall provide the capability to characterize, group (by physics, scale, model, etc.), and format / reduce data for internal use and export / transfer to external applications. This will include providing capabilities to archive, retrieve, extract, manipulate, and transfer large amounts of data that will be used in modeling and analysis of applications.

5.5.2 VERA shall provide the capability to manipulate data so that it supports modern automated V&V / UQ. As needed, VERA shall provide the capability for data clustering, scenario aggregation, and pattern recognition to support effective data storage and enable effective data mining.

5.5.3 VERA shall provide the capability to enable secure / protected mechanisms for data access, processing, analysis, and use of CASL-owned data and data protected by CASL nondisclosure agreements (NDAs). These capabilities shall be conducted in accordance with the approved CASL Technology Control Plan (TCP).

5.6 For instances where the VERA software provides the capability for end users to add user specified and / or proprietary information the VERA environment shall provide protection capability for end user supplied information and data.

5.7 VERA shall provide research user capabilities to support modeling and investigation of new concepts / emerging technologies and rapid prototyping of proposed design changes. (Note – this requirement represents a long-term objective of VERA. Thus, specific requirements applicable to meeting this objective are anticipated to be developed as research user needs are identified.)

6. QUALITY ASSURANCE REQUIREMENTS

The requirements provided below represent high level general requirements that are capable of supporting multiple and diverse application. It is recognized that specific requirements may be dependent upon the individual application. Thus, these requirements are intended to permit a graded application based upon the intended usage of the software, e.g. exploratory research vs. safety analysis.

6.1 VERA software development shall be performed in accordance with practices and policies described in and controlled by a VERA Software Development Specification that is approved and controlled under the responsibility of the Virtual Reactor Integration (VRI) Focus Area (FA) Lead. When possible, appropriate, and practical, VERA software development should also conform to DOE Order 414.1C, “Quality Assurance”, which also conforms to ASME NQA-1, the nuclear power industry standard for quality assurance of nuclear related software. While it is recognized that VERA will not immediately be utilized for safety-related calculations, early conformance in these standards will assist future users in gaining regulatory approval of any methods derived from or using the VERA software suite.

6.2 Testing Plan

6.2.1 VERA software testing shall be performed under a written software testing plan that is approved and controlled under the responsibility of the VRI FA Lead.

6.2.2 All versions of VERA that will be externally released by CASL shall be tested, verified, and validated to conform to a formal written software testing plan developed for each software release. Each such testing plan shall contain explicit criteria and documentation of results for the following:

- system functionality including description of VERA foundational capabilities addressed in the release and capabilities to address identified Challenge Problems.
- system reliability including capabilities to identify and resolve system errors,
- testability including specification of standard test cases

- performance including guidance on expected execution times for standard test problems under specified hardware configurations.

6.2.3 All VERA testing plans shall be approved and controlled under the responsibility of the VRI FA Lead with review and concurrence of the AMA FA Lead.

6.2.4 Acceptance of VERA test results shall be approved by the CASL Senior Leadership Team (SLT) prior to software release.

6.3 Modifications and changes to VERA software, review and approval.

6.3.1 All materials modeling, performance and optimization methods used in VERA software shall be approved and controlled by the Materials Performance and Optimization (MPO) Focus Area (FA) Lead.

6.3.2 All reactor physics and thermal-hydraulics based models used in VERA software shall be approved and controlled by the applicable Focus Area (FA) Lead (identified below). This includes models and numerical methods that address the following phenomena modeled in VERA

- Core Physics including radiation transport, cross sections and depletion (Radiation Transport – RTM)
- Fuel Performance (Materials Performance and Optimization – MPO)
- Core and Reactor Vessel Thermal Hydraulics Models (Thermal Hydraulics Modeling – THM)
- Reactor Water Chemistry (Materials & Performance Optimization – MPO)
- Core and Reactor Vessel / Internals Thermo-Mechanics (Virtual Reactor Integration – VRI)
- Fluid Structures Interaction (Virtual Reactor Integration – VRI)

6.3.3 All software tools and methodologies for verifying, calibrating, and / or validating VERA software, models, and data shall be approved and controlled by the VUQ FA Lead.

6.4 VERA Software Release Requirements

6.4.1 VERA software releases by CASL shall be scheduled and controlled by the VRI FA Lead.

6.4.2 VERA software shall only be released by CASL after successful completion of the approved software testing plan as described in 6.2.1 through 6.2.3.

6.4.3 All external releases of VERA software (both major and minor as described in 6.4.4 – 6.4.6 below Define major and minor?) shall comply with established export control requirements and proprietary data release constraints.

6.4.4 All external major releases of VERA software shall be approved by the CASL Director.

6.4.5 All external minor releases of VERA software shall be approved by the VRI FA Lead, with notification to CASL Director and SLT.

6.4.6 All external releases of VERA software to resolve software bugs shall be approved by the VRI FA Lead, with notification to CASL Director and SLT.

6.5 Documentation and Records

CASL related documents shall be controlled and managed by the CASL Records Management system and associated processes for version control and archival.

6.5.1 Physics-based models, mathematical formulations, and numerical solution algorithms integrated into VERA shall be documented in the code theory and models manuals and code V&V report as part of the VERA basis documentation. As a minimum this documentation shall include the following:

- theoretical / mathematical relationships,
- material properties,
- numerical solution methods,
- initial and boundary conditions,
- closure laws,
- verification (including range of validity),
- validation (including range of validity).

6.5.2 Mesh generation procedures used shall be documented in the VERA basis documentation.

6.6 VERA user documentation in the code user manual shall provide detailed instructions to support user setup and operation. This shall include instructions for the following:

- User system minimum requirements (i.e. processor, memory, graphics, etc.
- Installation and Execution procedures including test problems' inputs and outputs
- Input Instructions (including format, parameter, command and control requirements) including Sample Input Descriptions
- Application of User Defined Models
- Restart Instructions
- Post-processor Instructions
- Error Messages
- Frequently Asked Questions (FAQ)
- User Tutorials (Use of Sample Problems)

6.7 CASL shall provide continuing means and fora for user support and training. These should include the following:

- Comprehensive applications training on use of VERA for end user application.
- Provide capability for internet and phone based technical support to address user issues in real-time.
- Provide fora ongoing interactions with technical user community (including industry, regulatory authorities and academia) via courses, symposia, and seminars hosted by CASL (or CASL partner institutions).

7. VERIFICATION AND VALIDATION / UNCERTAINTY QUANTIFICATION REQUIREMENTS

7.1 Physics-based and correlation-based mathematical models selected for integration into VERA shall be evaluated for verification and validation requirements. This shall include, at a minimum, consideration of the following:

- Identification of uncertain parameters and their uncertainty distributions.
- Representation of uncertainties in model form, numerics, initial conditions, and boundary conditions.
- Identification of potential calibration and validation data and their usage.
- Development and application of verification test problems.
- Development of a hierarchical validation approach that includes the necessary model couplings and upscaling.
- Range of validity for each physics-based model.

The results of these evaluations shall be documented and incorporated into the individual model development work plan.

7.2 Software models integrated into VERA shall be evaluated for verification and validation requirements. This shall include, at a minimum, consideration of the following:

- Geometric Models
- Core Neutron Physics Models
- Thermal Hydraulics Models
  - Clad-Coolant Heat Transfer
  - Coolant Enthalpy
  - Subcooled Boiling
  - Turbulent Excitation Forces
- Materials Models
  - Fuel Constitutive and Physical Models / Materials Properties (including pellet, clad, and grids)
  - Clad Constitutive and Physical Models / Materials Properties
  - RPV Internals Constitutive and Physical Models / Materials Properties
  - RPV Constitutive and Physical Models / Materials Properties
- Structural Mechanical Models
  - Fuel Deformation and Failure (including contributors from pellet, clad and grids)
  - Reactor Internals Deformation and Failure
  - Fluid – Structure Interactions
- Chemistry Models
  - Reactor Coolant Chemistry
  - Material Surface Chemistry (including corrosion)
- One-way and multi-directional (through physics coupling) feature coverage of the VERA verification test suite.
- Fuel Performance / Behavior Models

The results of these evaluations shall be documented and incorporated into the individual model development work plan.

7.3 The VUQ process shall validate VERA predictions for each challenge problem by quantification of uncertainties originating from key modeling parameters, models, numerics, initial conditions, and boundary conditions. The VUQ process also shall verify the uncertainties are properly propagated through intermediate calculations and the predictions obtained and their uncertainties correspond to available operational or testing data that represent the phenomena that were modeled. These activities shall be conducted in accordance with the approved CASL Validation Plan. Figure 3 provides a schematic of the validation and uncertainty quantification hierarchy process that will be followed for each challenge problem.

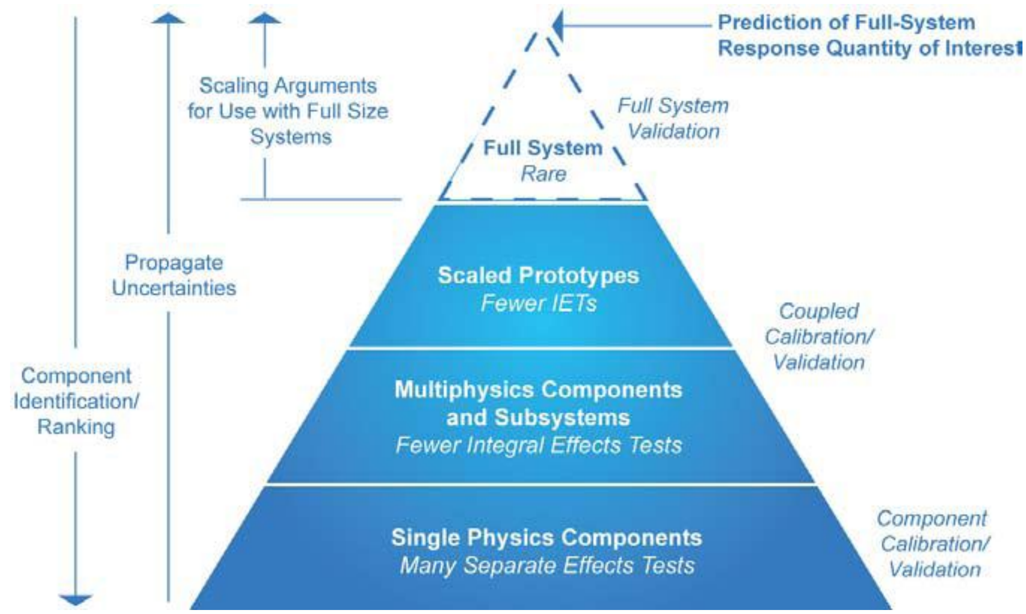

Figure 3: Validation Hierarchy Process to be Applied to Each Challenge Problem

8. VERA REQUIREMENTS MANAGEMENT

2.2 Requirements Planning

The process of requirements planning is implemented through the following actions.

8.1.1 Elicitation

Requirements elicitation is performed by reformulating the four basic types of requirements (business, functional, quality, and design) into a series of questions to present to VERA stakeholders. The first task with respect to the elicitation process is to identify an appropriate sample of interviewees and formulate several questions per requirement for presentation to them. Next answers are sought to these questions from the selected interviewees (with responses obtained through e-mail, phone calls, meetings / interviews, workshops or a combination of these techniques). The responses are documented and verified by the interviewees to ensure that the answers correctly reflected the opinion of the person interviewed.

8.1.2 Analysis

Analysis is the process by which gaps or missing requirements are identified. Models (such as state diagrams, information / class diagrams, data flow diagrams, Phenomena Identification and Ranking Tables (PIRT), sensitivity analysis etc.) may be used to analyze requirements, confirm or modify scope and ensure consistency.

8.1.3 Prioritization

Results of the analysis conducted in step 8.1.3 are then used to set priorities (typically based on a set of predefined attributes such as scale, cost, benefit, risk, etc.). These prioritizations should be conducted using a formally approved methodology (such as the Analytic Hierarchy Process (AHP), decision tress, maturity evaluation, etc.) by the SLT and documented.

8.1.4 Validation

Validation is the process of determining whether the specified requirements are appropriate, correct and sufficient to achieve the specified objectives. Requirements may be validated through peer reviews, test case creation, or target / estimation alignment. The validation process ascertains the extent to which the requirements are unambiguous, testable, technically correct, within project scope, modifiable, feasible, traceable, clearly written, and acceptable to all stakeholders.

8.1.5 Specification Format

Requirements shall be documented. They may be specified in various formats such as templates (text or models), user manuals, test cases, or prototypes dependent upon the nature of the particular requirement.

2.3 Requirements Development

Requirements are managed by the actions of scrubbing, tracking changes, and matching scope.

8.2.1 Scrubbing

Specified requirements are scrubbed by eliminating those that are identified / validates as not important. The scrubbing process also simplifies those requirements that may be unnecessarily complicated. Scrubbing occurs via a requirements review conducted under the direction of the AMA FA Lead.

8.2.2 Change Management

Changes in requirements shall be documented, tracked, and approved via a VERA Change Board working under the direction of the AMA FA Lead.

8.2.3 Scope Matching

In considering changes to requirements, attention must be paid to the impact the change has on benefits, cost, risk, schedule, quality, resource allocation, timing, and stability. The AMA FA Lead has responsibility for the conduct of scope matching for the VERA product.

2.4 Requirements Management

Requirements development and management is an ongoing process with necessary supporting activities planned in advance. The AMA FA Lead owns and executes requirements development and management for the VERA software. Requirements management shall be controlled and documented in a requirements plan owned by the AMA FA Lead.

APPENDIX A: VERA FOUNDATIONAL CAPABILITIES

This appendix provides a discussion of the VERA foundational capabilities that have been identified to permit VERA to function as a core simulator for PWR NPPs. The intent of specifying these specific capabilities is to focus VERA development to achieve this level of generic analytical capability by 31 December 2013 such that the core VERA application (designated as VERA-CS) will be capable of performing analyses and simulations to address the benchmark problems. These benchmark problems, which were originally developed for core neutronics in the report "VERA Technical Requirements by Component" (CASL-2011-0074-000-CI) are as specified below. In these specifications the core neutronics benchmarks are, at this point in time, more fully developed than the similar benchmarks for either thermal hydraulics or fuel performance. Also, the benchmarks specified here are high level and do not contain detailed specifications for technical content, data sources, or verification / validation / uncertainty quantification requirements. To address these issues, detailed specifications will be developed for each of the benchmarks identified below to provide technical descriptions of the benchmark problem and data (geometry, material, etc.) necessary to evaluate it. (Note that these will be similar is scope and content to the Challenge Problem Technical Specifications which provide this level of detail for the Challenge Problems). As these technical benchmark specifications are developed, this Appendix will be updated (with commensurate SLT review and approval) to reflect the enhanced requirements. Similar to the approach to address the Challenge Problems, in addressing the benchmark problems, it is recommended that a scale-up sequence consisting of 3x3 rods, single-assembly, coupling, multi-assembly, and full-core be used to conduct the individual benchmark evaluations.

Core Neutronics Benchmarks

Benchmark 1: 2D Hot-Zero-Power (HZP) Pin Cell

Benchmark 1 is a simple two-dimensional pin cell eigenvalue calculation without thermal-hydraulic or fuel temperature feedback.

Benchmark 2: 2D HZP Lattices

Benchmark 2 is a two-dimensional slice of a 17x17 PWR assembly (typically referred to as a lattice). The assembly contains fuel rods, control rod guide tubes, an instrument tube, and inter-assembly gaps. Output includes eigenvalue and pin power distributions. There is no thermal-hydraulic or fuel temperature feedback.

Benchmark 3: 3D HZP Assembly

Benchmark 3 is a three-dimensional 17x17 PWR assembly, which includes axial heterogeneity such as low enriched axial blankets, gas plenums, spacer grids, and upper and lower reflector regions. Output includes eigenvalue and 3-D pin power distributions. There is no thermal-hydraulic or fuel temperature feedback.

Benchmark 4: HZP 3x3 Assembly with CRD Worth

Benchmark 4 is a three-dimensional 3x3 configuration of 17x17 PWR assemblies with one assembly containing control rods. The assemblies are arranged in a typical checkerboard loading pattern. Output includes eigenvalue, control rod worth as a function of axial position, and 3-D pin power distributions. There is no thermal-hydraulic or fuel temperature feedback.

Benchmark 5: Physical Reactor Zero Power Physics Tests (ZPPT)

Benchmark 5 is the prediction of startup Zero Power Physics Tests (ZPPT) results for Cycle 1 of a Westinghouse 4-loop 17x17 physical reactor. The tests include measurement of critical boron concentration, isothermal temperature coefficient, control bank worths, and soluble boron worth. The tests are performed at zero-power no-xenon conditions without thermal-hydraulic or fuel temperature feedback. We note that because NPP startup data typically is collected for this condition, this benchmark serves as a useful point for VERA validation and verification (V&V) benchmarking activities.

Benchmark 6: Hot Full Power (HFP) BOL Assembly

Benchmark 6 is a three-dimensional 17x17 PWR assembly with thermal-hydraulic and fuel temperature feedback. This problem is performed at Beginning-of-Life (BOL) without depletion effects, including fission product poisoning such as xenon and samarium.

Benchmark 7: HFP BOC Physical Reactor with xenon

Benchmark 7 is the simulation of equilibrium HFP conditions of BOC Cycle 1 of a Westinghouse 4-loop 17x17 physical reactor, including quarter-core thermal-hydraulic feedback, fuel temperature feedback, and fission product poisoning.

Benchmark 8: Physical Reactor Startup Flux Maps

Benchmark 8 is the prediction of startup power escalation testing (PET) results for Cycle 1 of a Westinghouse 4-loop 17x17 physical reactor. The PET tests measure the three-dimensional reaction rate distribution in a portion of the core's instrument tubes at various times during the approach to HFP at BOC. We note that because NPP startup data typically is collected for this condition, this benchmark also serves as a useful point for VERA V&V benchmarking activities.

Benchmark 9: Physical Reactor Depletion

Benchmark 9 is the full simulation of Cycle 1 of a Westinghouse 4-loop 17x17 physical reactor. This problem includes critical boron searches and fuel depletion. Again, since operating NPP data typically is collected for this condition, this benchmark also serves as a useful point for VERA V&V benchmarking activities.

Benchmark 10: Physical Reactor Refueling

Benchmark 10 performs the fuel shuffling from Cycle 1 to Cycle 2 of a Westinghouse 4-loop 17x17 physical reactor.

Core Thermal Hydraulics Benchmarks

In the development of the VERA software, the CASL development plan will address modeling of thermal hydraulic phenomena in the following order:

1) single phase flow,
2) single phase flow with sub-cooled nucleate boiling,
3) two phase flow.

Thus, the core thermal hydraulic benchmark problems are ordered to reflect this planned development sequence through single phase flow with sub-cooled boiling. (Note that separate benchmark problems to address full two phase flow and transient conditions will be developed to support VERA releases scheduled to occur after the 31 December 2013 target supported by the requirements addressed in this Appendix.)

Benchmark 1: Single Phase Simple Channel Pressure Drop
Benchmark 1 is a simple single channel test case that compares calculated single phase flow pressure drop to measured data. This benchmark is used to confirm the basic momentum equation predictions and constitutive models (such as wall friction).

Benchmark 2: Single Phase Bundle Pressure Drops and Flow Distributions
Benchmark 2 will compare calculated single phase pressure drop profiles to data. This test is used to confirm the basic field equations and constitutive models for more complex flow fields. This benchmark also will apply data from rod bundle experiments to confirm the ability to determine flow (e.g. velocity) redistribution due to blockages at various locations within the bundle for single phase flow conditions. The benchmark addresses typical modern PWR bundle geometries for plant operating conditions.

Benchmark 3: Single Phase Heat Conduction
Benchmark 3 compares steady state fuel rod temperatures computed by VERA conduction model(s) against analytic solutions under single phase flow conditions. For cases where subchannel models are used, this benchmark will evaluate the heat transfer correlations used to relate the wall surface temperature to the wall heat flux under single phase flow conditions. Separate effects tests for different heat transfer regimes can be used to provide axial profiles of surface temperatures for benchmarking against the computed temperatures.

Benchmark 4: Sub-Cooled Boiling Simple Channel Pressure Drop
Benchmark 4 is a simple single channel test case to evaluate pressure drop for the case of single-phase flow with subcooled boiling. This benchmark is used to confirm the basic momentum equation predictions and constitutive models (such as wall friction) and the results can be compared to those obtained in Benchmark 1.

Benchmark 5 Sub-Cooled Boiling Pressure Drops in Bundles
Benchmark 5 addresses single-phase pressure drop under sub-cooled boiling. This test is used to confirm the basic field equations and constitutive models for more complex flow fields. The benchmark addresses typical modern PWR bundle geometries for plant operating conditions.

Benchmark 6: Single Channel and Lattice Sub-Cooled Boiling Void Fractions
Benchmark 6 will compare void profiles for pressures ranging from several hundred psia to near PWR operating conditions. The tests will confirm the onset of subcooled boiling predicted by available models and will also confirm the validity of void profiles over the length of the channel. A

variety of inlet sub-coolings, pressures and wall heat fluxes will be compared. Additionally, this benchmark.will evaluate void fractions for predefined fuel lattices and can be applied in cases where data at this level are available. A variety of inlet sub-coolings, pressures and wall heat fluxes will be compared.

Benchmark 7: Heat Conduction for Single Phase with Sub-Cooled Boiling
Benchmark 7 compares steady state fuel rod temperatures computed by VERA conduction model(s) against analytic solutions under single phase flow conditions under the presence of sub-cooled nucleate boiling. For cases where subchannel models are used, this benchmark will evaluate the heat transfer correlations used to relate the wall surface temperature to the wall heat flux under conditions of single phase flow with sub-cooled boiling. Separate effects tests for different heat transfer regimes can be used to provide axial profiles of surface temperatures for benchmarking against the computed temperatures.

<u>Fuel Performance Benchmarks</u>

Benchmark 1: Steady State Fuel Rod Operation

A 2-D axisymmetric steady state fuel rod will be modeled. It will be operated for two cycles, with startup and shutdown conditions using FEA methods. Standard UO2 fuel with Zircaloy-4 cladding will serve to obtain temperature distributions given axial varying linear heat rate and appropriate cladding outside thermal boundary conditions. For this case, simple calculation of cladding surface temperature distribution would be sufficient (or, if available, linkage to thermal hydraulic conditions would be better). This benchmark problem assumes that appropriate fuel-to-gap and internal gas modeling is performed. The stress and strain state of the fuel, cladding and gaps will be determined and reported.

Benchmark 2: High-Burnup Fuel Rod Modeling

The same model as the previous benchmark will be extended to appropriately model fuel, cladding, and internal voids as they reach burnup greater the 40 GWd/MTU. Here the cladding material properties should be dependent of fluence and the fuel properties dependent on burnup. Fission gas production and release will be estimated as will the compositions of the internal gas volume to determine dependent properties of this gas. Oxidation on the outside of the cladding will be determined and reported.

Benchmark 3: Transient Fuel Rod Modeling

Building upon the two previous benchmarks, the response of a fuel rod will be determined for sharp increases in power due to normal operational transients or those associated with design basis accidents.

Benchmark 4: 3D Fuel Rod Modeling

The modeling capabilities required to perform the previous benchmark cases will extend to 3-dimentional FEA modeling. Here the thermal boundary conditions shall very axially and azimuthally with time.

The following provides a detailed compilation of technical capabilities that have been identified as necessary to achieve this level of core simulator capability within the identified development schedule. The intent of providing these capabilities to support effective prioritization within each CASL FA and effective and efficient resource allocation by the CASL SLT to achieve this level of generic functionality of the VERA-C product. Comment At the beginning of this Appendix, page 19, the core VERA application was designated as VERA-CS. Now and in the following it has become C, please be consistent, BTY what does S stand for? We note that additional capabilities identified to achieve emerging or changing objectives or to address other LWR designs (e.g. BWRs and SMRs) will be developed and specified in future revisions to the VRD.

1. COUPLED PHYSICS

1.1 VERA-C shall provide the following coupling capabilities:
- a) 2-way channel flow and transport neutronics
- b) 2-way CFD and transport neutronics
- c) 2-way rod fuel temperatures and transport neutronics

1.2 VERA-C shall provide capability to converge non-linear solutions coupled with fuel rod heat generation from the nuclear physics models.

1.3 VERA-C shall provide capability to converge non-linear solutions coupled from the nuclear physics and thermal-hydraulics (T/H) model solutions.

2. INDIVIDUAL PHYSICS REQUIREMENTS

2.1 Nuclear / Core Physics

2.1.1 Steady-State

VERA-C shall provide to capability to perform the following steady state reactor physics calculations.

2.1.1.1 Calculate steady-state neutron flux over entire geometry.

2.1.1.2 Calculate 3D power distribution with pin-level resolution.

2.1.1.3 Calculate 3D exposure distribution.

2.1.1.4 Calculate 3D fluence distribution in fuel.

2.1.1.5 Calculate reaction rates (including power distribution and in-core detector responses).

2.1.1.6 Provide capability to perform capability to steady-state searches on critical eigenvalue and critical boron concentration.

2.1.1.7 Provide capability to converge non-linear solution coupled with coolant density/temperature from T/H components and fuel temperatures from fuel performance model.

2.1.1.8 Provide capability to account for different isotopic values of the fission spectrum (χ).

2.1.2 Cross-Sections

VERA-C shall provide to capability to perform the following cross-section calculations.

2.1.2.1 Generate macroscopic multi-group neutron cross sections for nuclear physics model.

2.1.2.2 Provide capability to perform resonance cross section calculations in a particular group structure (e.g. 200+ groups or continuous energy) and collapse cross sections to a smaller group structure to be used in the transport solution (e.g. 20 or 40 groups).

2.1.2.3 Provide accurate cross sections for resonance materials that:

a) account for fuel pins with multiple radial and azimuthal regions, each with separate isotopic concentrations and fuel temperatures,
b) account for resonance isotopes in cladding and structural materials (e.g. zirconium),
c) account for resonance isotopes in burnable absorbers,
d) account for surrounding pin geometry (e.g., with Dancoff factors, sub-group cross sections, or some other appropriate model).

2.1.2.4 Generate microscopic cross sections for soluble boron in coolant.

2.1.3 Depletion

VERA-C shall provide to capability to perform the following depletion calculations.

2.1.3.1 Calculate isotope depletion by region using 3D flux solution and depletion time step size.

2.1.3.2 Allow fuel pins to be depleted in user-configurable depletion regions, which may be different than the flux solution mesh. Allow for multiple radial and azimuthal depletion regions in each pin.

2.1.3.3 Provide ability to model slow transients (pseudo-steady-state), such as xenon peaks.

2.1.3.4 Provide model to allow reasonable depletion steps for strong absorber materials (e.g. gadolinia).

2.2 Thermal Hydraulics

VERA-C shall provide the following thermal-hydraulics (T/H) capabilities.

2.2.1 Provide 3D maps of coolant temperatures as well as evaluations of pressure drops and fluid densities to support coupled subchannel analysis capability.

2.2.2 Provide 3D maps of coolant temperatures and flow velocities as well as evaluations of pressure drops and fluid densities to support coupled CFD analysis capability.

2.2.3 Calculate clad surface temperature.

2.2.4 Calculate cross flow (3D flow paths).

2.2.5 Provide capability to model turbulent mixing, subcooled boiling and mass flux on a sub-channel basis.

2.2.6 Provide an option for “fast” thermal-hydraulic solution for routine core analysis (e.g., sub-channel model).

2.3 Fuel Rod Thermo-mechanics

VERA-C shall provide the capability to properly characterize the behavior and materials for fuel, cladding, internal voids and gaps. VERA-C also shall provide capability to determine displacements, temperatures, and internal pressures as the constituent models contained in VERA-C are applied and the geometry of the fuel rod system changes with time.

2.3.1 Provide capability to perform fuel behavior and performance evaluations of the following as a function of operating conditions (power density, coolant thermal-hydraulics, and chemistry) over the in-core life cycle using appropriate fuel material property modeling.

2.3.1.1 Fuel material properties that are required (with some as function of burn up and chemical composition) include:

a) specific heat, enthalpy, emissivity and melting temperature,
b) thermal conductivity as a function of burn up and burnable poison concentration,
c) thermal expansion,
d) solid swelling,
e) Young's modulus and shear modulus,
f) compressive yield stress,
g) fracture strength,
h) thermal and irradiation creep.

2.3.1.2 Fuel behavior models include:

a) densification, pellet cracking, and relocation,
b) fission gas production and release,
c) fission gaseous swelling,
d) burnable poison He release,
e) isotopic transmutation and decay,
f) microstructure evolution,
g) oxygen transport.

2.3.2 Calculate fuel temperatures in each fuel pellet and fuel cladding ensuring rod surface temperature is converged with thermal-hydraulics solution.

2.3.3 Provide capability to perform cladding behavior and performance evaluations of the following as a function of operating conditions (power density, coolant thermal-hydraulics, and chemistry) over the in-core life cycle using appropriate cladding material modeling.

2.3.3.1 Thermal properties:
a) Specific heat capacity, thermal conductivity, and melting temperature,
b) Oxide conductivity and emissivity.

2.3.3.2 Mechanical properties:
a) thermal expansion,
b) Young's and shear modulus for isotropic cladding,
c) yield stress and plastic strain hardening,
d) annealing of cold work / irradiation damage,
e) mechanical limits, fracture and failure,
f) thermal and irradiation creep,
g) irradiation growth and swelling,
h) Meyer hardness.

2.3.3.3 Behavioral properties:
a) microstructure evolution,
b) low and high temperature oxidation (may be from linked component),
c) hydrogen pickup,
d) hydrogen diffusion and hydride formation,
e) CRUD formation (may be from linked component).

2.3.4 Provide capability to perform fuel-to-cladding behavior and performance evaluations of the following as a function of operating conditions (power density, coolant thermal-hydraulics, and chemistry) over the in-core life cycle using appropriate cladding material modeling.

2.3.4.1 Thermal properties:
a) gas thermal conductivity,
b) gas viscosity,
c) temperature jump distance.

2.3.4.2 Mechanical properties:
a) friction coefficient,
b) contact sliding.

2.3.4.3 Behavioral properties:
a) open and solid gap conductivity,
b) internal pressure,
c) plenum elastic spring,
d) pellet – clad bonding.

2.3.5 Provide capability to model any number of fuel rods ranging (I believe you had a Freudian slip here ☺) from single-rod model to full-core model.

a) The full core model may be simplified relative to single rod models and shall include an option for utilizing "fast" fuel temperature and clad surface temperature models for routine core analysis and account for crud thermal conductivity and thickness.

b) Provide capability to focus in on user specified regions of interest.

2.4 Structural

For the purpose of achieving the capability to address the benchmark problems, there are no specific structural modeling capabilities specified for VERA-C. However, where structural models, information, and interactions are required to accomplish specific calculations within individual physics components of VERA-C, these capabilities shall be included within the respective physics models. COMMENT: I believe we need to have structural modeling capabilities if we want a complete product.

2.5 Material Models and Properites

Since VERA will consist of a diverse integration / coupling of several codes and models, at this stage of the development of VERA, the most significant issue with respect to material models and properties is the need for unification of how they are applied / used in the respective physics codes. This is required to permit VERA to effectively support the following:

- ensure consistency during the conduct of multi-physics simulations,
- provide the ability to perturb for sensitivity studies, and
- provide the ability to properly propagate uncertainties and permit effective uncertainty quantification (UQ).

Thus, for each constituent element and model contained in VERA the following requirements shall be followed.

2.5.1 Define all material properties used within each model / code integrated into VERA.

2.5.2 Document what material properties are used within each model / code integrated into VERA.

It should be noted that in the longer term it will likely be beneficial or necessary to develop a suite of common material properties / model libraries for integration into VERA. Examples of such material models / properties include

- material densities,
- thermal conductivities,
- Young’s modulus,
- yield stress,
- ultimate stress,
- strain hardening modulus,
- thermal creep rates,
- irradiation creep rates,
- irradiation growth rates,
- oxidation rates,

- thermal expansion coefficients.

Additionally, reactor coolant properties / models (e.g. steam table properties) for subcooled liquid, saturated liquid and vapor, and superheated vapor shall be included / documented for critical properties including enthalpy, density, surface tension, viscosity, etc..

2.6 Uncertainty Quantification

VERA-C shall provide generic capability the following uncertainty quantification and analysis capabilities.

2.6.1 Performance of sensitivity studies of key input variables.

2.6.2 Performance of sensitivity studies of key correlations.

2.6.3 Capability to obtain ranges of key variables and apply to assess / validate results.

2.7 Supporting Requirements

The following subsections provide general requirements that are necessary to support multi-physics modeling and analysis in VERA-C. For each code and physics-based model integrated into VERA-C, these requirements shall be evaluated and incorporated into the integration. We note that different models will require different levels of fidelity to account for the components / physics applicable to the specific problem being addressed.

2.7.1 General Modeling Capability

VERA-C shall be capable of supporting physical reactor model development / integration to the level appropriate to the specific physics being modeled.

2.7.1.1 Support modeling of core baffle, internals and externals.

2.7.1.2 Support modeling of upper and lower tie plates.

2.7.1.3 Support modeling of spacer grids.

2.7.1.4 Support modeling of control rods and removable burnable absorbers.

2.7.1.5 Provide ability to model partial core configurations (one fuel assembly, 3x3 fuel assemblies, etc.).

2.7.1.6 Provide ability to model quarter-core configurations and full-core configurations.

2.7.2 General Simulation Capabilities

VERA-C shall be capable of supporting general physical reactor simulations to the level appropriate to the specific physics being modeled.

2.7.2.1 Provide ability to model partial-core configurations (one assembly, multiple-assemblies, quarter-core).

2.7.2.2 Support modeling of features of modern PWR fuel designs (14x14 through 17x17 including geometry, grids, water rods, IFBA, etc.).

2.7.2.3 Provide ability to transfer required data between components (e.g., via LIME).

2.7.2.4 Provide ability to load applications and launch jobs on targeted computer systems.

2.7.2.5 Provide capability to save a calculation at a given statepoint (i.e. at a given power, flow, isotopic content, geometric configuration, etc.).

2.7.2.6 Provide capability to restart a calculation from a given statepoint.

2.7.2.7 Provide ability to shuffle the core (physically move fuel assemblies in core, discharge fuel assemblies, and insert fresh fuel assemblies).

2.7.3 Input / Output Capabilities

VERA-C shall provide standardized input / output capabilities to support end-user implementation. The intent of this section is to permit users to interface with VERA using a standard format for providing input data and viewing and storing output results.

2.7.3.1 Provide capabilities for end-users to retrieve, store, and transfer / export simulation output data in predefined user selected formats and provide traceability tags (e.g. execution date and time, codes and versions used, compiler used, computer platform used, etc).

2.7.3.2 Provide capabilities for end-users to manipulate, store and transfer visualizations of simulation outputs and provide traceability tags.

2.7.3.3 Provide the capability to enable secure / protected mechanisms for data access, processing, analysis, and use of CASL-owned data and data protected by CASL nondisclosure agreements (NDAs).

2.7.3.4 Provide the capability to display 2D and 3D data using all mesh formats used by the components.

2.7.3.5 Support user-selectable ASCII output edits of all major physics results for the fuel system and coolant (power, density, isotopics, temperature, stress, strain, pressure, etc.), including:

a) 2D and 3D edits by assembly,
b) 2D and 3D edits by pin,
c) core averaged values,
d) average axial distributions by assembly,
e) average axial distributions of entire core,
f) 3D pin peaking factors by assembly (i.e. F_q edits),
g) 2D pin peaking factors by assembly (i.e. F_{dh} edits).

2.7.3.6 Provide user-selectable edits of all major core distributions by fuel pin.

2.7.4 Usability

VERA-C shall provide the following information to support end-user implementation.

2.7.4.1 Provide appropriate documentation for use / running of coupled physics codes.

2.7.4.2 Provide documentation for application to each benchmark problem.

APPROVALS

______________________________________ ______________
Douglas Kothe – CASL Director Date

______________________________________ ______________
Ronaldo Szilard – CASL Deputy Director Date

______________________________________ ______________
Paul Turinsky – CASL Chief Scientist Date

______________________________________ ______________
Mario Carelli – CASL Chief Strategy Officer Date

TBD