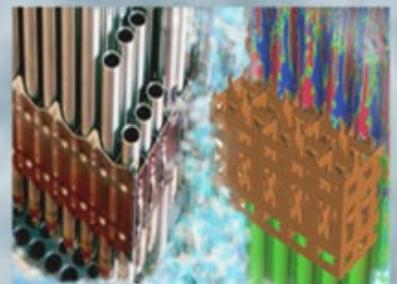
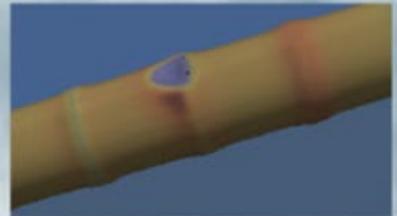
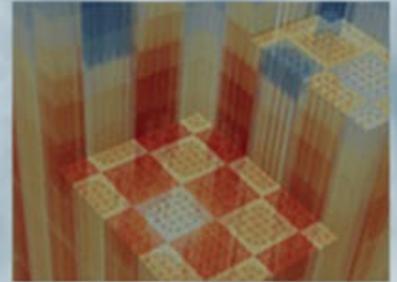


Consortium for Advanced Simulation of Light Water Reactors

CASL Phase II Summary Report

September 2020



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MESSAGE FROM THE CASL DIRECTOR

On behalf of CASL, I am pleased to present this final report covering Phase II for the period 2015-2020, which provides a summary of achievements and impacts in the areas of research and development, technology deployment, education and workforce development. The Virtual Environment for Reactor Applications (VERA), the product of CASL, has matured and is being widely deployed as an integrated, high performance computing platform for performing multi-physics simulation for advanced Light Water Reactors. The CASL challenge problems, defined at the outside of the CASL, has expanded the advanced simulation capabilities encompassed by VERA for a wide range of applications. This includes not only solution of the CASL challenge problems, such as crud and pellet-clad interaction, but development of first-of-a-kind analyses for accident tolerant fuels and plant lifetime extension.



The unique partnerships built by CASL brought together a diverse team of talented individuals working in a collaborative environment across the national laboratories, academia and industry. The key to such collaboration is having a shared vision, a line of sight from each individual contributor and technical focus area towards common goals, and excellence in execution. There have been hundreds of contributors to the CASL program during the history of the hub who were brought together under a “one roof” virtual environment with the goal of providing tools and capabilities that have not only high value but high impact with respect to addressing the design and operational challenges of the current, as well as future, nuclear fleet.

To this end, the last years of CASL increased industry engagement with a focus on providing the knowledge and technology transfer to industry to assure codes are, in the words of the CASL Industry Council, “used and useful”. This report contains a wide array of industry applications and high impact and high value use cases developed in conjunction with industry partners. The deployment of VERA has been facilitated by the creation of the VERA Users Group and the issuance of the first commercial software licenses for the nuclear industry. A focused collaboration effort with the Nuclear Regulatory Commission on the use of advanced modeling and simulation tools in a regulatory environment has laid a pathway for the use of VERA in licensing for applications in advanced light water reactors, advanced technology fuels, high-burnup and high-enriched fuels, and plant lifetime extension. VERA support for development and deployment of advanced technology will be the legacy of CASL for the nuclear industry moving forward.

To date, CASL has simulated 170 operating fuel cycles across 28 reactors representing the full spectrum of Pressurized Water Reactors (PWRs) and operating fuel designs within the US nuclear fleet. Noteworthy, is that VERA is being used not only as a benchmark tool for previous cycles of operation but as a reference solution in the mode of making highly accurate ‘blind predictions’ (the goal standard for all predictive simulation), including the startup of Watts Bar 2 and the first four AP1000® units in China. By all performance metrics, CASL can be considered a success.

As CASL Director and former Chief Scientist, I continue to be impressed by the strength and breadth of technical talent with whom I have had the pleasure of working across the DOE laboratory complex, universities, and industry. I would like to thank the hundreds of scientists, engineers, software developers, and nuclear analysts who have contributed to the success of CASL and the VERA code suite.

The management and technical leadership teams within CASL over the history of the hub have been outstanding. Led by former CASL Directors Doug Kothe and Jess Gehin and Chief Scientist Paul Turinsky, the CASL hub from its early days of inception through the Phase II renewal established an organization and CASL culture of technical excellence and accountability that maintained focused on delivery of the CASL mission. Ascending to leadership within CASL I was greatly aided by their knowledge, mentorship and advice that allowed for seamless transition of the CASL program from research and development towards deployment. During this pivot, I was was greatly aided by Scott Palmtag who took on the new role of Chief Technologist and Jason Hales as Deputy Director to deliver the CASL end state vision.

I also recognize the CASL Board of Directors, chaired most recently by former DOE Deputy Assistant Secretary and NRC Commissioner Dr. Pete Lyons, who provided invaluable advice on CASL activities. I also extend my thanks to the CASL Science Council, chaired by Dr. Bill Oberkampf, provided continous feedback which was particularly important during the final years of CASL that resulted in a mature VERA product. Finally, I acknowledge the CASL Industry Council, led by IC Chair Bob St. Clair of Duke Energy and IC Executive Director Erik Mader of EPRI, whose ongoing efforts have helped assure a VERA end product that can and will be adopted by industry as well as the standing up of the VERA Users Group.

It is also important to recognize the strong support CASL received from DOE NE that included Shane Johnson, former Deputy Assistant Secretary for Reactor Fleet and Advanced Reactor Deployment (NE-5), Alice Caponiti (NE-5), and CASL program managers that included Alex Larzelere, Tansel Selekler, Dan Funk ,and most recently, Dave Henderson. In addition, I would like to recognize the strong efforts by the NRC to deliver on the CASL and NRC collaboration, including the leadership team of Ray Furstenuau, Mike Case, Kim Webber within NRC Research, Senior Advisor Cynthia Jones, and program manager Lucas Kyriazdis.

Sincerely,

A handwritten signature in black ink that reads "David J. Kropaczek". The signature is written in a cursive, flowing style.

Dr. David J. Kropaczek, Director

The Consortium for Advanced Simulation of Light Water Reactors

Founding Partners

Oak Ridge National Laboratory
 Idaho National Laboratory
 Los Alamos National Laboratory
 Sandia National Laboratory
 University of Michigan
 North Carolina State University
 Massachusetts Institute of Technology
 Electric Power Research Institute
 Tennessee Valley Authority
 Westinghouse Electric Company



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ACRONYMS

AFIR	Autoclave Fetting and Impact Rig
AMA	Advanced Modeling Applications focus area
ANS	American Nuclear Society
AOO	anticipated operational occurrences
ATF	accident-tolerant fuel
BOD	Board of Directors
BWR	boiling water reactor
CASL	Consortium for Advanced Simulation of Light Water Reactors
CFD	computational fluid dynamics
CHF	critical heat flux
CILC	crud-induced localized corrosion
CIPS	crud-induced power shift
CRAB	Comprehensive Reactor Analysis Bundle
DNB	Departure from Nucleate Boiling
DOE	US Department of Energy
DPA	displacements per atom
EPRI	Electric Power Research Institute
EXC	ex-core Applications
EWM	engineering wear model
FMC	Fuels Materials and Chemistry focus area
FY	fiscal year
GAIN	Gateway for Innovation in Nuclear
GEN-II	CASL Generation II DNB framework
GTRF	grid-to-rod fretting
HBCU	Historical Black Colleges and Universities
HBU	high burnup fuel
HE	high enriched fuel
HPC	high performance computing
HZP	hot Zero Power
INL	Idaho National Laboratory
LANL	Los Alamos National Laboratory
LOCA	Loss of Coolant Accident
LWR	Light Water Reactor
MIT	Massachusetts Institute of Technology
M&S	Modeling and Simulation
NCSU	North Carolina State University
NEAMS	Nuclear Energy Advanced Modeling and Simulation
NMVG	Non-Mixing Vane Grid
NQA-1	Nuclear Quality Assurance-1 standard

NRC	US Nuclear Regulatory Commission
ORNL	Oak Ridge National Laboratory
PCI	pellet-clad interaction
PCMM	Predictive Code Maturity Model
PHI	Physics Integration focus area
PWR	pressurized water reactor
R&D	research and development
REF	VERA reference calculation
REU	Research Experience for Undergraduates
RIA	Reactivity Insertion Accident
RSICC	Radiation Safety Information Computational Center
RTM	Radiation Transport Methods focus area
SCC	stress corrosion cracking
SLB	steamline break
SNL	Sandia National Laboratory
SMR	Small Modular Reactor
SPERT	Special Power Excursion Reactor Test
THM	Thermal Hydraulics Methods focus area
TVA	Tennessee Valley Authority
UIUC	University of Illinois at Urbana-Champaign
UM	University of Michigan
UTK	University of Tennessee, Knoxville
VERA	Virtual Environment for Reactor Applications
VOCC	Virtual Office, Community and Computing
VVUQ	verification, validation and uncertainty quantification
VUG	VERA Users Group
VVI	Verification and Validation Implementation focus area
WBN1	Watts Bar Nuclear Unit 1
WBN2	Watts Bar Nuclear Unit 2
WEC	Westinghouse Electric Company

PART 1: CASL ENERGY INNOVATION HUB

DOE ENERGY INNOVATION HUB CONCEPT

The Consortium for Advanced Simulation of Light Water Reactors (CASL) was established as one of the Department of Energy's first "Energy Innovation Hubs" that focused on accelerating research to address critical problems in key energy areas. As outlined by U.S. DOE Energy Secretary Steven Chu in 2010, the Hub concept is based on "multi-disciplinary, highly collaborative teams ideally working under one roof to solve priority technology challenges" with the goal of taking scientific discovery to technological development and commercial deployment. As stated in 2010 by Undersecretary for Energy and the Environment, Kristina Johnson, the Hubs were designed to "create a research atmosphere with a fierce sense of urgency to deliver solutions."

Modeled on the proactive approach to science management exemplified by the Manhattan Project and AT&T's legendary Bell Laboratories, the characteristics of the DOE Hub model are best defined as outstanding and independent scientific leadership based on a "light" federal touch with a focus on delivering technologies that can change the U.S. "energy game". To aid in this journey, a CASL Board of Directors provided oversight and recommendations on management, planning, and science and technology strategy. Independent technical review and feedback on CASL research and development (R&D) activities was provided by a Science Council, comprised of external experts in each of the technical areas addressed by CASL, and an Industry Council, comprised of key industry stakeholders who provided continuous feedback on the relevancy of CASL activities as well as technology deployment of CASL developed products.

The focus of the CASL Energy Innovation Hub was on advanced modeling and simulation (M&S) to address challenges facing the existing fleet of operating Light Water Reactors (LWRs). The bulk of current operating nuclear power generation in the U.S. was established in earnest in the 1970s and 1980s with many reactors having gone through a first license renewal beyond their original 40-year lifetime. During this same period, the operating performance of the existing fleet has continued to improve with increased availability, increased capacity factor, especially through power uprates, and continued safety improvements. In 2020, nuclear generation, even with recent plant retirements, contributes >20% to the nation's energy mix. The CASL mission to "provide leading edge modeling and simulation capabilities to improve the performance of currently operating LWRs" would address not only existing challenges to the existing fleet but would lay the groundwork for the next generation of advanced reactors.



Figure 1. Former DOE Energy Secretary Steven Chu

CASL VISION

The CASL vision, established in 2010, was:

To predict with confidence the performance and assured safety of nuclear reactors, through comprehensive, science-based modeling and simulation technology deployed and applied broadly by the United States nuclear energy industry.

This vision has remained constant over the entire ten years of CASL. To achieve this vision, CASL adopted overarching goals to:

- Promote an enhanced scientific basis and understanding of reactor operations by replacing design and analysis tools that are based on limited experimental data with more robust science-based predictive capabilities;
- Develop a highly integrated multiphysics M&S environment based on high-fidelity tools;
- Incorporate uncertainty quantification into the M&S environment development process;
- Educate today's industry professionals in the use of advanced M&S tools through direct engagement in CASL activities, and develop the next generation of engineers through use of appropriate curricula at partner universities; and
- Engage the US Nuclear Regulatory Commission (NRC) to help facilitate eventual industry use of the CASL tools to support licensing.

Phase I of CASL focused primarily on challenge problems facing Pressurized Water Reactors (PWRs) that comprise 2/3 of U.S. operating nuclear reactors. This focus drove the scientific understanding and simulation capability development for a broad range of multiphysics phenomena encompassed by the Virtual Environment for Reactor Analysis (VERA). In testimony to the Senate Energy & Water Development Hearing on the Future of Nuclear Power on September 14, 2016, former U.S. Secretary of Energy Ernest Moniz (Figure 2) noted "We have been successful in improving modeling and simulation to enhance the performance of currently operating light water reactors through the Consortium for Advanced Simulation of Light Water Reactors (CASL), one of the Department's Energy Innovation Hubs, and a program I was honored to serve as the Chairman of the Board for its first two years."

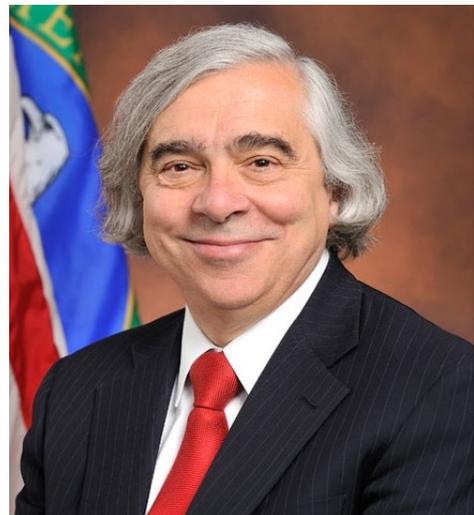


Figure 2. Former DOE Energy Secretary Ernest Moniz

Phase II of CASL focused on finalizing development and deployment of CASL tools for PWR analysis and extending the program's tools for use in Small Modular Reactor (SMR) operation and Boiling Water Reactor (BWR) analysis. In February 2018, the CASL program was authorized to receive additional funds to focus on the use of advanced modeling and

simulation tools in a regulatory environment which brought the NRC in as a collaborator on VERA development.

STRATEGIC PARTNERSHIPS

The success of the CASL program was driven by the unique partnerships developed among world-class experts in science and engineering drawn from across the nuclear industry, national laboratories, and academia under a “one roof” collaboration model that enabled a coordinated attack on challenge problems facing the nuclear industry. During its lifetime, CASL engaged hundreds of collaborators on a yearly basis that included physical scientists, nuclear analysts and engineers, applied mathematicians, and software developers, all working together to advance the state-of-the-art in advanced M&S capabilities and tools. This focus on solving specific problems provided a “line of sight” from the efforts of individual contributors to the broader program goals that drove technology deployment for the benefit of the US nuclear industry.

To accommodate the hundreds of geographically distributed hub contributors, CASL implemented unprecedented tools for physical and virtual collaboration. The Virtual Office, Community and Computing (VOCC) laboratory, established at Oak Ridge National Laboratory (ORNL), consisted of unique computing and telecommuting infrastructure that promoted seamless collaboration and critical thinking. VOCC interactive immersive visualization environments (Figure 3) fostered a deeper insight and understanding into the CASL challenge problems enabling technology innovation to rapidly proceed.



Figure 3. CASL VOCC Immersive Visualization Cave

CASL was built upon the strength of ten founding partner organizations with support from a wide breadth of additional contributing partners from industry, government laboratories, and academia. ORNL, the lead CASL institution was founded to develop the world’s first nuclear fuel cycle and today is DOE’s largest science and energy laboratory. ORNL has world-leading capabilities in computing and computational science and substantial programs and resource in nuclear energy research and development (R&D), as well as a record of accomplishment in leading large-scale scientific collaborations.

Idaho National Laboratory, Los Alamos National Laboratory, and Sandia National Laboratories provided exceptional strengths and broad expertise in the areas of nuclear energy, physical sciences, applied mathematics, transformational high-performance computing, and algorithm development for the solution of complex problems. Academic partners North Carolina State University (NCSU), the University of Michigan (UM), and the Massachusetts Institute of Technology (MIT) are leaders in nuclear engineering R&D and education.

CASL industry partners included Westinghouse Electric Company (WEC), a founder and world leader in commercial nuclear energy, Tennessee Valley Authority (TVA), one of the leading nuclear utilities in the U.S. with 7 operating reactors (including the Watts Bar Units

1 and 2 reactors), and the Electric Power Research Institute (EPRI), a leading research organization that works closely with the U.S. nuclear industry to identify and address issues and technology gaps through collaborative R&D programs.

CASL additionally leveraged a broad range of industry and science advisors through implementation of an independent Industry Council and Science Council to review and advise on the relevance and quality of CASL R&D activities. The mission of the Industry Council was to ensure that CASL capabilities and tools were “used and useful” to the nuclear industry. As shown in Figure 4, the CASL industry council represented the full breadth of nuclear industry stakeholders include nuclear utilities, fuel and nuclear hardware vendors, engineering design, service and research organizations, independent providers of software analysis



Figure 4. CASL Industry Council member organizations

tools. Ex-officio members of the CASL industry council included the CASL Board of Directors and DOE. The CASL industry included both domestic and international members who represent key organizations important to the sustainability of the current operating fleet and future nuclear builds.

The CASL Science Council was comprised of internationally recognized experts in nuclear modeling and simulation and provided feedback on R&D in each of the key CASL technical areas. This included such areas as fuel performance, thermal-hydraulics, nuclear data, radiation transport, chemistry, multiphysics integration, verification, validation and uncertainty quantification, and high performance computing (HPC). The Science Council was a key source of critical feedback for CASL technical activities and provided objective, independent oversight to the technical focus areas. The CASL Industry and Science Councils met semiannually with one meeting held independently and one held as a joint meeting between the two groups (Figure 5). The joint meeting allowed feedback received from each council to be considered in the context of both relevancy and technical output quality. Individual Science Council members also met yearly with their respective focus areas to provide feedback on annual budget and technical milestone planning.

The CASL Board of Directors (BOD) consisted of representatives of the executive leadership of the CASL founding partners as well as multiple internationally recognized leaders in R&D, industry, or government with extraordinary records of achievement. The CASL BOD served as both an advisory and oversight body for the ORNL Laboratory Director and the CASL senior leadership team on issues related to management, performance, strategic direction, and institutional interfaces within CASL. The BOD worked to ensure the execution of CASL operational and R&D plans provide maximum benefit to

key stakeholders, such as DOE and the CASL Industry Council. The CASL BOD met monthly which allowed emerging issues to be addressed in a timely manner.



Figure 5. Joint CASL Industry and Science Council Meeting – Oak Ridge National Laboratory, October 2016

CASL MANAGEMENT AND ORGANIZATION

CASL implemented several effective management strategies that evolved during the tenure of CASL to address emerging issues as they arose as well as maintain an agile organization focused on the execution of the CASL mission. In addition to the oversight provided by the Industry and Science Councils as well as CASL Board of Directors, CASL had an integrated Senior Leadership Team (SLT) that consisted of the CASL Director, with full line authority and accountability for all CASL activities, a Deputy Director, to drive program planning, performance and assessment, and CASL Chief Scientist (and later Chief Technologist) to drive the science, applied research, and technology deployment. The SLT was supported by R&D focus areas responsible for the core science and engineering elements that evolved over time that were each led by a focus area lead and deputy and CASL challenge problem integrators. This evolution of the focus areas occurred as the CASL technical activities moved from basic science and research, to applied research and engineering, and finally to technology deployment.

Utilizing a virtual one-roof approach enabled by the VOCC, integrated project management allowed for well-informed and timely decision-making, integrated planning and tracking of milestone scope, schedule and budget. Because CASL had a known and fixed budget, a multi-year strategy could be formulated and executed. Critical to the success of the CASL organization was maintaining a line of sight with an eye towards solving the challenge problems and remaining agile with respect to course corrections on R&D activities. Motivation of the CASL team was especially important given the high level of focus and evolving requirements, which required everchanging skill sets in the CASL program. To this end, recognition of key CASL contributors was made through focus area leadership opportunities (as they became available) and direct awards (i.e. CASL Knight and Directors Awards).

EDUCATING THE NEXT GENERATION OF NUCLEAR PROFESSIONALS

The mission of the CASL Education Program was the education of the next generation of LWR designers, scientists and nuclear power professionals. The objectives of the program were to ensure that CASL results and technology are integrated into university undergraduate and graduate course curricula and to encourage the transfer of CASL technologies to industry users. Activities that supported these goals included:

- CASL Undergraduate Research Scholars program,
- Summer internships at CASL partner laboratories,
- CASL Summer Research Experience for Undergraduates (REU),
- Development of new courses at participating universities, and
- CASL Institute / Certificate Program

The CASL Undergraduate Research Scholars program matched top students with CASL faculty mentors to engage in CASL research projects during the academic year. Nearly half of the 40 CASL scholars over the hub period attended graduate school to continue their research. During the summers, CASL supported a suite of summer internships at ORNL and other CASL partner laboratories (LANL, SNL, and INL). Students participating in summer internships were directly mentored by CASL researchers, providing a unique educational experience connected directly to ongoing CASL activities and inspiring many to students complete advanced degrees.



Figure 6. CASL REU Presentation
NC State University, 2018

The CASL Summer Research Experience for Undergraduates provided an additional opportunity for top students from Historically Black Colleges and Universities (HBCU) to engage in CASL research activities with CASL faculty mentors and present their work to a broad audience (Figure 6). Several HBCU students sponsored by CASL have gone on to pursue Ph.D. degrees.

The CASL Institute is a two-week in-depth, hands-on course for faculty, graduate students and engineering professionals with an interest in CASL research and the application of CASL tools for the solution of practical nuclear industry problems. The Institute introduced

participants to CASL, the VERA framework and component physics packages. Upon completion of the course and a team project, students earn the CASL-VERA Certificate which also qualifies for credit for the Professional Engineering continuation education. The CASL Institute has been held four times, twice at ORNL and twice at NC State University, and provided students with modern HPC resources within a hosted environment.



Figure 7. First CASL Institute - Oak Ridge National Laboratory, Summer 2016

With its various initiatives, the CASL Education Program has served 289 undergraduate students, graduate students and industry shareholders from 31 institutions since its inception.

PART 2. VIRTUAL ENVIRONMENT FOR REACTOR APPLICATIONS

The Virtual Environment Environment for Reactor Applications (VERA) represents the cutting edge in nuclear reactor modeling and simulation and can be used to solve a variety of reactor performance challenges through the modeling of multiphysics phenomena. VERA integrates within a single environment the relevant physics of nuclear reactors including neutronics (neutron and gamma transport), thermal-hydraulics, fuel performance and chemistry on a detailed fuel rod-by-rod basis that allow for modeling of complex reactor behavior. VERA integrates physics components based on science-based models, state-of-the-art numerical methods, and modern computational science. The VERA models are verified and validated using data from operating reactors, single-effects experiments, and integral tests. VERA’s high fidelity, high resolution coupled solutions provide an accurate representation of the reactor’s behavior and feedback mechanisms and is being used to quantitatively advance understanding beyond existing industry methods. VERA was recognized as an R&D100 Award recipient in 2016 [1] for its innovation in the field of advanced modeling and simulation.

VERA EXISTING CAPABILITIES AND CODE SUITE

VERA is optimized for efficient execution on multiple platforms, including leadership-class computers, advanced architecture platforms now under development, and industrial engineering workstation clusters. Figure 8 displays the components of the VERA code suite along with the external interfaces to codes that support VERA research and provide interoperability reactor systems codes [2].

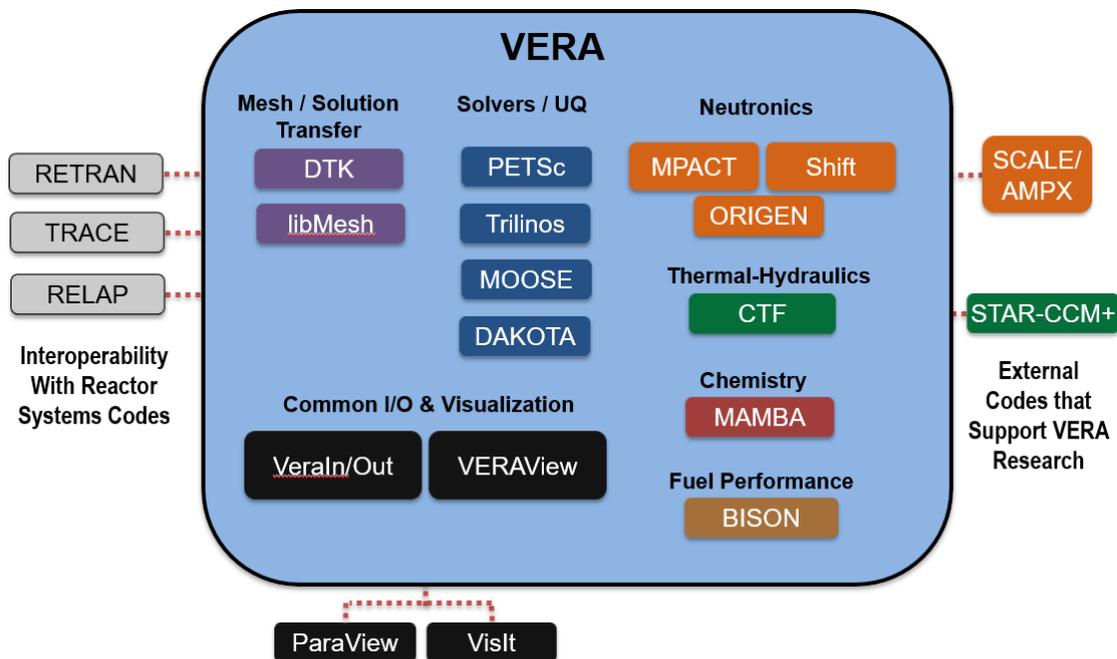


Figure 8. VERA Code Suite

The VERA code suite was developed to model in high fidelity the behavior of LWRs for the purpose of solving challenge problems for the existing nuclear operating fleet. Such challenge problems cover a broad range of issues related to reactor operations (crud, pellet-clad-interaction) and licensing (loss of coolant accident, reactivity insertion accident,

departure from nucleate boiling). From a modeling perspective, this required a deeper understanding of the physics relevant to each problem (i.e. neutronics, fuel performance, thermal-hydraulics, chemistry) as well as an understanding of the interaction between physics, often considered separately in reactor analysis. VERA solves all physics fully resolved with multi-physics coupling which captures the interdependencies among physics phenomena what would traditionally be handled as boundary conditions to single physics codes. For example, fuel rod simulation requires knowledge of the bulk fluid density and neutronic power. Similarly, the thermal-hydraulic density calculations require knowledge of the fuel rod surface heat flux and neutronic direct gamma energy deposition in the coolant. Neutronic feedback depends on detailed knowledge of all number densities and temperature as relates to nuclear cross sections which depends on the fuel, thermal-hydraulic, and chemistry (i.e. crud) simulation. VERA resolves all physics implicitly in a consistent manner, allowing for high fidelity and physics resolved solutions to be achieved.

The original focus of VERA was on the reactor core which is comprised of the fuel rods, burnable absorbers, control rods, detectors, assemblies, coolant and support structures. This has enabled a large range of applications that includes core design, core follow, operations, and transient licensing applications. More recently, VERA has incorporated the Shift code for performing ex-core calculations (i.e. neutron dose beyond the core) that has expanded the range of VERA capability to include vessel fluence analysis, core structural component lifetime analysis, and analyses involving ex-core signals (secondary source and core shuffle simulations).

VERA has been well-validated against a broad range of reactors types, core sizes, lattices and burnable designs within the PWR operating fleet. This represents approximately 65% of the US operating fleet. For BWRs, representing the remainder of the US operating fleet, VERA continues to be developed including modeling enhancements to address high core void conditions characteristic of BWR behavior.

The primary codes within VERA are now described.

NEUTRONICS

The MPACT code [3] is designed to perform high-fidelity LWR analysis using whole-core pin-resolved neutron transport calculations on modern parallel-computing hardware. This is accomplished by solving the integral form of the Boltzmann transport equation for the heterogeneous reactor problem in which the detailed geometrical configuration of fuel components, such as the pellet and cladding, are explicitly retained. The cross section data needed for the neutron transport calculation are obtained directly from a 51 energy group cross section library, which has traditionally been used by lattice physics codes to generate few-group homogenized cross sections for nodal core simulators. Hence, MPACT involves neither *a priori* homogenization nor group condensation for the full core spatial solution. The code consists of several modules which provide the functionality necessary to solve steady-state eigenvalue problems. Several transport capabilities are available within MPACT including both 2-D and 3-D Method of Characteristics. A three-dimensional whole core solution based on the 2-D and 1-D solution method provides the capability for full core depletion calculations.

Shift [4] is a continuous energy Monte Carlo radiation transport code for performing high fidelity, high resolution calculations for neutron and gamma transport problems that may be executed as either a fixed source or eigenvalue mode of calculation. The eigenvalue

calculation is used to provide reference solutions for MPACT and is used in the verification of the solver, especially the multigroup energy resolution. The fixed source problem is used in ex-core calculations where the converged MPACT solution provides the neutron sources. VERA ex-core calculations are used for solution of deep-penetration problems in reactor structural materials, detector responses, and dose calculations for irradiation measurements. Shift includes use of a deterministic transport method (adjoint) for improving the efficiency of ex-core transport calculations.

ORIGEN [5] is an isotope generation and depletion code that solves the nuclear transmutation equations with a matrix exponential. ORIGEN integrates seamlessly with the MPACT flux calculation and calculates time-dependent concentrations, activities, and radiation source terms for a large number of isotopes simultaneously generated or depleted by neutron transmutation, fission, and radioactive decay. ORIGEN tracks hundreds of isotopes within VERA on a sub rod-by-rod basis as a means of capturing the fuel depletion effects with core exposure which are fed back through material composition changes.

THERMAL-HYDRAULICS

CTF [6] is a modernized version of the time-dependent, thermal-hydraulics subchannel code COBRA-TF that was originally developed in the early 1980s at Pacific Northwest National Laboratory. CTF uses a two-fluid, three field modeling approach (fluid film, fluid drops and vapor) for modeling fluid flow and heat transfer. CTF includes a wide range of flow-regime dependent closure models for capturing complex two-phase flow behavior, which includes rod-to-fluid heat transfer, interphase heat and mass transfer, wall and interphase drag, turbulent mixing and void drift, grid droplet breakup, and grid heat transfer enhancement effects. CTF can accurately simulate flow distributions including cross-flow effects from turbulent mixing and lateral pressure gradients caused by power distributions or mechanical design differences within assemblies and within a reactor core.

CTF also solves the time-dependent heat conduction in the fuel for the fuel temperature, with explicit meshing of the fuel pellet and gap, and surface heat flux which is resolved implicitly with the two-phase flow solution. CTF is coupled to MPACT through the volumetric heat source of the fuel and provides accurate local fuel temperatures, density and void distributions which are used in the cross section feedback. Such feedback can affect the local flux spectrum, and subsequently local cross sections, which determines the accurate prediction of local pin powers.

FUEL PERFORMANCE

BISON [7] is a finite element-based nuclear fuel performance code applicable to a variety of fuel forms including light water reactor fuel rods, TRISO particle fuel, and metallic rod and plate fuel. It solves the fully-coupled equations of thermo-mechanics and species diffusion, for 1-D spherical, 1-D layered, 2-D axisymmetric, 2-D plane strain, or 3-D geometries. Fuel models are included to describe temperature and burnup dependent thermal properties, fission product swelling, densification, thermal and irradiation creep, fracture, and fission gas production and release. Plasticity, irradiation growth, and thermal and irradiation creep models are implemented for clad materials. Models are also available to simulate gap heat transfer, mechanical contact, and the evolution of the gap/plenum pressure with plenum volume, gas temperature, and fission gas addition. BISON includes models for UO₂ irradiation fuel behavior (e.g., thermal conductivity degradation), Zircaloy cladding behavior (e.g., cladding creep), and gap behavior (e.g., reduced conductance due to fission gas release). BISON is used to assess the thermomechanical behavior of the fuel as a function

of irradiation history and has one-way coupling to MPACT via the volumetric heat source of the fuel and CTF bulk fluid conditions.

CHEMISTRY

MAMBA [8] simulates the time-dependent, three-dimensional crud growth along the surface of each fuel rod in the reactor. MAMBA is used to perform crud and accompanying boron precipitation calculations which have been shown to be a factor in both fuel rod mechanical performance, through crud induced localized corrosion, and reactor operations, through crud induced power shift. MAMBA is coupled to CTF through the fuel surface heat flux and bulk fluid conditions which are boundary conditions to the crud growth and erosion calculation. In turn, MAMBA provides feedback to CTF through conductivity changes due to the crud layer and feedback to MPACT through the localized boron deposition.

PART 3: NUCLEAR INDUSTRY PERFORMANCE CHALLENGES

The nuclear industry employs a variety of science and engineering analysis techniques to understand and predict the performance of materials, components and subsystems involved in the diverse aspects of electric power generation. These analysis techniques, originating as far back as the 1960s and 1970s, have evolved over the past several decades as analytical methods have advanced and have been validated against experimental data from test reactors, commercial power reactors and unirradiated test loops.

Traditional industry analysis methods, especially for regulatory licensing, are typically based on bounding, conservative assumptions that enables complex, coupled physics simulations to be performed in a simplified manner. Such simplifications have served the industry well in supporting the safe operation of nuclear reactors and assured the reliable performance of nuclear fuel. However, the drive for more economical operation of nuclear power plants is often limited by such conservative analysis when it comes to increased capacity factor through power uprate, increased fuel cycle efficiency through higher fuel burnup, reduced maintenance through longer cycle lengths, and lifetime extension. The introduction of high fidelity and fully resolved multiphysics simulation offers a unique opportunity to change the paradigm for M&S, thereby allowing for margin recovery in nuclear analyses based on rigorous verification, validation, and uncertainty quantification (VVUQ).

CHALLENGE PROBLEM OVERVIEW

The CASL challenge problems were the most challenging problems facing the nuclear industry for which an advanced modeling and simulation capability could be applied. The challenge problems addressed issues in reactor operation, fuel management, licensing, and materials performance. These issues have a high economic impact on fuel cycle costs, capacity factors, and plant lifetimes where the opportunity in terms of reduced costs and increased revenue are in the hundreds of millions of dollars.

CASL focused on several key performance challenges over the period of the Hub with each challenge problem describing a particular issue and relevant set of phenomena of important to its understanding and solution (Figure 9). Three of the challenge problems relate to postulated accident scenarios (i.e. reactivity insertion accident (RIA), loss of coolant accident (LOCA), and departure from nucleate boiling (DNB)) while the other three relate to normal operations. Pellet-clad interaction (PCI), for example, may occur during operational maneuvers and is a particular concern for load follow operation. Grid-to-rod fretting (GTRF) is an issue with fuel that arises due to fuel excitation that may occur within reactor core coolant flow fields. Crud is the buildup of deposits on the fuel surface which can lead to fuel failure due to crud-induced localized corrosion (CILC). In addition, the presence of crud may result in a phenomena known as crud-induced power shift (CIPS) due to absorption of boron from the coolant into the crud layer. Because boron is a reactivity poison this has an effect similar to that of a control rod insertion, CIPS creates unanticipated power swings that can lead to violation of operating limits and forced derate during operations.

Each of the challenge problems requires detailed multiphysics and rod-by-rod detail to accurately model the reactor behavior. The multiphysics describes the tightly coupled interaction of different single physics models such as fuel and cladding performance, thermal-hydraulics, neutronics, and chemistry. Important to note is that the same single physics models apply to several of the challenge problems. For example, neutronics and

thermal-hydraulics is required for all of the challenge problems while fuel and clad performance is critical to all challenge problems involving fuel failures.

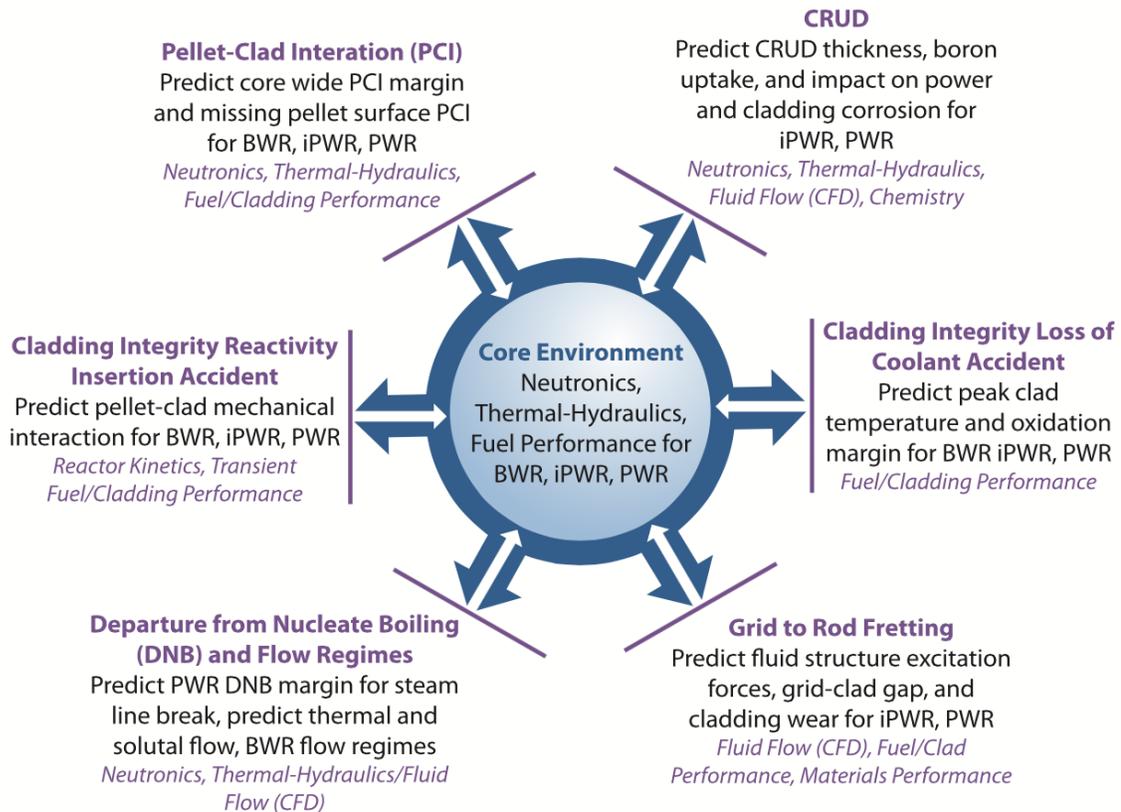


Figure 9. CASL Challenge Problems

CASL technical activities were divided into six focus areas with the mission to perform the fundamental research, software development, and applications required to drive the capability development within the VERA code suite and address the CASL challenge problems. The focus areas included:

- Advanced Modeling Applications (AMA) - responsible for the application of VERA to industry-focused problems, including challenge problems, test stands, and applications demonstration. AMA coordinated with the other focus areas on requirements for VERA capabilities while serving as the bridge to the nuclear industry end users.
- Physics Integration (PHI) - responsible for multiphysics coupling and software integration of the single physics models and codes (MPACT, Shift, ORIGEN, CTF, BISON and MAMBA) developed within CASL within a unified software framework. PHI also had responsibility for the CTF subchannel code development. PHI collaborated with the other focus areas to deliver usable tools for performing analyses guided by the functional requirements for the CASL challenge problems.
- Radiation Transport Methods (RTM) - responsible MPACT, Shift and ORIGEN neutronics modeling capabilities for neutron transport, fission and depletion within the reactor fuel and core. RTM activities included development of 3-D radiation transport models, nuclear data libraries and spatial kinetics methods, including delayed neutrons and isotopic depletion and decay.

- Fuels Materials and Chemistry (FMC) – responsible for BISON and MAMBA materials performance models for fuel, cladding, and fuel assembly structural materials as well as the clad surface chemistry, especially the deposition of species transported in the primary coolant. FMC activities included development of the fundamental models for fuel and clad evolution, fission gas release, and crud growth with boron uptake.
- Thermal Hydraulics Methods (THM) - responsible for thermal-hydraulic modeling capabilities for computational fluid dynamics (CFD) with a focus on the development of single and two-phase closure relationships. This included integrations within the STAR-CCM+ code with applications to critical heat flux (CHF) and BWR high pressure, high void flow predictions. THM supported the CTF subchannel code development through high-fidelity CFD simulations of two-phase flow which informed development of CTF phenomenological models, such as turbulent kinetic energy, needed for the crud challenge problem.
- Verification and Validation Implementation (VVI) – responsible for the development, and execution of VVUQ activities for the VERA software. VVI activities included development of the VERA predictive code maturity model (PCMM) and its application for continuous assessment of VERA maturity with respect to solution of the challenge problems.

Within CASL, the focus on challenge problems drove capability development that enabled the solution of many problems and new applications of CASL tools that were not explicitly defined at the outset of the program. A prime example is the use of VERA for performing ex-core analysis for fluence which is important to reactor lifetime extension. This application arose out of neutronic capability development. Another example is the development of CASL tools and capabilities for accident tolerant fuel (ATF). Furthermore, while the challenge problems primarily focused on PWRs analogous issues exist for BWRs. Thus, CASL tools and capabilities will continue to have broad applicability across a range of new LWR challenge problems as they arise.

CRUD CHALLENGE PROBLEM

The top challenge problem within CASL has been and remains a solution for crud, the growth of deposits on fuel rod surfaces, which manifests as either crud-induced localized corrosion (CILC) or crud-induced power shift (CIPS) during the reactor fuel cycle of operation. CIPS results from the precipitation of lithium tetraborate within the crud layer and can dramatically affect the axial power distribution to the point of plant derate and violation of thermal margins. Conservative bounding analyses to prevent formation of crud have resulted in reduced thermal limits (i.e. less steaming rates) which increases fuel cycle costs through a need to flatten the core power distribution (i.e. loading more fresh fuel assemblies). Such bounding analyses are based on 30 years of operating experience, empirical and scale test measurement data, and coarse mesh single physics thermal-hydraulic and crud growth models that have been extensively tuned based on the operating fleet performance. An accurate determination of crud margin has the direct benefit of reducing fuel cycle costs.

VERA provides a solution for crud that involves modeling in high fidelity the complex multiphysics phenomena related to crud that includes high resolution modeling of: 1) crud

growth and boron uptake within the crud layer, 2) neutronic impact of boron on the local and global axial power shape, 3) the depletion of boron in the crud layer, and 4) thermal-hydraulic subcooled boiling and the impact of crud growth and erosion due to fuel mixing vanes. The VERA code suite models crud growth needed for CILC and CIPS on a rod-by-rod basis with the 3-D simulation of crud profile as well as the boron uptake within the crud layers. This provides unprecedented detail assessment of crud growth and crud boron behavior as well as the local and global impacts of crud growth on power and subcooled boiling. CASL R&D activities related to crud are detailed in the report “CASL Research and Development Activities and Results for the CIPS challenge problem [9]

An advanced (CILC) screening capability [10] has been developed within VERA that allows for detailed evaluation of the local fuel corrosion evolution during the fuel cycle. The work focused on the development and implementation of advanced models for crud buildup coupled with higher resolution CFD informed thermal-hydraulic detail. This first-of-a-kind capability allows the capture of fuel rod azimuthal flow effects due to grids and spacers on corrosion. Figure 10 displays the results for CILC analysis performed for the Seabrook nuclear power plant for Cycle 5. Shown are the rod-by-rod maximum calculated corrosion thickness at each axial level within the reactor core.

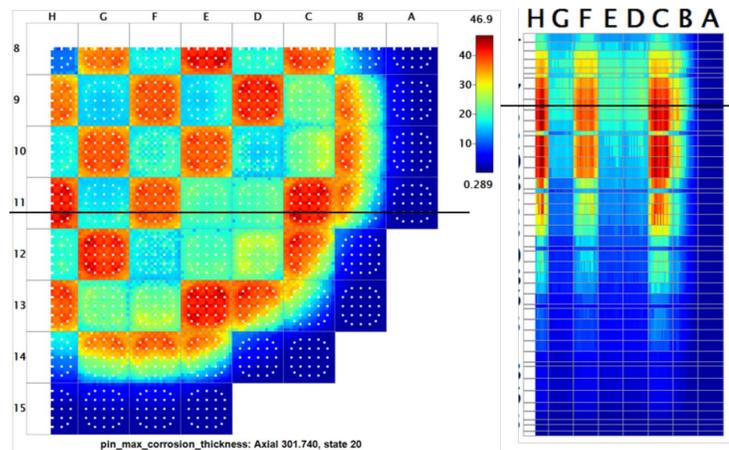


Figure 10. VERA Seabrook Cycle 5 distribution of maximum corrosion thickness

A challenge of modeling crud at the level of detail provided by VERA is the lack of data “at power” within operating reactors, the sparsity and quality of data that does exist (i.e. crud scrape data), and the applicability of measured data obtained within crud test facilities to operating reactor conditions. For example, the solubility of boron, which impacts the uptake of boron in the crud layer, makes measurement in the lab extremely difficult. To this end a significant effort has been put forth using formal calibration methods whereby unknown crud parameters are inferred based on at power, integral measurements (i.e. flux maps). These formal calibration methods, including the establishment of uncertainty bounds on calibrated parameters, are a necessity for accurate prediction of crud. Methodologies developed for crud calibration within CASL have been developed and demonstrated in the report “Inference of Crud Model Parameters from Plant Data” [11]. A particular challenge, is that conservative operation over the past decades means that many plants that are susceptible to CIPS have not experienced CIPS in recent years. Thus, the calibration of crud utilizing individual plant data necessarily includes a significant portion of data which shows little to no crud effect. Also, given the nature of calibration it is equally important to not only predict the onset of CIPS but also to not predict crud were none exists (the dominant, null scenario). The calibration methodology accounts for both scenarios.

The calibratable parameters for crud include those that are plant independent (fundamental to the crud kinetics) and those that are plant specific (the iron and nickel particulate source term). The source term depends on mass balances performed for the reactor system of

interest, component lifetime, water chemistry management, and fuel cleaning performed between fuel cycles. A generic source term simply does not exist although similar source term behavior would be expected to be similar for plants within the same class (e.g. Westinghouse 4-Loop PWR). Because prediction of crud for a given plant highly depends on understanding the source term, working with users and utilities to establish the source term for specific reactors is extremely important to fully realize the benefits of VERA to industry for crud applications.

Having established a source term and benchmarked VERA against previous cycles of operation, VERA has been shown to be a usable for identifying core locations susceptible to CIPS and using VERA to perform core redesign to mitigate the impact of crud. During cycle operation, crud appears first in locations where local steaming is high due to higher local power, usually occurring in fresh fuel. As the cycle progresses, burnable poisons deplete and can increase power locally in other locations, thus producing additional high local steaming and hence, more crud. However, the soluble boron also plays a role and maintaining a lower boron for control can reduce the boron uptake in the crud layer. All these factors can be mitigated by design.

DEPARTURE FROM NUCLEATE BOILING CHALLENGE PROBLEM

DNB and CHF represent a boiling crisis during reactor operation that causes a sharp rise in clad surface temperature due to localized vapor generation at the clad surface and degraded heat transfer. DNB can lead directly to fuel failure. Understanding of DNB is important not only for normal operations but anticipated operational occurrences (AOOs) as well as accident scenarios. The mechanisms for DNB are quite complex and rely on large-scale measurement and empirical correlation for its prediction, which can be quite expensive and can hinder new fuel product designs.

The DNB challenge problem focused on developing, demonstrating, and assessing advanced computational fluid dynamics (CFD) based capability for the prediction of two-phase flow and DNB in PWR fuel. The prediction of DNB within CFD is highly dependent on the physical modeling of mechanisms for vapor generation and bubble hydrodynamic behavior that are encompassed by CFD closure relations. Examples of such closure relations developed within CASL include new models for heat flux partitioning, lateral void redistribution, near wall bubble interaction effects, and bubble induced turbulence. A key aspect of this work is the development of improved wall heat partitioning models and closure relations for dispersed vapor phase interaction with the liquid carrier phase.

The CASL two-phase, CFD model is an advanced first-principle based formulation for two-phase flow phenomena which includes the CASL delivery of new experimental data to deliver and assess its formulation. The resultant closure models were brought together within the CASL Generation II DNB (GEN-II) framework [12] that formed the basis for validation activities against measured PWR assembly test data for critical heat flux. As shown in Figure 11, the CASL strategy for closure development utilized data generated from high resolution direct numerical simulation as well as high resolution, two-phase flow experimental data.

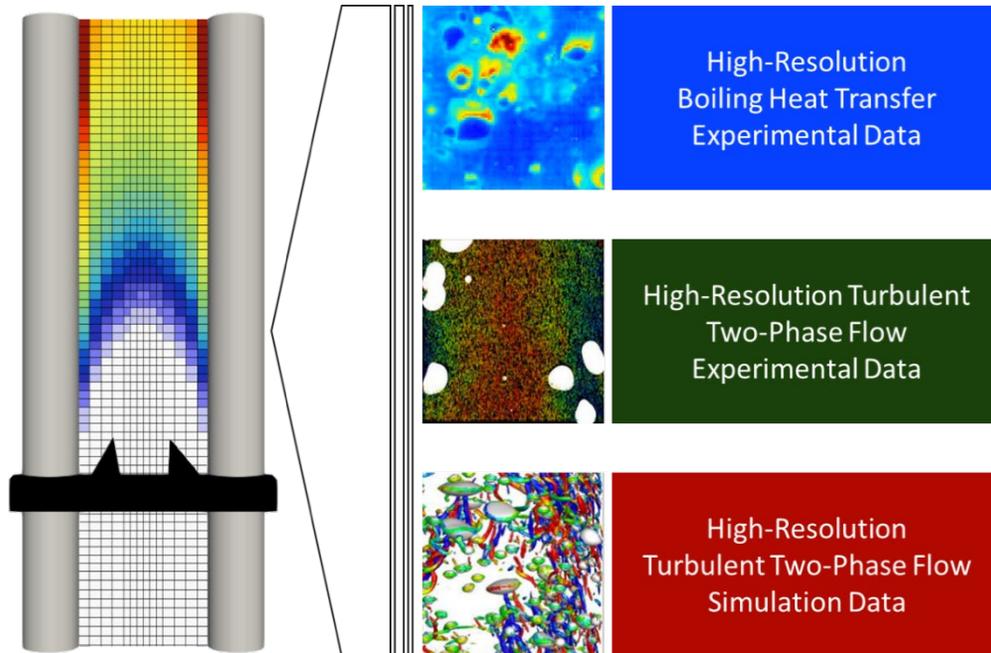


Figure 11. CASL strategy for closure development was based on the use of high fidelity, direct numerical simulation combined with high resolution two-phase flow experimental data

This included:

- High resolution experiments with varying surface characteristics for DNB model development
- Completion and assessment of closure models for GEN-II Heat Partitioning representation
- Advancement and assessment of GEN-II method to include surface effects.

The results demonstrate a fundamental advancement in CFD two-phase flow M&S with the ability to include the effect of surface characteristics on the boiling predictions from first principle bases. Validation of CFD predicted critical heat flux results for non-mixing vane grid (NMVG) and mixing vane grid (MVG) spacers demonstrate significant progress toward a fully predictive DNB capability. Figure 12 shows the CFD prediction of DNB for the full-scale CHF tests. The PWR test assembly (5x5, NMVG) with each measurement corresponds to the condition of critical heat flux (CHF). The ability to

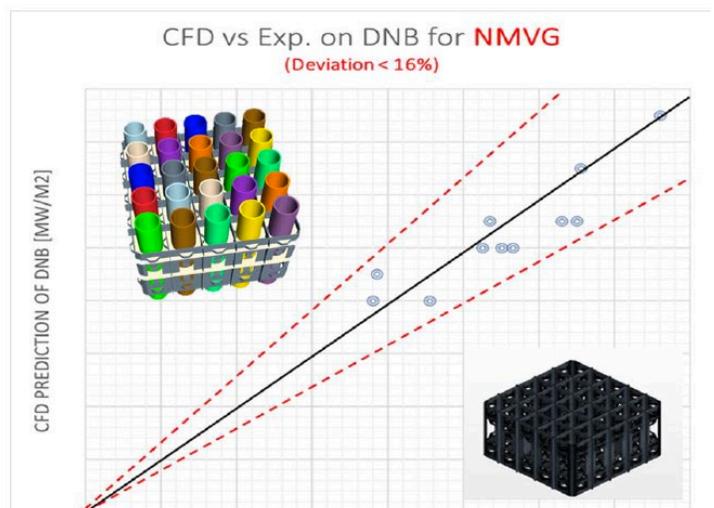


Figure 12. Two-phase flow CFD prediction of DNB against full-scale CHF tests

predict rod surface effects within two-phase CFD will allow for modeling of rod aging as well as ATF fuel concepts.

REACTIVITY INSERTION ACCIDENT CHALLENGE PROBLEM

RIA as a challenge problem arose from the need for the nuclear industry to address an emerging regulatory issue regarding the effect of high fuel burnup and its effect on degraded fuel and cladding performance. In 2016, the NRC issued the draft regulatory guide DG-1327, “PWR control rod Ejection and BWR control rod drop accidents,” [13] that established acceptable fuel cladding failure thresholds for ductile failure, brittle failure, and pellet-clad mechanical interaction (PCMI) during RIA events (in addition to radionuclide release fractions for use in assessing radiological consequences).

The VERA code suite includes transient, 3D, multiphysics modeling capabilities that enable higher fidelity for RIA than is currently used by the industry in NRC-approved codes and methodologies. The validation of VERA with respect to RIA includes a comprehensive selection of tests from available domestic and international test facilities including the SPERT III transient tests for neutronic validation and the CABRI and NSRR tests for fuel performance validation [14, 15].

A large-scale VERA analysis was performed for the AP1000® with the intent of demonstrating RIA simulation within an industry production environment. The two concerns of RIA are the deposited fuel enthalpy (cal/g) during the transient and the resulting risk of DNB post peak fuel temperature as the energy leaves the fuel and is deposited in the coolant. The analysis considered a real-world problem formulation, including conservative assumptions to maximize the ejected rod worth and deposited energy in the fuel rods of highest burnup. This is consistent with the goal of demonstrating a high-fidelity RIA modeling capability to support the industry resolution of regulatory issues associated with high-burnup fuel as per NRC DG-1327.

The limiting RIA initiating condition for the AP1000® occurs at hot zero power (HZP) with all rods inserted. Figure 13 displays the fuel rod resolved core power distribution at the limiting point of the transient where the fuel is most susceptible to DNB. To analyze the thermomechanical fuel performance, the highest power and burnup fuel rods were selected for detailed analysis based on the transient power history. Fine resolution, 2-D (r-z) axisymmetric modeling using 15 radial and 1000 axial mesh resolution was performed. Figure 14 displays the maximum fuel enthalpy and energy deposition as a function of transient time for the fuel rod with the maximum rod power. Note that the maximum enthalpy occurs just after the rod power peak pulse.

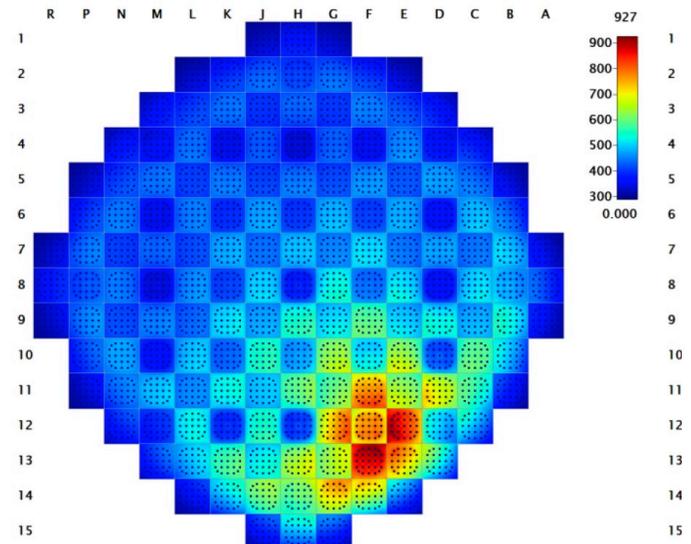


Figure 13. AP1000® detailed RIA power distribution at the limiting DNB condition

The VERA simulations required 25.8 hours of execution time on 6840 processors on the INL Falcon cluster. While computationally intensive, this is nevertheless within reach for industry use. Applications of the CASL RIA modeling and simulation capabilities are expected to be reference calculations, determination of margins to regulatory figures-of-merit, evaluation of RIA test results, providing simulation results to fill gaps in the RIA experimental testing database, and potentially to replace or augment licensing methodologies. The progress to date show that transient licensing applications with VERA are achievable for such applications as ATF fuel.

Industry applications of the CASL RIA M&S capabilities are expected to be implementation in reference calculations, determination of margins to regulatory figures of merit, evaluation of RIA test results, provision of simulation results to fill gaps in the RIA experimental testing database, and potentially replacement or augmentation of licensing methodologies. Current emerging applications for RIA include ATF and high-enriched and high-burnup fuel.

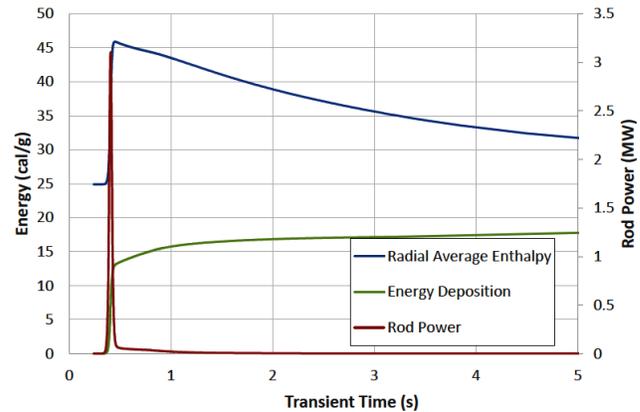


Figure 14. AP1000® RIA fuel rod enthalpy and energy deposition evolution

PELLET-CLAD INTERACTION CHALLENGE PROBLEM

The PCI challenge problem addresses pellet-clad mechanical interaction (PCMI) and stress corrosion cracking (SCC), a chemical effect activated by corrosive fission products, such as Iodine. The mechanisms of PCI which can lead to failure encompasses both SCC and PCMI and their interactions. PCI is a high concern during flexible power operations, also known as loading following events, where rapid power changes during a power maneuver may put undue stress on the fuel. Large local power gradients introduced by control rod insertions may exacerbate the potential for PCI failures.

A detailed description of the capabilities developed for the PCI challenge problem focus primarily on BISON materials and fuel behavior models [16] and included models for fuel swelling and fission gas release, fuel-cladding interface, cladding mechanical behavior and fuel pellet geometrical evolution (fuel pellet cracking and manufacturing defects such as missing pellet surface).

VERA analysis of fuel performance for flexible power operations allows for detailed rod-by-rod analysis performed utilizing coupled core simulation and fuel performance capabilities. VERA capabilities for PCI were demonstrated through analyses for Watts Bar Nuclear Unit 1 (WBN-1) Cycles 6 and 7 that included fuel cladding failures that, at the time, were believed to have been caused by PCI (Figure 15).

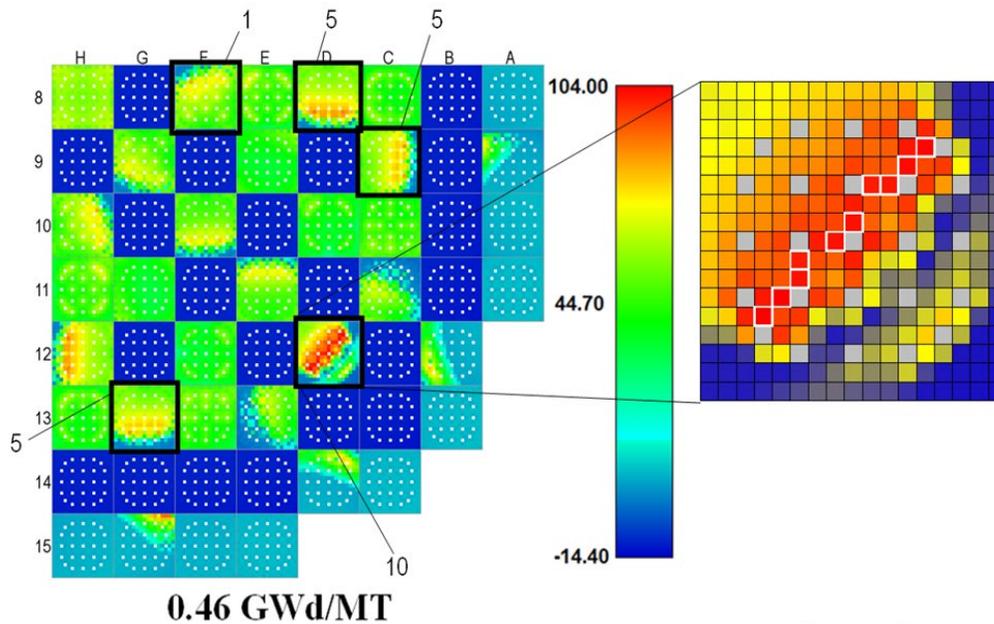


Figure 15. WBN-1 Cycle 6 with core wide cladding hoop stress distribution with limiting rods selected for further analysis

Quarter-core VERA simulations were used to calculate maximum, minimum, average, and integral quantities of interest across each fuel rod. The fuel performance calculation was performed with a layered one-dimensional screening method for thermo-mechanical performance followed by a high resolution calculation for selected rods. Displayed in Figure 15 are the core wide VERA hoop stress calculated by BISON on a rod-by-rod basis with a highlight of the rods within the limiting assemblies that were selected for a more detailed analysis in (r-z), (r- θ), and (r- θ -z) geometry using the full-core analysis power histories.

As a result, the analysis indicated the failures were likely caused by an external factor, such as missing pellet surfaces, rather than by classical PCI. The analyses were also able to distinguish between the behavior of Cycle 6, which had a relatively simple power history, and the Cycle 7 history where the presence of CIPS drove rapid changes in fuel temperature and stress distributions.

LOSS OF COOLANT ACCIDENT CHALLENGE PROBLEM

The loss of coolant accident (LOCA) is a limiting design basis accident for LWRs that requires reliable predictions of fuel rod integrity to assure that safety with respect to radioactive releases is maintained. Within the framework of VERA, the LOCA challenge problem focused on the required fuel performance capabilities in BISON for simulating the fuel and clad behavior over time. This included models for specific LOCA phenomena as well as separate and integral effects tests to be used for validation. The key material and behavior models required to address transient high-temperature phenomena occurring during LOCAs for PWRs have been implemented [17].

Models were developed specifically for UO₂ fuel forms, Zircaloy cladding and water coolant. Simulation of clad evolution and failure include models for LOCA phenomena of interest that include high-temperature steam oxidation, crystallographic phase transformation, high-temperature clad creep, and energy deposition in the clad due to the exothermic steam

oxidation reaction that occurs at high temperature. The clad failure model includes four different burst criteria. For the UO_2 fuel form, mechanistic models for fission gas swelling and release were developed and extended to treat the burst release that represents the effect of grain-boundary separation due to microcracking. Evolving material interfaces is critically important to the LOCA transient behavior and to this end an extended finite element method was developed to address issues such as axial relocation of the fuel stack, central void formation, oxide layer evolution and mechanical contact. Models also include high burnup structure evolution which is extremely important as the nuclear industry moves in the direction of high-burnup fuel.

A substantial number of separate effects validation cases (48 tests from 5 experimental series) have been completed to compare BISON predictions to measured ballooning and burst behavior for Zircaloy cladding. Such experiments include a wide variety of pressures, temperatures and loading rates. These experiments involve all fuel and cladding phenomena relevant to LOCA conditions, and can include complexities associated with irradiated fuel relative to fresh fuel. Integral validation tests included five experiments (7 rods) that have been considered to date including simulated fuel (ZrO_2) and both fresh and high-burnup UO_2 . Test rods ranged from rodlets to full length commercial PWR fuel rods. Predictions of burst temperature, pressure and burst time are in general agreement with experiment.

The demonstration of BISON for real-world LOCA analysis was performed under collaboration with the NRC where one of the collaboration topics was modeling and simulation capabilities for ATF. To this end, fuel clad and fuel form models were developed for near-term ATF concepts. For the fuel clad, BISON models were developed for chromium-coated clad and FeCrAl [18] while ATF fuel form development included models for Cr_2O_3 -doped and uranium silicide (U_3Si_2) fuel [19]. An important part of this effort was validation and uncertainty quantification for the ATF models developed. Figure 16 displays the validation for the BISON fission gas release model for chromium-doped fuel which agrees quite well with experiment.

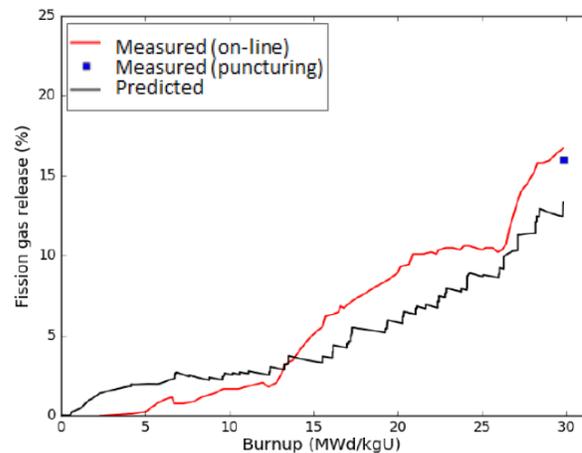


Figure 16. BISON fission gas release prediction for chromium-doped fuel

To demonstrate a complete a full LOCA simulation, BISON was coupled to the NRC system code TRACE under the NRC's Comprehensive Reactor Analysis Bundle (CRAB) which enabled a full LOCA simulation to be performed with validation against the LOFT L2-5 set of LOCA experiments [20]. LOFT was a series of transient experiments, including 24 nuclear experiments reflective of PWR small-, intermediate- and large-break LOCAs conducted between 1976 and 1983 at INL. BISON-TRACE results for peak cladding temperature over the LOCA accident progression showed reasonable comparisons to measurement.

GRID-TO-ROD FRETTING CHALLENGE PROBLEM

Grid-To-Rod Fretting (GTRF) is a phenomenon whereby coolant flow induces vibrations within the structural components of the fuel assembly and the fuel rods, resulting in surface cladding wear that can lead to fuel failure. Fretting fuel failures produce radioactive species releases into the coolant and may lead to unplanned outages and lost generation to address the failed fuel issues. Fretting damage typically occurs at the location of the fuel grids and is a function of a number of variables such as surface oxide film growth and removal rates, operating conditions of the reactor and accumulated fuel burnup.

CASL has developed a stage-wise GTRF engineering wear model (EWM) that is based on structural mechanics modeling of the GTRF phenomena combined with extensive CFD modeling of the fluid and interactions [21]. The EWM includes materials science-based wear factor based on different operating scenarios and its effect on fretting wear on the structural components. GTRF capabilities that have been developed include 3D multiphysics simulation based on structural and CFD models for the interactions of the fuel clad, grid and coolant and advanced material response models. Figure 17 displays the distribution of fuel grid dimple pressure as a function of irradiation displacement per atom (dpa).

As shown, there is a significant variability over time that can affect grid to fuel rod contact.

The need for experimental data arises from the complex behavior of the wear coefficient which is a function of the alloy composition of the cladding and grid materials, surface conditions (e.g., oxidation), contact geometry, water temperature, fluid chemistry, and flow rate (inducing vibration). Within the operating environment of a nuclear reactor it is extremely difficult to quantify and most non-reactor, wear tests fall short of the temperature, coolant pressure and chemistry environment characteristic of nuclear fuel as well as the complex types of structural fretting and impact motions. Experimentally determined cladding wear coefficients were obtained based on a novel autoclave fretting and impact device that was developed to provide experimental validation data for the EWM.

CASL developed the Autoclave Fretting and Impact Rig (AFIR) to provide for a well-controlled, realistic testing of parameters (contact geometry, load, oscillation frequency and amplitude) in PWR environments. AFIR provides a well-controlled, realistic test environment for a range of testing parameters such as contact geometry, load, oscillation frequency and amplitude with temperatures up to 220 deg-C. In each test, commercial Zr-based alloy cladding and grid provided a realistic environment reflective of PWR fuel. Results have been used to validate the EWM and has allowed for greater understanding of material mechanical interactions in a reactor environment, including effects of surface

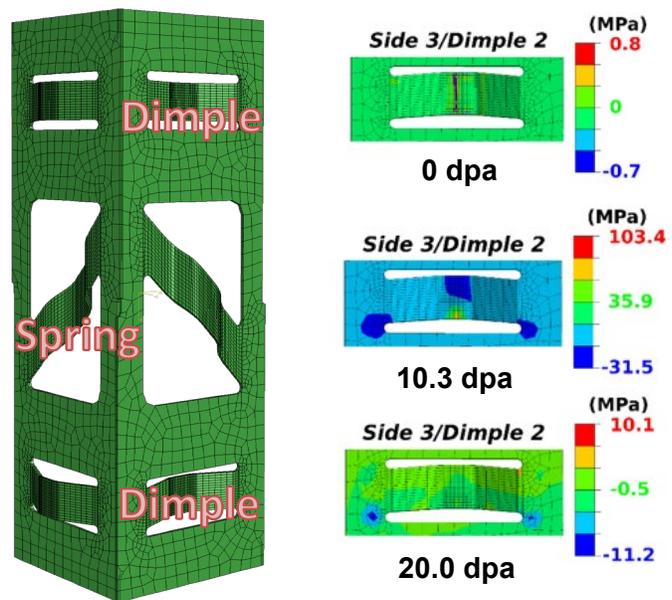


Figure 17. Distribution of fuel grid dimple pressure as a function of irradiation dpa

treatments on fuel rods and grids and the role of corrosion on wear rates. The completion of the GTRF challenge problem provides a foundation for analyzing future reactor materials, such as new accident tolerant fuel claddings.

PART 4: VERA DEPLOYMENT TO INDUSTRY

A significant effort was put forth in the final years of CASL to complete work on the CASL challenge problems as well as pivot towards activities to enable broad VERA deployment to industry. Guidance was provided by the CASL Industry Council, Science Council, and Board of Directors to achieve the objectives outlined in the initial CASL proposal and renewal application, as reflected in the following end-state vision for the program:

By the end of the CASL operational period, CASL will have successfully developed and deployed advanced M&S technologies that can be used with confidence to solve the CASL challenge problems and address future nuclear energy industry challenges, emerging issues, and evolving opportunities.

To this end, a significant effort was made to work with CASL industry partners on the development of new VERA use cases and demonstration of novel applications. In addition, efforts were made to mature the VERA software to the point of making VERA “used and useful”. Activities aligned with these goals included developing and successfully implementing an NQA-1 compliant software quality program for VERA, creating the VERA Users Group, executing a success path that led to issuance of the first VERA commercial licenses, and providing access to high performance computing (HPC) resource through DOE for those VERA users lacking in-house HPC computing capability.

The transition of CASL to an integrated modeling and simulation with the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program began with the development of the program plan “DOE-NE ModSimX Program Plan, Rev 3.1” [22]. This plan defines the future research areas for LWR advanced M&S activities and includes capability development for two-phase flow, with an emphasis on advanced LWR deployment, advanced technology fuels, and lifetime component analysis. The transition began in FY20 during which time there was an overlap of CASL completion activities as well as new scope that leveraged CASL activities in the primary research focus areas of the integrated program. VERA continues to remain the platform for all LWR development activities which allows for continued VERA capability development that will benefit existing and future VERA users.

A key aspect of the integrated program was the establishment of an LWR Industry Council which was created in FY20. The LWR Industry Council serves a similar role to the CASL Industry Council in providing feedback to the program and assuring relevance of LWR R&D activities to the nuclear industry. It is noted that the LWR Industry Council serves as an advisory group for future M&S capability development and has a different role from the VERA Users Group (described below) which was created to provide sustainability for the VERA software.

VERA USERS GROUP

The strategy for VERA deployment to industry is built upon an active VERA Users Group (VUG) and VERA commercial licensing to VUG organizations. The goal is to build an active user base which is achieved through direct use of the VERA software for applications of relevance to each VUG organization.

The VUG, created in 2019, is organized as a partnership between industry users of the VERA code suite and ORNL. The VUG is vital in providing the resources to the industry for

the continued use and application of VERA for the benefit of the US nuclear fleet. The VUG was provided funding of \$3M by DOE in 2019 to initiate activities with the intent that the VUG would become self-sustaining within the time frame of several years. This would be achieved through the collection of annual VUG fees to provide continued support of the VERA software. At the point of collecting fees, the VUG will be moved from ORNL to a private entity.

As illustrated in Figure 18, the goal of the VUG is to sustain the use of VERA through industry engagement for the post-CASL period. It will achieve this through:

- Successful deployment and implementation of VERA by the nuclear industry, including facilitating software licenses
- Sustainability of VERA by providing software maintenance, software quality assurance, training, code support, and HPC access for users of LWR applications
- Building on current CASL accomplishments and drive new innovations for the LWR fleet through sharing of user application experiences and feedback
- Promoting industry participation in the DOE GAIN and industry funding opportunities
- Representing LWR stakeholders in the integrated CASL and NEAMS program

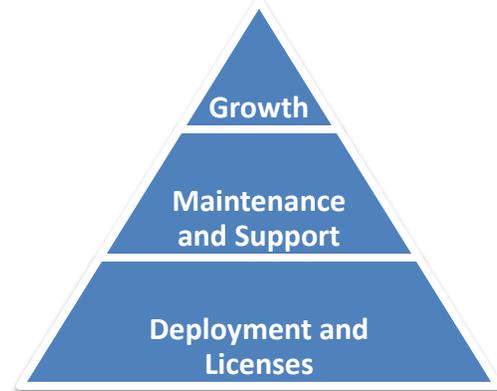


Figure 18. VERA Sustainability Model

Key activities for the VUG include:

- Providing a forum for VERA users to share knowledge and provide feedback on VERA development,
- Providing user support through training, workshops and access to expert knowledge of VERA use,
- Maintaining the VERA NQA-1 software quality assurance program, including control, bug fixes, and error reporting,
- Fostering industry collaboration and promote best practices among VERA users,
- Establishing and providing software license agreements,
- Providing installation support for VERA, and
- Facilitating VUG member access to DOE HPC resource for VERA remote execution

The current membership of the VUG as of September 2020 is 68 members from 23 organizations representing a broad spectrum of the nuclear industry (utilities, fuel and hardware vendors, research organizations, and service companies). In addition, the NRC is a member of the VUG.

VERA COMMERCIAL LICENSING

The VERA licensing strategy is focused on wide-spread deployment of VERA to industry to support the design, operations, optimization, and continued safe operation of the current and next-generation LWR fleet. From a licensing perspective and the VUG, it is important to focus on VERA organizational licenses that will remove barriers to adoption by industry. Commercial licenses going beyond the R&D licenses that have been and will continue to be issued to universities and the DOE laboratories to support continued R&D using VERA going forward.

The goal for the commercial organizational licenses is to build a user base for a broad range of industry applications, many of which have already been demonstrated as part of the CASL program. Through the VUG, those industry applications will be shared among the VERA community, with the goal of developing the user base and accelerating the realized value, in the short term (three years) for the US nuclear industry. The EPRI license was the first commercial VERA license for the US nuclear industry issued in 2019 and included all software within the VERA code suite. There are currently six VERA commercial licenses issued with another eleven pending as of September 2020.

NQA-1 COMPLIANCE

As part of the deployment of VERA for production use an initiative was undertaken to bring VERA under the American Society of Mechanical Engineers NQA-1 software quality assurance standard. The goal of this effort was to eliminate a primary barrier for adoption of VERA by the nuclear industry as well as the NRC. The VERA NQA-1 program plan replaces the previous CASL Quality Assurance program. The VERA NQA-1 program for the software development process recognizes a graded approach for software quality level based on the software maturity. In this manner, both production level software, as well as follow on VERA research level software, is maintained under quality control. This is fully discussed in the “VERA Quality Assurance Program Plan” [23] as shown in Figure 19. A successful external audit of VERA (exclusive of BISON) was performed at ORNL in August 2019. An additional successful audit of BISON occurred at INL in February 2020. VERA users must be members of the VUG to have access to the NQA-1 program, including software error reporting.

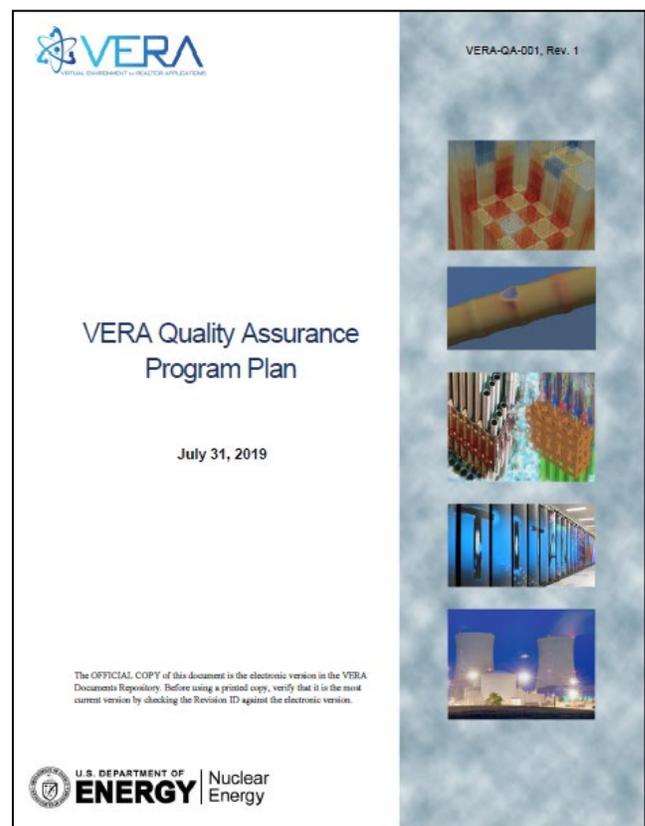


Figure 19. VERA NQA-1 Quality Assurance Program Plan

VERA INDUSTRY USE CASES

Numerous VERA analyses have been performed in the area of design, operations, licensing, and component lifetime analysis. The CASL program has been focused on the solution of challenge problems and this has driven VERA applications that were aligned with industry needs. A survey conducted among the CASL Industry Council members in 2018 (Table 1) was used to focus VERA development towards those application of highest value and impact to industry. Shown in the survey are those who provided data, commitment to use VERA, availability of HPC computing resource, and their interest in specific areas of VERA application including, crud analysis (CRUD), ex-core analysis (EXC), RIA, PCI, LOCA, and use for VERA reference calculations (REF) for benchmarking of industry methods is also included.

	Provided Data	Will use VERA	Has Computer	CRUD	EXC	RIA	PCI	DNB	LOCA	ATF	REF
APS	X			X							
Duke	X	?		X	X					X	
Exelon	X						X				X
JSI	X	X									X
SCANA	X	X									X
Southern	X			X							
TVA	X	X		X	X						X
EPRI	X	X	X	X	X		X			X	
Framatome	X	X	X	X	X					X	
NNL	X	X	X								X
NuScale	X	X	X	X	X						X
PNNL	X	X	X								X
Rolls-Royce		X	X								X
Studsvik	X										
Westinghouse	X	X	X	X	X	X	X	X	X	X	X

Table 1. CASL Industry Council Survey (2018)

Of the primary VERA application areas, it is clear that CRUD, EXC and REF are the top priorities followed by ATF and PCI. It is noted that while RIA and LOCA show little interest this has changed significantly in the past 2 years with the desire of the nuclear industry to move toward high-enriched and high-burnup fuel to achieve longer and more economical fuel cycles. Also, with the creation of the VERA Users Group, additional organizations have been added to the list with different priorities. Also note that RIA and LOCA represent the extreme of transient VERA applications for licensing and there are a host of other licensing applications that are enabled through solution of the RIA challenge problem. The introduction of ATF into operating reactors necessarily requires licensing for all NRC Chapter 15 events which presents a new opportunity for VERA going forward.

A summary of industry use cases for VERA was defined by Westinghouse in partnership with CASL and was provided in the publication at the TOPFUEL 2018 meeting, held in Prague at the end of September 2018. The paper titled "Industry Use of CASL Tools" [24] presents several VERA applications including:

- AP1000® reactor control rod ejection accident
- DNB evaluation of PWR main steamline break event
- PWR DNB margin improvement
- CFD based thermal-hydraulic applications
- Fuel rod applications of CASL tools
- Advanced analysis of crud

It is noted that many of these applications have been reported on previously within CASL. However, the paper focuses on the specific industry applications of the CASL technology and “value story” by highlighting the full spectrum of CASL capabilities and potential benefits to industry.

Further details of specific application areas considered of high impact to VUG members are now described in greater detail.

PART 5: VERA INDUSTRY APPLICATIONS

VERA ANALYSIS FOR CORE FOLLOW AND STARTUP PHYSICS

VERA applications represent a broad spectrum of design and operating conditions for the current and future operating fleet. The analyses performed represent a key component of the VERA V&V plan [25] and assures confidence in the robustness of the software's physics, geometry, and numerical solvers. Steady-state core follow and startup physics analysis, which confirms reactivity and thermal margin as well as cycle energy production capability is the starting point for all other VERA applications.

Table 2 shows the plant, operating cycles, reactor, and fuel type for which VERA benchmarking was performed. This list represents nearly the full spectrum of PWR reactors and operating fuel designs within the US nuclear fleet as well as the advanced LWR reactor designs, such as the NuScale SMR. The list represents reactors of different sizes, power density, cycle energy production, fuel products, burnable absorbers and core loading pattern design strategies. Note that each plant on the list has different requirements based on energy production requirements, requirements for load follow or coast down, its maintenance and fueling outage schedule, and fuel product transitions (which may impose additional constraints on thermal operating margins).

	Plant	Cycles	Reactor and Fuel Type
1	AP1000	1-5	W Gen III+ 2-loop 17x17 XL
2	Byron 1	17-21	W 4-loop 17x17
3	Callaway	1-12	W 4-loop 17x17
4	Catawba 1	1-9	W 4-loop 17x17
5	Catawba 2	8-22	W 4-loop 17x17
6	Davis-Besse	12-15	B&W 15x15
7	Farley	23-27	W 3-loop 17x17
8	Haiyang	1	W Gen III+ 2-loop 17x17 XL
9	Krško	1-3,24-28	W 2-loop 16x16
10	NuScale	1-8	SMR
11	Oconee 3	25-30	B&W 15x15
12	Palo Verde 2	1-16	CE System 80 16x16
13	Sanmen	1	W Gen III+ 2-loop 17x17 XL
14	Seabrook	1-5	W 4-loop 17x17
15	Shearon Harris	Surrogate	W 3-loop 17x17
16	South Texas 2	1-8	W 4-loop 17x17 XL
17	Three Mile Island	1-10	B&W 15x15
18	V.C. Summer	17-24	W 3-loop 17x17
19	Vogtle 1	9-15	W 4-loop 17x17
20	Watts Bar 1	1-18	W 4-loop 17x17
21	Watts Bar 2	1-2	W 4-loop 17x17

Table 2. VERA Fleet Validation

In addition to the plants shown in Table 2, Westinghouse successfully performed their own, independent assessment of VERA on a range of plants which is described in the report “Benchmark of VERA Predictions at Steady State Conditions vs. Measurements at Westinghouses Nuclear Power Plants” [26]. As described in the report “Having confidence in these predictions is the foundation for incorporating the CASL tools in the commercial nuclear industry workflow to, inter alia, improve fuel reliability and operability, investigate core anomalies, enhance fuel cycle economics, and extend plant life.” A total of eleven plants representing 27 fuel cycles were benchmarked against startup physics measurements (HFP critical boron, rod worths, and isothermal temperature coefficient (ITC)) and core follow measurements as a function of cycle depletion (hot full power (HFP) critical boron, flux maps). The conclusion was that VERA is a solid platform with differences in measured to predicted (M-P) results generally very good.

VERA ANALYSIS OF NEW PLANT BUILDS

Of particular note, is that VERA is being used not only as a benchmark tool for previous cycles of operation but as a reference solution in the mode of making ‘blind predictions’ for future reactor operations. Most notable are the recent reactor startup examples for Watts Bar Nuclear Unit 2 (WBN-2), which achieved initial criticality in May 2016, and the Sanmen and Haiyang Nuclear Power Stations in China. Sanmen and Haiyang are the first implementations of the advanced AP1000® reactor developed by Westinghouse (4 units) and achieved initial criticality during the period from June 2018 through January 2019 [27].

TVA’s WBN-2 is the first new reactor to come online in the United States in nearly two decades, and it presented a perfect opportunity to test VERA capabilities on a modern reactor design. CASL analysts used VERA tools and the INL Falcon computing platform to perform high-fidelity physics calculations before startup and ongoing simulations as the plant increased power toward commercial operations.

WBN-2 is a traditional Westinghouse four-loop PWR of similar design to its sister WBN-1. The fuel-loading pattern is similar to other first cycle designs like WBN-1, but this is the first time that integral fuel burnable absorber and wet annular burnable absorber have been used in an initial startup. Another new feature included in WBN-2 is the use of fixed vanadium in-core detectors, rather than the moveable fission chambers used in most previous Westinghouse plants of this type.

VERA was able to predict important startup parameters and follow control rod bank positioning during power ascension with a very high degree of accuracy. Additionally, the power ascension calculations were performed at close to real time, demonstrating VERA’s ability to produce results that can be used to quickly analyze emerging issues that might arise during normal plant operations. A summary of VERA prediction results are shown in Table 3 and are considered excellent and well within the uncertainty of industry predictive accuracy.

Parameter	Difference from Measurement
Initial Critical Boron	-2 ppmB
Total / Max Bank Worth	0.7 ± 1.4% / 3.0%
Isothermal Temperature Coefficient	-0.8 pcm/°F
HZP Critical Boron Concentrations	-7 ± 3.3 ppmB
At-Power Critical Boron Concentrations	-37 ± 11.1 ppmB
In-Core Detector Segments: Total / Radial / Axial RMS	4.4% / 2.6% / 2.5%
In-Core Detector Currents: All wires / Long Wires RMS	3.3% / 2.7%

Table 3. Watts Bar Unit 2 - VERA Prediction Results

VERA predictions Sanmen and Haiyang [26] also showed excellent agreement with both global and local measured data. Table 4 displays the startup physics test results and VERA predictions for the first four AP1000® cores which are similar in accuracy to the WBN-2 results. Note that because the AP1000® core are identical the VERA predictions are identical and the variation of differences between measured and predicted values reflect the uncertainties in measurement and as-built data. The near-perfect VERA agreement with measurement confirmed the Westinghouse design values for the AP1000® first cores.

Plant	HZP Boron (M-P) (ppm)	ITC (M-P) (pcm/F)
A	-13	-0.27
B	6	-0.46
C	-14	-0.19
D	-14	+0.07
Avg Δ	-9	-0.21
Stdev Δ	8	0.19

Table 4. AP1000® - VERA Startup Physics Test Results

VERA CRUD ANALYSIS

A collaborative Test Stand for the application of VERA to the NuScale SMR design was completed in FY18. This was an exceptional opportunity for CASL to apply VERA capabilities for a new reactor concept in support of the nuclear industry. The goal of the Test Stand was an assessment of crud behavior for the NuScale reactor core which is impacted by flow driven by natural circulation as per Figure 20.

VERA was demonstrated to be able to accurately model the nuclear performance of the NuScale core, including the steel block reflector, based on comparison with Monte Carlo reference solutions [28]. An analysis of the NuScale reactor characteristics identified differences from large PWRs that could impact crud formation. This includes a lower coolant flow rate, an iron-rich crud source in comparison to a Nickel-rich crud source in currently operating PWRs. As no operational data yet exists, sensitivity analyses were performed with respect to model parameters that allowed for increased understanding of design crud deposition, including the impact of such terms as the spacer grid pressure loss coefficient and the spacer grid blockage coefficient.

The report titled “Core Design Optimization with CIPS Risk Analysis” [29] demonstrated the process of performing core design using VERA for CIPS risk mitigation. To this end, a 24 month, high enrichment (6 w/o U^{235}) core design was developed for WBN-1 Cycle 17 that showed high risk for CIPS beyond the existing 18 month fuel cycle. Traditional CIPS analyses for these cores would evaluate the risk and/or margin to CIPS by examining the total boron mass in the crud. Figure 21 displays the boron distribution for one of the alternate core designs which clearly shows the concentration of boron limited to a handful of assemblies. As a design issue, this is readily addressed by decreasing the local power (via burnable poisons or reduced enrichment) or fuel shuffling to lower power regions. A key conclusion, is that the distribution of boron and not necessarily the total boron is the key factor in CIPS behavior. Simple core design changes produced a 30% reduction in the amount of axial power distribution shift over the cycle.

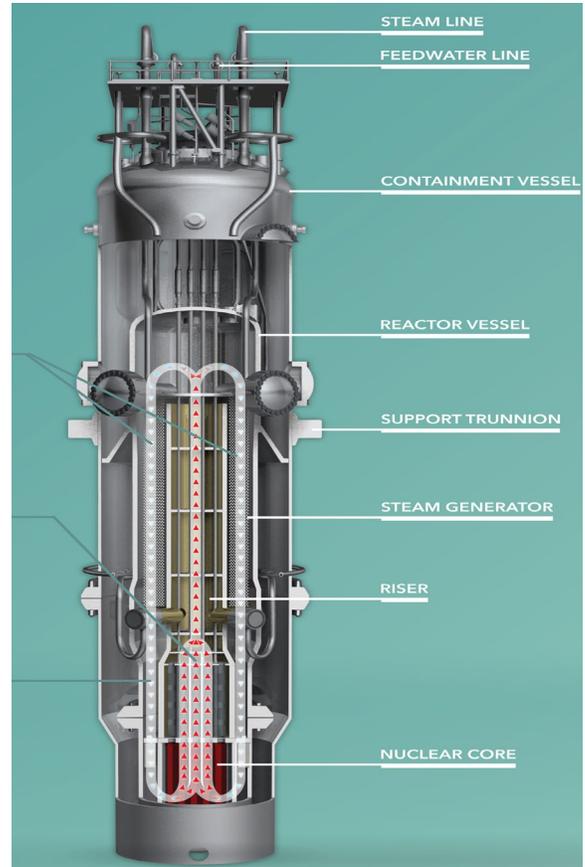


Figure 20. NuScale SMR Design Flow Circulation

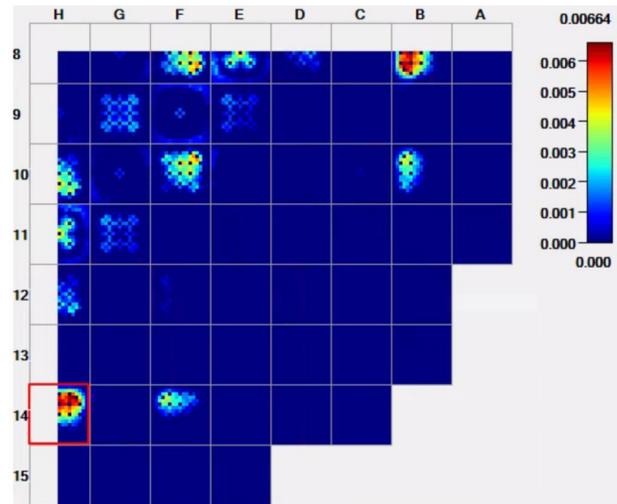


Figure 21. Alternate Design Boron Distribution at 350 EFPD (305 cm elevation)

VERA EX-CORE ANALYSIS

The integration of the Shift Monte Carlo code within the VERA framework resulted in an integrated capability for performing highly detailed ex-vessel fluence analysis with a broad range of applications. The CASL report “Demonstration of Comprehensive Ex-Vessel Fluence Capability” [30] summarizes the recent developments of VERA and describes several benchmark activities in the application areas of vessel fluence (beltline and nozzle region), detector response sensitivity to moderator density, and source range detector response during reactor startup.

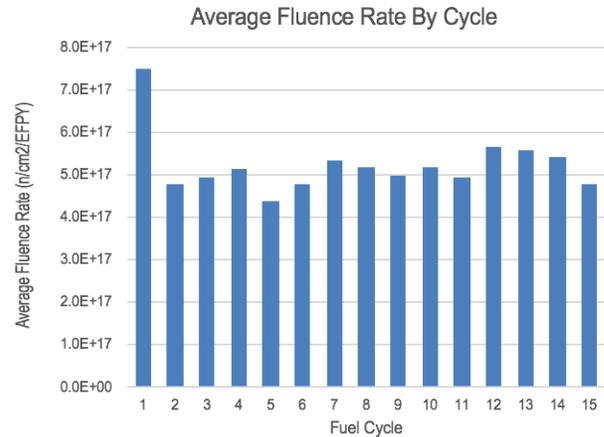


Figure 22. Watts Bar Unit 1 Fluence (Cycles 1-15)

CASL collaborated with TVA to simulate the vessel fluence of WBN-1 over cycles 1-15 (Figure 22). Because of the parallelization provided by Shift and the optimized coupling within VERA, a minimal increase in compute runtime was demonstrated through inclusion of the additional Shift ex-core calculation. From the user perspective, this demonstrated that a material fluence may be obtained directly as part of a VERA simulation. This contrasts with current industry practice of needing to run separate code packages. Running separate code packages is very complex and often involve high levels of approximation including the assumed reactor source terms and the dimensionality of the transport solvers (such as 2-D/1-D synthesis methods).

As shown in Figure 22, one sees a significant variation of fluence between fuel cycles (-14% to +11%) which reflects the differences in reload design strategy, such as that due to fuel placement on the core periphery. A best-estimate fluence using cycle specific source terms can reduce uncertainties, identify excess margins to lifetime limits, and inform future core design strategies to minimize vessel damage.

Detailed fluence analysis was also performed using measured coupon data from Davis-Besse Cycle 6 [31]. This work was performed utilizing VERA models developed by Framatome. These models were then expanded upon, creating detailed Shift models for the benchmark of Davis-Besse in-vessel capsule dosimetry (wires measured reaction rates) and cavity dosimetry (foils measured reaction rates) measurements. Table 5 displays the Shift calculated to measured reaction rates for the measured quantities which show excellent with measured reaction rates. The use of an accurate source, specifically the pin powers in the core periphery locations which is calculated by VERA, is considered a key contributor to the excellent results.

Reaction	Shift C/M
$^{238}\text{U}(n,f)^{137}\text{Cs}$	0.9671
$^{238}\text{U}(n,f)^{137}\text{Cs}$	1.0050
$^{237}\text{Np}(n,f)^{137}\text{Cs}$	0.9815
$^{237}\text{Np}(n,f)^{137}\text{Cs}$	1.0010
$^{58}\text{Ni}(n,p)^{58}\text{Co}$	1.0300
$^{58}\text{Ni}(n,p)^{58}\text{Co}$	1.0340
$^{54}\text{Fe}(n,p)^{54}\text{Mn}$	1.0440
$^{54}\text{Fe}(n,p)^{54}\text{Mn}$	1.0500
Average =	1.014

Table 5. VERA Predicted Reaction Rates for Davis-Besse, Cycle 6

A novel application of VERA to ex-core detectors was done in collaboration with TVA and modeled the core behavior during the refueling outage [32]. This is a sub-critical, source-driven problem that includes the modeling of activated secondary source rods that are important to the source signal. The placement of secondary sources is important to the ex-core detectors ability to identify potential core mis-loadings during the fuel reload and shuffle sequence. As shown in Figure 24, the VERA sub-critical thermal neutron flux quantifies the regions of influence for the two secondary sources. Initial comparison against measured data demonstrated excellent agreement with the predictions of the ex-core detector response. Further validation included modeling the detector response with high accuracy for the partially loaded core shuffle sequence.

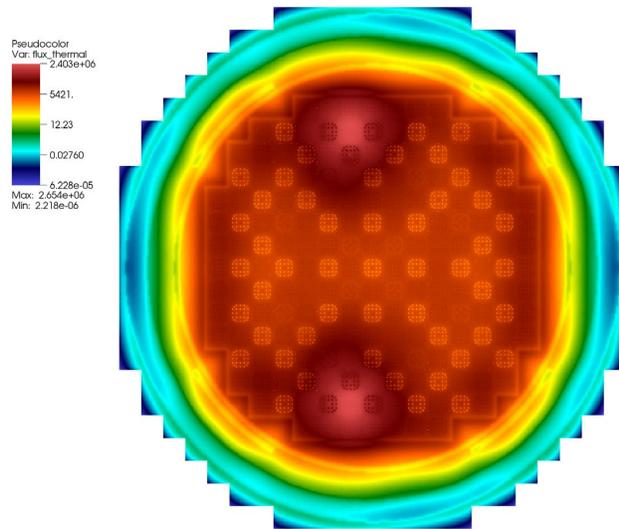


Figure 23. Sub-critical thermal neutron flux for Watts Bar Unit 1, Cycle 8 when fully loaded

A number of other ex-core analyses have been performed. CASL collaborated with Duke Energy [33] on the use of VERA to analyze the ex-core detector response with respect to reactor downcomer coolant density which influences the detector signal due to neutron attenuation. Results were benchmarked against industry methods and shown to be consistent with existing modeling methodologies. EPRI [34] applied for VERA for fluence analysis in four areas: surveillance capsules, reactor pressure vessel beltline, core baffle (i.e. baffle bolts) and the reactor pressure vessel outlet nozzle.

VERA TRANSIENT AND LICENSING ANALYSIS

VERA transient capability with fully coupled fuel, subchannel thermal-hydraulics, and neutronics expands the range of VERA applications to AOOs as well as design basis accidents. This includes reactivity initiated transients such as RIA, flow and temperature transients such as loss of flow accident and main steamline break, and large and small-break LOCA. It is recognized that licensing of VERA for such events is a prohibitive expensive endeavor for existing fuel products unless the margin recovery can be translated into sufficient economic benefit. Examples of economic benefit are additional operational flexibility, power uprate, or new fuel products that provide additional fuel cycle cost efficiencies. Both ATF, high-enriched and high-burnup fuel offer opportunities in this arena for use of VERA in licensing applications because of the potential economic benefit to the operating fleet. To this end, VERA has been demonstrated on a number of transient applications, including RIA and steamline.

Industry applications of the CASL RIA modeling and simulation capabilities are expected to be implemented in reference calculations, determination of margins to regulatory figures of merit, evaluation of RIA test results, provision of simulation results to fill gaps in the RIA experimental testing database, and potentially replacement or augmentation of licensing

methodologies. Current emerging applications for RIA include ATF and high-enriched and high-burnup fuel.

The steamline break accident is a hot zero power (HZP) cooldown event whereby an increase in steam flow reduces reactor coolant system pressure and temperature through an increase secondary side heat transfer. The result is a positive reactivity insertion which rapidly increases core power that in turn increases the risk of local boiling and DNB. Two scenarios are relevant to SLB – the case of loss of offsite power (i.e. natural circulation in the absence of cooling pumps) and full pump operation (high flow). VERA was used to model these two scenarios in order to analyze which case was more limiting in terms of minimum DNB margin [35]. This analysis was important to confirming assumptions in the existing design basis licensing methodology. Figure 24 displays the results of these analysis which utilized

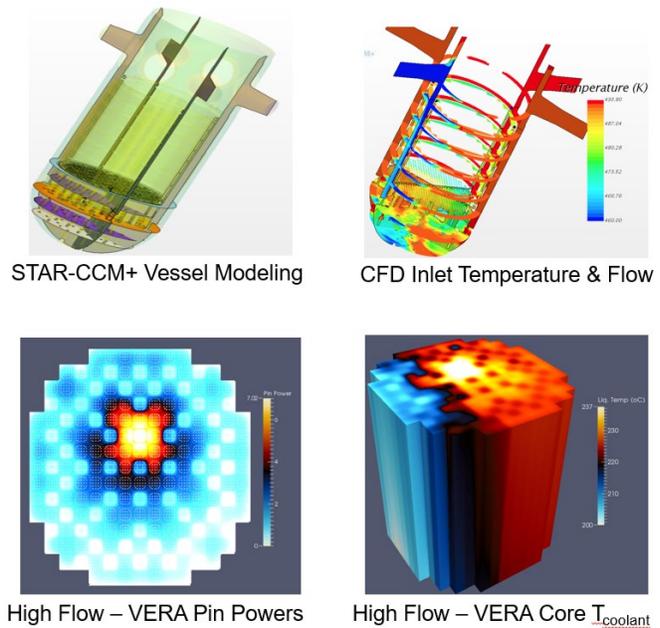


Figure 24. VERA modeling for Steamline Break (high flow scenario shown)

system CFD modeling to provide the core inlet temperature and flow distributions for VERA, which then calculated the detailed pin-by-pin power, flow and temperature distributions throughout the core. Results confirmed, consistent with the assumptions utilized in the current design basis licensing, that the high flow scenario was more limiting because of due a significantly higher limiting surface heat flux under forced flow versus natural circulation conditions. This is a good example of how the high fidelity, high resolution capabilities of VERA have been used in licensing activities.

VERA SIMULATION FOR BOILING WATER REACTORS

VERA capabilities were developed with a near-term focus on PWRs while maintaining a line of sight towards simulation of BWRs. In terms of modeling, BWRs are much more complex due to the high void, high pressure two-phase flow regimes characteristic of BWR operation. CASL made significant progress on CFD two-phase flow modeling for PWRs, advancing the closure model development to the point of a first of a kind capability for prediction of DNB. CASL work extended the closure model development for PWRs to the BWR flow regimes, most notably annular flow, with early work showing great promise but limited by a lack of experimental two-phase flow data that CASL sought to fill. Continued development of two-phase flow capabilities are a high priority and are being addressed in the integrated M&S program.

Nevertheless, while the focus of VERA was primarily PWRs, VERA is uniquely positioned to address the M&S challenges of BWRs. Characteristic of BWRs are complex two-phase flow phenomena and the use of control blades and flow for reactivity and power distribution control. Current industry codes for BWRs have been, from the very beginning, based on multiphysics coupled solutions with various modeling approximations made to

accommodate the limitations of computing capability. Such approximation introduces higher uncertainties in power distribution and reactivity predictions and as a result, require higher margins to operational and safety limits. The excess margin was used to perform power uprates by the nuclear industry over the past two decades with some BWR uprates as high as 20% adding significantly to the installed nuclear capacity in the absence of new reactor builds.

In October 2019, the DOE Office of Nuclear Energy funded a two year project titled “Modeling and Analysis of Exelon BWRs for Eigenvalue & Thermal Limits Predictability” led by Exelon and ORNL with participation of INL, Global Nuclear Fuel (GNF) and three universities, NCSU, University of Michigan, and University of Illinois Urbana-Champaign (UIUC) [36]. The primary objective of this project was to enhance the capabilities of VERA to support the detailed modeling and simulation of BWRs. This work commenced in fiscal year (FY) 20 and will continue through FY21 and involves maturing the VERA simulation capabilities for BWR analysis including validation against existing BWR operating data for reactors currently operating within the U.S. fleet using modern fuel designs.

Figure 26 displays the results of VERA for the rod-wise void distribution within a 16 bundle core slice consisting a 4 control cells. A control cell consists of 4 fuel bundles oriented in reflective symmetry towards either a central cruciform control blade (inserted between bundles) or a fixed detector location. The fuel bundles are based on the GE14 product and consist of a 10x10 lattice of full and part length fuel rods with two large, interior water rods to provide neutron moderation in the upper portion of the fuel bundle. As shown, VERA captures the significant void gradient that exists both axially and radially within the bundle adjacent to the blade insertion. This has implications for both local power but also global reactivity predictions. Given that current industry codes model void based on one-dimensional axial models in each bundle, VERA represents a step function in analytical modeling capability for BWRs.

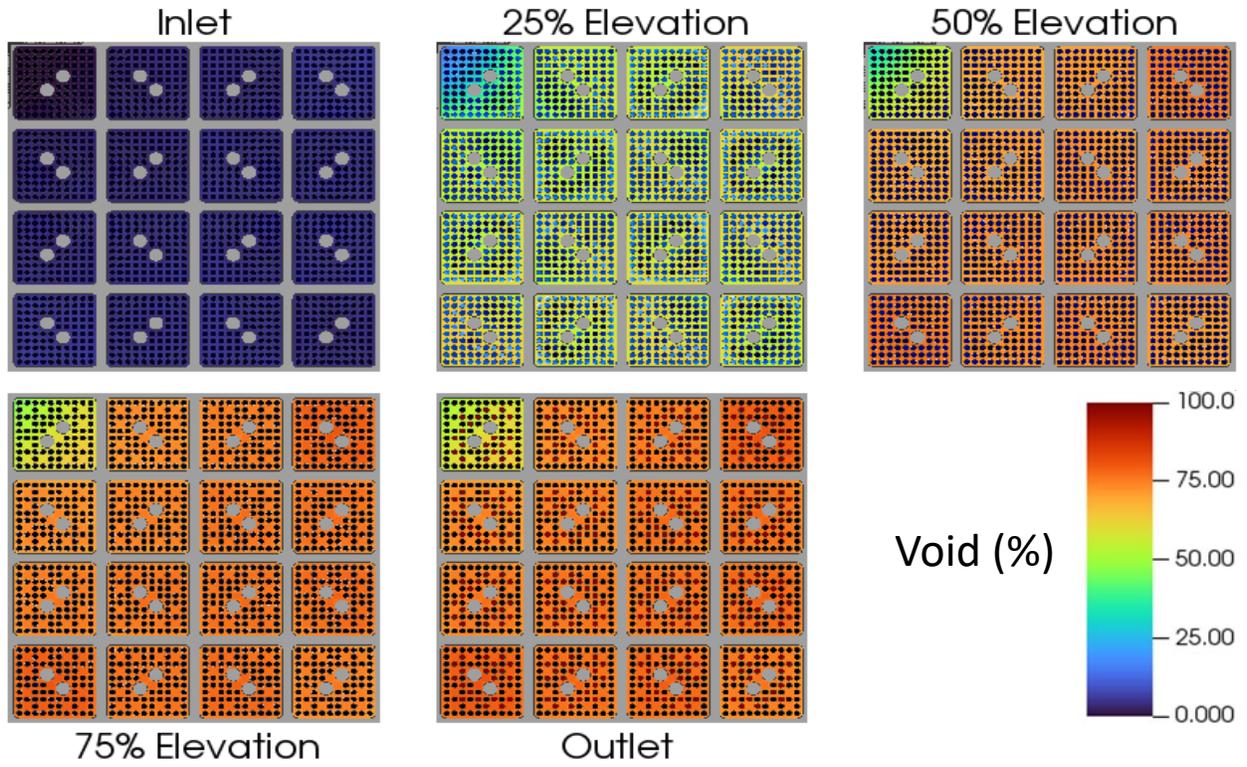


Figure 25. VERA BWR rod-wise void distribution (4x4 bundle configuration), partial control blade insertion, upper left corner of bundle (1,1)

PART 6: RETURN ON TAXPAYER INVESTMENT

CASL worked to ensure that the program produced a strong return on taxpayer investment and that funding provided by DOE-NE was carefully managed. The primary measure of return on investment is the successful completion of CASL's planned technical work that results in impactful outcomes for the nuclear industry. Regarding financial management, CASL's work was executed through contracts established by ORNL with CASL partner organizations. Yearly budget and technical planning was performed by the CASL technical focus areas in alignment with CASL yearly program goals established by the CASL senior leadership team. Financial and technical milestones were tracked on a monthly basis to assure that work performed was consistent with contractual scope of work with deliverables based on submission of completion memo and technical milestone reports. Work was reviewed by the CASL focus area leads for the specific technical area as well as the senior leadership team. The uncertain nature of R&D activities with respect to guaranteed outcomes when coupled with a high focus on periodic review allowed course corrections to be made as needed on continuous basis. A subset of technical milestones (11) were established in conjunction with DOE as reportable milestones for each fiscal year that included both technical activities as well as deliverables related to the VERA software.

PERFORMANCE METRICS

CASL program expenditures over the 10 year hub history included spending of \$232M that is categorized in Table 6 by costs for Management, Operations and Infrastructure (18%), Research and Development (75%), and VERA deployment (7%). Note that the expenditures shown exclude funding distributed separately by DOE through the Small Business Innovation Research and Small Business Technology Transfer programs as well as DOE program costs for the Federal Lab Consortium, Office of Technology Transfer, and IAEA peaceful uses program.

CASL Spending Categories	Costs (\$K)	% Total Cost
Management, Operations & Infrastructure		
Program Management	\$ 20,051	8.66%
VOCC & Infrastructure	\$ 16,204	7.00%
CASL Education Program	\$ 4,899	2.12%
Research and Development		
Laboratories	\$ 96,384	41.61%
Universities	\$ 50,539	21.82%
Industry	\$ 28,360	12.24%
VERA Deployment		
Test Stands, NQA-1, Release, Support	\$ 12,180	5.26%
VERA Users Group	\$ 3,000	1.30%
TOTAL	\$ 231,618	100.00%

Table 6. CASL Research, Development and Deployment Expenditures

CASL expenditures are further broken down to include the R&D distribution by laboratories, universities and industry, the CASL education program (2%), and VOCC and Infrastructure

(7%). Note that the expenditures include NRC funding (\$5M), funding related to the Exelon FOA (\$5M), and the VERA Users Group (\$3M) all of which were included in the CASL program activities. It is noted that there is planned carryover for the FOA (funded for FY20-FY21) and the VUG (planned for FY20-FY22).

CASL research and development expenditures of \$175M included significant funding provided to both universities (29%) and industry (16%). This excludes the additional funding for universities received under the CASL Education Program. University funding included direct R&D funding for 20 partner universities while industry funding for 26 organizations and contracted individuals. DOE laboratory funding included the CASL founding partners (ORNL, INL, SNL and LANL) as well as Argonne National laboratory and Pacific Northwest National Laboratory. Note that the CASL Industry Council was comprised of member organizations the bulk of which received no direct funding under CASL.

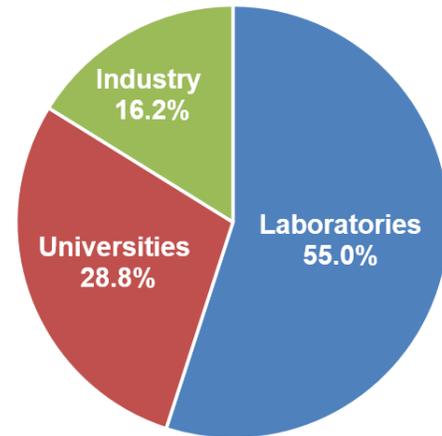


Figure 26. R&D Expenditures by Partner Category

A summary of CASL technical output is provided in Table 7 for the 10 year Hub period. It includes the number of VERA licenses, distributed as individual licenses through the Radiation Safety Information Computational Center (RSICC) and commercial license, publications, technical reports, invited talks, and CASL education program participation. The technical output in terms of R&D technical and milestone reports, number of students educated, and VERA individual licenses represents a significant achievement for the CASL Hub.

Task Description	Total
VERA individual R&D licenses	397
VERA commercial licenses (6 issued and 11 pending as of September 2020)	17
Journal & Conference Publications	1,160
Invited talks	905
Milestone reports	1,482
Programmatic & Technical Reports	879
CASL Education Program Students	289
CASL Education Program Institutions	31

Table 7. CASL Technical Output

CASL SYMPOSIUM

The CASL Symposium is the crowning technical event for the CASL Hub celebrating the 10 year history and achievements of the CASL consortium. The CASL Symposium is to be held as an embedded American Nuclear Society (ANS) topical meeting held in conjunction with the ANS Virtual Winter meeting, November 15-19, 2020. As shown in Table 8 the CASL Symposium includes 290

CASL Symposium Metrics	Total
Total organizations	33
Total papers	84
Total authors	290
Total panels	8
Total panelists	47

Table 8. CASL Symposium Metrics ANS Winter Meeting 2020

authors and panelists 33 organizations representing academia, industry, laboratories, and the NRC.

The format of the CASL Symposium is identical to the ANS National meeting with peer-reviewed technical papers and panels presented in a conference format.

NRC COLLABORATION

In 2018, the FY18 Omnibus Spending Bill included language that allotted a portion of the CASL funding to collaborate “with the Nuclear Regulatory Commission to evaluate the use of high-fidelity modeling and simulation tools in the regulatory environment.” To this end, a program plan was developed in conjunction with NRC, starting in late 2018, to achieve this mandate. The program plan, titled “DOE and NRC Collaboration on the Use of CASL Tools in a Regulatory Environment” [37] identifies the objectives, key collaboration areas, and specific milestones that were part of the CASL planning process for FY19 and FY20.

The primary objective of the program plan was the use of existing capabilities of CASL to demonstrate the potential benefits that advanced modeling and simulation can have in the NRC’s regulatory framework through collaboration. The high-level activities include:

- Direct collaboration with the NRC on advanced modeling and simulation, including knowledge and technology transfer,
- Evaluate the existing capability, within VERA, for core and fuel performance analyses of current PWR/BWR concepts,
- Evaluate the existing capability, within VERA, for advanced fuel concepts such as chromium-coated Zr-based claddings, chromium-doped UO₂ fuels, FeCrAl claddings, and U₃Si₂ fuels.

Table 5 displays the primary Tasks for the CASL and NRC collaboration. Tasks 1 through 7, exclusive of Task 6, have been developed to provide new capabilities to the NRC through training, knowledge & software transfer, linkage of NRC and DOE codes, development and documentation of new material property models for advanced fuels and materials (especially for ATF), and benchmarking of high-fidelity solutions to NRC’s methods. Task 6 was developed to provide NRC with an industry perspective on the application of VERA from the viewpoint of economic and commercial benefits. A total of 35 milestones for the 7 task areas were established and delivered in a collaborative manner between the DOE and NRC.

Task	Task Description
1	Positioning NRC for evaluation of CASL software use in a regulatory environment
2	Advanced fuel materials models development, UQ and documentation
3	Generation of benchmark progression problems for current & advanced fuel reloads
4	Comprehensive Reactor Analysis Bundle (CRAB) development for TRACE-BISON
5	Establishment of CFD two-phase flow capabilities for software in use at NRC
6	Development of a report on industry application of VERA for PWR reload design
7	VERA ex-core capability development and NRC collaboration

Table 9. CASL and NRC Primary Collaboration Tasks

For each of the Tasks 1 through 7, exclusive of Task 6, NRC points of contacts were assigned to facilitate the collaboration activities which involved working closely with DOE personnel towards the completion of each task. Collaboration took on many forms and included: 1) providing continual technical review and feedback on each task, 2) exercising DOE software through performance of independent analysis, 3) engagement of broader NRC personnel, especially in the Office of Nuclear Reactor Regulation (NRR), to facilitate knowledge transfer via workshops and seminars, and 4) software activities involving NRC code coupling with DOE codes, such as defining of software requirements and coupling specification, as well as direct coding activities.

The DOE and NRC collaboration on the use of advanced modeling and simulation in a regulatory environment has been fruitful. The collaborations initiated within the CASL program have continued within the integrated CASL and NEAMS program. There has been significant progress towards NRC personnel gaining experience with the CASL developed tools and VERA code suite through VERA industry training and hands-on code execution (Figure 27). DOE has stood up the Sawtooth cluster where all codes of interest to the NRC reside and available for use, under NQA-1 quality assurance.



Figure 27. VERA Training at Oak Ridge National Laboratory (February 2019)

The collaboration with the NRC has involved a number of code linkages of NRC codes with DOE codes. Notably, the NRC's fuel performance code, FAST, and NRC's systems code TRACE. CRAB coupling based on MOOSE multi-apps was successfully demonstrated for BISON and TRACE which was also important for ATF and the LOCA challenge problem. VERA linkage was also performed with FAST leveraging the ECI library of TRACE and the data interface interfaces developed under CRAB. Whole-core pin-by-pin calculations for

FAST coupled through VERA have been demonstrated with the interface and visualization tool, VERA-View, made available to NRC through the VERA distribution.

PART 7: VERA FUTURE CAPABILITY DEVELOPMENT

TWO-PHASE FLOW AND ADVANCED LWRS

The VERA capability for PWR steady-state and transient reactor and ex-core analysis is quite mature with numerous applications demonstrated for reactors within the current operating fleet. Advanced LWRs include large-scale systems, such as the Westinghouse AP1000®, and a number of small modular reactors (SMRs) that continue to be developed and are expected to be deployed in the near future. SMRs are characterized by simplified design features, such as integrated reactor vessel and steam generators, off the shelf components, and factory completed module construction. SMRs being developed include designs by NuScale, Holtec (SMR-160), and General Electric (BWRX-300). Advanced passive safety systems are the hallmark of advanced LWRs. An example of passive safety is the reliance on physical phenomenon, such as natural circulation, to remove decay heat from the reactor core instead of cooling pumps which require a source of external power.

Full system modeling beyond the core remains a priority as a means to provide complete analysis for current operating as well as advanced LWRs with passive safety systems. Preliminary coupling of VERA to TRACE has been performed as part of the CASL NRC collaboration with explicit boundary conditions (time lagged). However, to fully resolve the transient solutions implicit coupling approaches need to be implemented. This capability is needed for the introduction of advanced fuel products (i.e. ATF, high-burnup fuel, high-enriched fuel) which would require transient licensing for postulated accident scenarios. In addition, the NRC through their CASL collaboration has expressed a strong interest for implicit systems coupling with CTF, the thermal-hydraulic code within the VERA code suite.

The extension of VERA to BWRs is being performed under a two-year funding project performed in collaboration with Exelon. This is addressing two-phase flow modeling, including the effects of coupled neutronic and thermal-hydraulic feedback, especially as it relates to prediction of reactivity and thermal margins. Accurate power predictions for problems characterized by significant voiding within the reactor core and systems depend on accurate modeling of the moderator density feedback on the neutronic conditions. In addition, reliance on natural circulation flow, a key feature of passive safety for both BWR and advanced LWR designs, introduces further complexity for two-phase flow modeling. Therefore, for LWRs operating in highly voided conditions improvements in simulation capabilities resulting from changes in the neutron spectrum from changes in neutron moderation is extremely important to better understand reactivity, fuel depletion and isotope inventory, and operating cycle length.

To this end, the following capabilities for VERA are identified:

- Fully coupled, multiphysics modeling of BWR core behavior including control blade operational behavior, bypass flow modeling, and complex fuel geometry (water rods/boxes/crosses, part length rods, gad and enrichment zoning).
- Validation of LWR capabilities against current BWR operating reactor data (cycle energy capability, reactivity and thermal margins) to support advanced LWR reactor designs, using data spanning the range of power and flow conditions as well as shutdown criticality.

- Application of BWR modeling for power/flow exclusion zones, power uprate (high void) conditions and thermal-hydraulic stability (transient modeling) (Identified as a high priority NRC need)
- Demonstration of modeling natural circulation for PWR and BWR SMR, including system response to thermal-hydraulic instabilities.

Another key area of research is the development of fluid models that are applicable for all two-phase flow regimes, from subcooled boiling through dry out, under both forced convection and natural circulation. This will build on work performed within CASL for modeling of BWR two-phase flow in the annular flow regime [38]. These will be critical to the successful prediction of core void and power distributions within the reactor as well as the transient system response. Such closure development is needed for purposes of both CFD, reactor core subchannel simulation, and systems analysis for design basis events.

ADVANCED TECHNOLOGY FUELS

Advanced technology fuels refers to both Accident Tolerant Fuel (ATF) as well as advanced fuel products, such as high-burnup (HBU) and high-enriched (HE) fuel based on current UO_2 -Zircaloy fuel. ATF has the potential to enhance overall safety for the current nuclear operating fleet while providing significant economic benefits through a reduction in nuclear generation costs. The stated requirements for ATFs are improved plant safety performance with respect to loss of active cooling (i.e. improved coping time) during design basis accident and beyond design basis accident scenarios such as long-term station blackout. In addition, ATFs should demonstrate equivalent performance during normal operations and AOOs. The strategy for development and deployment of ATF is based on an aggressive goal of introducing reload quantities of ATF in commercial reactors in the 2025-2026 time frame. This will entail the assessment of ATF performance under normal and off-normal conditions for PWR and BWR reactors and NRC licensing of ATF for partial core reloads to affirm the safety benefits of ATF.

In addition to ATF, all US utilities are considering extension of existing fuel burnup based on UO_2 -Zircaloy beyond the existing licensing burnup limits of 62 GWd/t to 75 GWd/t. HBU is an economic incentive to reduce fuel cycle costs by increasing overall batch discharge burnup. In addition, HBU can be used in tandem with increases in batch enrichment beyond the existing 5 w/o to economically extend fuel cycle lengths (e.g. 18 months to 2 years) for the dominant class of PWR reactors within the US operating fleet.

VERA should be well-suited to analyze all advanced technology fuels envisioned for the current and future operating fleet. Two main focus areas for advanced technology fuels as relates to VERA are identified. The first is based on assuring that VERA is capable of modeling the key phenomena of interest, including validation through experiments such as TREAT, and the second is based on assuring that VERA is capable of modeling all anticipated licensing and operational scenarios. Goals include:

- Validation of near-term (e.g. chromium-coated and FeCrAl clad, chromium-doped fuel forms) and long-term ATF fuel concepts (e.g. SiC clad, U_3Si_2 and UN fuel forms) for key physics parameters (e.g. fission gas release, conductivity)
- Fuel performance model development and validation to support extending the burnup of LWR fuel from 62 GWd/t to 75 GWd/t

- In tandem with enrichment increases >5 w/o, high-burnup fuel assessment of core performance for extended fuel cycles (>2 years) for licensing scenarios such as LOCA
- Integration of LWR core analysis capability with systems codes to simulate PWR and BWR licensing transient events, including post-CHF modeling, for ATF fuel transition cores and full core reloads (Identified as a high priority NRC need).
- Application of LWR capability for limiting licensing events for ATF fuel for PWR and BWR operating cores targeted for first advanced technology fuel reloads (lead test rods and assemblies, transition and full core)
- Validation of LWR predictive capability using reactor operational data for first insertion of advanced technology fuels into PWR and BWR operating cores

REACTOR AND COMPONENT LIFETIME ANALYSIS

Advanced M&S for nuclear materials component damage when combined with data analytics and time-dependent reliability analysis offers a significant opportunity to reduce the maintenance costs for nuclear power plants while increasing reactor availability due to fewer unplanned outages. A key area of potential use of data analytics in conjunction with advanced M&S is with respect to reactor materials degradation due to mechanical and thermal cycling as well as a high radiation environment. This is important for assessing and managing component damage and is part of normal plant maintenance. For example, propagation of micro-cracks could be modeled with advanced M&S and supplemented with measured plant data, such as vibrational frequencies, to better inform the risk profile for component repair or replacement. This would allow utilities to improve performance and reduce production costs via a more focused effort on maintenance planning in a proactive manner. VERA is well-positioned to become the platform for performing such real-time analysis of reactor behavior. The use of VERA as a ‘digital twin’ that can be used in core monitoring with real time data collection (via the plant process computer) is very attractive in this regard as it would provide further value for VERA as a projection and potential plant upset recovery tool.

The ability of VERA to calculate fluences based on a high resolution, time-dependent source term distribution for the reactor core has been demonstrated for the vessel beltline and shown to be highly accurate using measured coupons. This same capability can be translated to all reactor and plant components whose lifetime may be limited by radiation damage. This includes not only the reactor core structural components and vessel subject to neutron damage but also regions such as the concrete shield that are subject to damage via gamma dose. The capability of VERA to provide the complete neutron and gamma distributions for the reactor core therefore provides a unique opportunity in the area of component aging and lifetime extension.

Materials damage codes for component steels and concrete rely upon fluence as input to their radiation damage models. Straightforward one-way coupling of VERA to such codes allows for determination of the true fluence fluence analyses based on ‘representative’ fuel loading patterns that are assumed to be conservatively bounding. However, such conservative assumption may be easily challenged based on changes to the fuel management strategy which depends highly on the fuel located in limiting core locations. For example, beltline fluence greatly depends on the power of the first few rows of fuel rods located on the periphery adjacent to the baffle. As future cores move to ATF and HBU/HE fuel

designs, the potential exists to invalidate existing conservative assumptions related to fluence or alternatively, provide additional margin to materials limits.

With respect to balance of plant modeling, coupling of VERA with a systems code such as TRACE, already described as a high priority, provides a complete simulation capability for the nuclear steam supply system (NSSS) that can be used to simulate the long term performance of not only the reactor core but also the system response changes required to perform normal reactor operational maneuvers. This includes a host of operational events such as load follow response, periodic testing, reactor coastdown, and AOOs. All such events induce mechanical and thermal cycling of components through changes in power, flow and temperature which have an impact on component lifetime. The use of VERA as a 'digital twin' to simulate in high resolution detail the behavior of all components within the NSSS provides a new opportunity for expanded use throughout the nuclear operating fleet.

A significant effort currently exists through the LWR Sustainability (LWR-S) program to provide advanced monitoring and diagnostic capabilities as a means to improve plant performance and extend plant operating lifetime. This has resulted in a wealth of data that is available for use to provide a deeper understanding of plant dynamics and performance as relates to operations as well as areas such as plant maintenance. The use of data analytics combined with VERA simulation offers the potential for improved predictions with reduced uncertainties where there is a lack of data for simulation model parameters. Such uncertainties may arise from incomplete knowledge that arises out of an ability to measure certain plant parameters or deviations that arise through normal processes such as reactor maintenance.

Specific goals include:

- Extension of LWR capability to allow for modeling of all reactor structural in-core and ex-core structures for neutron and gamma dose including coupling with material damage models for purposes of component lifetime assessment
- Validation of LWR predictive capabilities against reactor structural material damage data (e.g. vessel, shroud, concrete, core support components, top and bottom nozzles)
- Predictive component failure model development based on reactor operating history and measured component damage using ModSim combined with data analytics.
- Complete VERA integrated capability system, subsystem and component level modeling for simulation of overall system behavior
- Integration of VERA system modeling with dynamic component reliability modeling for optimization of plant operational maneuvering and maintenance schedule

CONCLUSIONS

CASL has completed its mission with the completion of the CASL challenge problems and maturation and deployment of VERA software code suite to industry. This has been achieved via key accomplishments associated with completion of CASL's challenge problems, development of new VERA capabilities such as VERA-Shift, and expansion of engagement with the nuclear industry through a growing list of new applications. The VERA Users Group has been stood up as the mechanism to continue VERA support post-CASL with a continuing maturation of the VERA as the user base has grown. Engagement with the NRC has been productive through establishment and execution of a formal collaboration program focused on the use of CASL tools in a regulatory environment.

The CASL program has fulfilled its end-state vision and has laid strong path towards establishing VERA as a set of tools widely used by industry, academia, and the national laboratories for advanced simulation and analysis of commercial LWRs. VERA development will continue through the CASL and NEAMS integrated program and will continue to engage the LWR community on future challenges facing the nuclear energy industry.

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