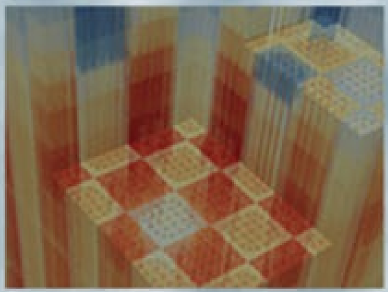
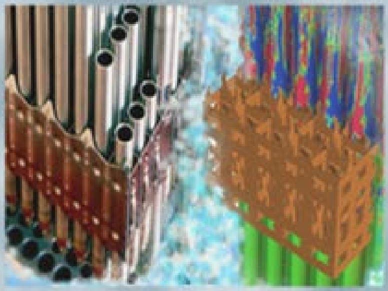
CASL-U-2020-1958-000
ORNL/SPR-2020/1761

Consortium for Advanced Simulation of Light Water Reactors



DOE and NRC Collaboration on the Use of CASL Tools in a Regulatory Environment

Status Report



July 2020

REVISION LOG

Revision	Date	Affected Pages	Revision Description
0	9/30/2020	All	Original

Document pages that are:

Unlimited: All

Export Controlled: None

IP/Proprietary/NDA Controlled: None

Sensitive Controlled: None

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ACRONYMS

AMA	Advanced Modeling Application Focus Area
ANL	Argonne National Laboratory
ANS	American Nuclear Society
ATF	accident-tolerant fuel
B&W	Babcock and Wilcox
BWR	boiling water reactor
CASL	Consortium for Advanced Simulation of Light Water Reactors
CE	Combustion Engineering
CFD	computational fluid dynamics
CRAB	comprehensive reactor analysis bundle
DNB	departure from nucleate boiling
DOE	US Department of Energy
DOE-NE	DOE Office of Nuclear Energy
FMC	Fuels Materials Chemistry Focus Area
FY	fiscal year
HFP	hot full power
HPC	high-performance computing
HZP	hot zero power
INL	Idaho National Laboratory
LOCA	loss-of-coolant accident
LWR	light water reactor
M&S	modeling and simulation
NEAMS	Nuclear Energy Advanced Modeling and Simulation
NQA	Nuclear Quality Assurance
NRC	US Nuclear Regulatory Commission
ORNL	Oak Ridge National Laboratory
PCMM	Predictive Code Maturity Model
PHI	Physics Integration Focus Area
PWR	pressurized water reactor
R&D	research and development
RIA	reactivity insertion accident
RTM	Radiation Transport Methods Focus Area
SMR	small modular reactor
THM	Thermal Hydraulics Methods Focus Area
TVA	Tennessee Valley Authority
VVUQ	verification, validation, and uncertainty quantification
VERA	Virtual Environment for Reactor Applications
VUG	VERA Users Group
WEC	Westinghouse Electric Company

INTRODUCTION

The Consortium for Advanced Simulation of Light Water Reactors (CASL) was established in July 2010, as the first US Department of Energy (DOE) Energy Innovation Hub. The consortium was initially funded for five years with the goal to develop advanced modeling and simulation (M&S) tools. These tools would be used to analyze issues associated with the operation of US commercial light water reactors (LWRs). During this period, the program focused primarily on capabilities that would solve challenges related to the operation of pressurized water reactors (PWR). In January 2015, the program was extended for an additional five years with the goal of 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) analyses.

In 2018, the FY18 Omnibus Spending Bill included language that allotted a portion of the CASL funding to collaborate "with the U.S. Nuclear Regulatory Commission to evaluate the use of high-fidelity modeling and simulation tools in the regulatory environment." From this, a program plan in late 2018, was developed in conjunction with the NRC. The program plan, titled "DOE and NRC Collaboration on the Use of CASL Tools in a Regulatory Environment" (CASL-I-2018-1623-000, 2018), identifies the objectives, key collaboration areas, and specific milestones that were part of the CASL planning process for FY19.

The primary objective of the NRC/CASL program plan was the use of existing CASL capabilities to demonstrate the potential benefits that advanced modeling and simulation can have in the NRC's regulatory framework. 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 concepts such as Cr-coated Zr-based claddings, Cr-doped UO_2 fuels, FeCrAl claddings, and U_3Si_2 fuels.

The NRC/CASL program plan is comprised of seven tasks and are tabulated in Table 1.

Table 1. CASL-NRC Collaboration Primary Tasks

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

With the exception of Task 6, Tasks 1 - 7, have been developed to provide new capabilities to the NRC through training, knowledge & software transfer, coupling of NRC and DOE codes, development and documentation of new material property models for advanced fuels and materials, 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. All milestones have been developed in a collaborative manner between the DOE and NRC.

NRC ENGAGEMENT

For all tasks in the NRC/CASL program plan apart from 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, which included:

1) providing continual technical reviews and feedback on tasks,
2) exercising DOE software through performance of independent analysis,
3) NRC engagement through workshops and seminars to facilitate knowledge transfer, and
4) code development activities such as code coupling between NRC & DOE codes.

MILESTONES

All deliverables related to the NRC / CASL program plan are categorized into seven major tasks, as defined in Table 1. Table 2 provides a brief description of each milestone defined as deliverables within the overall CASL program plans.

Table 2. CASL Milestones Related to NRC Collaboration

Task	CASL Milestone ID	CASL Milestone Description	Finish Date
1	ACT:AMA.US.P19.01	Support VERA releases and user requests (including Test Stands)	9/30/2019
1	ACT:AMA.US.P19.02	User Training	9/302019
1	L1.CASL.P19.01	NQA-1 Certification and Audit [see footnote]	9/30/2019
1	L3:PHI.PCI.P18.02	Document interface to couple external fuel performance codes (e.g. NRC code)	3/30/2019
1	L3:PHI.TRN.P19.01	Develop coupling interface to systems code for transient analysis (VERA/RELAP5)	9/30/2019
1	L3:AMA.NRC.P19.01	Develop two-way coupling between VERA and NRC's fuel performance code, FAST	8/19/2020
2	L3:FMC.FUEL.P19.08	NRC Engagement on advanced technology fuels (Zry coatings, FeCrAl, and doped UO_2)	9/30/2019
2	L2:FMC.FUEL.P19.01	Modeling of mechanical integrity of coated Zr-based cladding for accident tolerance	9/30/2019

2	L3:FMC.FUEL.P19.02	Modeling the thermo-mechanical behavior of chromium based coated zirconium alloys	9/30/2019
2	L3:FMC.FUEL.P19.03	Modeling fission gas release from doped oxide nuclear fuel	9/30/2019
2	L3:FMC.FUEL.P19.04	Modeling the plasticity and thermal creep of doped oxide nuclear fuel	9/30/2019
2	L3:FMC.FUEL.P19.05	Fission gas and creep in uranium silicide fuel	9/30/2019
2	L3:FMC.FUEL.P19.06	Material model development and validation for priority fuel concepts (doped UO2)	7/30/2019
2	L3:FMC.FUEL.P19.07	Material model development and validation for priority cladding concepts (Zry coatings and FeCrAl)	8/30/2019
2	L3:FMC.FUEL.P19.12	Data driven constitutive model for FeCrAl	9/30/2019
2	L3:FMC.FUEL.P19.13	Mesoscale Material Model Development for priority fuel concepts (doped UO_2)	8/30/2019
2	L3:AMA.NRC.P19.08	Steady-state benchmarking & documentation - Existing AMA plants	3/1/2020
2	L3:RTM.XSN.P18.01	Development of SAMPX 51 group ENDF/B-VIII.0 MPACT library to support FeCrAl, U_3Si_2, and SiC	2/28/2019
2	L3:PHI.ATF.P18.01	VERA enhancements to support Cr-coated claddings, Cr-doped fuels, FeCrAl, etc.	1/31/2019
2	L3:PHI.ATF.P18.02	Improvements to CTF Fuel to support Cr-coated claddings, Cr-doped fuels, FeCrAl, etc.	3/31/2020
3	L3:AMA.NRC.P18.02	PGP/VERA Comparisons for non-ATF	2/28/2019
3	L3:AMA.NRC.P19.02	PGP/VERA Comparisons for HALEU/HBU fuel with FeCrAl cladding and benchmarking application	8/31/2019
3	L3:AMA.NRC.P18.03	Develop Benchmark Problems for NRC code comparisons for U3Si2, Cr-coated claddings, and UN fuels.	3/31/2019
4	L2:FMC.P18.01	Demonstration of TRACE/Bison LOCA capability for LWR and FeCrAl fuel (FY19.CASL.003)	3/18/2019
5	L3:THM.NRC.P19.02	Establish DNB Test Stand at NRC	6/30/2020
5	L3:THM.NRC.P19.01	PETHeR Engineered Surface Boiling Tests to support characterization of surface effects	5/31/2020
5	L3:THM.NRC.P19.03	Revision and Validation of surface boiling closure models based on PETHeR testing	5/31/2020
6	L2:AMA.P19.05	Steady-state benchmarking & documentation - Westinghouse data and processes (FY19.CASL.011)	9/30/2019
6	L3:AMA.CP.P18.12	RIA application for Westinghouse and DG1327	3/1/2020
6	L3:AMA.NRC.P18.04	VERA application to PWR DNB-limiting conditions	3/1/2020
7	L3:AMA.RX.P18.04	Validation of VERA ex-core transport capability	3/1/2020
7	L3:AMA.RX.P19.01	Incorporation of VERA (SHIFT) neutron flux calculations into a RPV analysis with Grizzly	9/30/2019
7	L2:RTM.MCH.P19.02	Shift I/O optimization	9/30/2019
7	L3:RTM.MCH.P19.03	Shift usability updates for production release	9/3/2019

7	L3:AMA.RX.P19.04	Demonstration of Comprehensive Ex-Vessel Fluence Capability	10/31/2019

Note: NQA-1 certification and audit tasks were funded under Task 4 but will be grouped as part of Task 1 for purposes of the discussions

The following discussion provides a high-level summary for each task while providing references in the form of CASL reports.

TASK 1. POSITIONING THE NRC FOR EVALUATION OF CASL SOFTWARE USE IN A REGULATORY ENVIRONMENT

Task 1 provided the NRC with the initial knowledge needed to use VERA. Specific activities in Task 1 included:

- initiating a workshop on identifying potential NRC use of CASL tools,
- providing training courses for NRC staff on the CASL tools,
- maintaining builds of VERA on computing hardware available to the NRC, and
- providing the NRC user-support and expert knowledge to support the application of CASL tools.

Within Task 1, several meetings were held at NRC headquarters with the goal of refining the scope of the NRC/CASL program plan. In November 2018, the need for coupling TRACE and FAST to CASL tools were established and formalized as specific tasks in the program plan (i.e., extension of Task 1 and creation of Task 4). Task 1 was expanded to include the coupling of FAST & VERA (specifically CTF), where the coupling would leverage the MOOSE coupling interface.

TRAINING AND WORKSHOPS

In February 2019, a 3-day workshop was held on the use of the VERA platform. During this training, seven NRC personnel from both the Offices of Nuclear Regulatory Research and Nuclear Reactor Regulation attended, as part of a broader group that included 38 individuals representing 18 organizations.

The training included presentations by CASL researchers and developers via detailed course modules on VERA methods (e.g., single physics codes and multi-physics coupling). The workshop included hands-on access to the VERA software via the Lemhi cluster at Idaho National laboratory with a resource reservation that enabled rapid turnaround of parallel VERA executions (1,000 cores/run). Through participation of the training, NRC users have been provided accounts and login credentials for use of VERA. This have now been extended with access to the Sawtooth cluster that was stood up by INL in early 2019 along with the latest version of VERA (version 4.1), released under the VERA NQA-1 program in April 2020, available to NRC personnel.

With access to VERA, the NRC is also a member of the VERA Users' Group (VUG), which last met in May 2020. The VUG, comprised currently of 23 industry organizations,

is a forum for VERA users to share their experience in specific applications with the code suite to the general user-base, and to provide direct feedback on additional capability needs to the VERA development team. NRC is participating by exercising reactor core models released to the VERA user group for safety analysis-type simulations using both VERA and their traditional core analysis workflow. Use of VERA as a computational reference solution can help identify areas where legacy methods need to be refined and improved.
Additional workshops

have been held at NRC HQs. A workshop held in November 2019 showcased the use of VERA-Shift for external core calculations. Topics included the applicability of VERA-Shift for fluence analysis and methodologies for lifetime analyses. Other applications showcased during the workshop included the use of VERA-Shift for performing beyond the beltline region, including baffle bolt analyses and ex-core detector response function analysis.

The topic of verification, validation, and uncertainty quantification (VVUQ) is also a keen interest to the NRC. To support the NRC in this area, a workshop was held in Raleigh, NC on CASL's approach to VVUQ. This included detailed presentations on the CASL implementation of the Predictive Code Maturity Model (PCMM) for the VERA software, as well as sharing best practices and experiences in code and solution verification. Follow-on seminars are planned for the Fall 2020 on the topic of VVUQ for both the technical staff and NRC leadership with the goal of providing further knowledge transfer of CASL's best practices of VVUQ. Specific topics for the Fall 2020 seminars are to provide the NRC with practical applications of VVUQ; providing decision-makers with information on when to trust a model and simulation.

VERA NQA-1 PROGRAM IMPLEMENTATION

As part of the deployment of VERA, for production use, an initiative was undertaken to bring VERA under the NQA-1 software quality assurance standard, based on ASME NQA-1-2008, Quality Assurance Requirements for Nuclear Facility Applications and the NQA-1a-2009 Addenda. To this end, a VERA NQA-1 program plan was developed for all codes within the VERA code suite including MPACT, CTF, BISON, Shift and MAMBA. The NQA-1 program replaces the previous CASL Quality Assurance program and removed a primary barrier for adoption of VERA by the broader nuclear industry as well as NRC. The VERA NQA-1 program takes a graded approach to the software development process, recognizing several maturity levels (SQL1 through SQL4) for code development. This is fully discussed in the "VERA Quality Assurance Program Plan" (VERA-QA-001, Rev. 1) as shown in Figure 2. Note that BISON is an INL-developed fuel performance code and is developed under the INL software quality assurance program which follows a similar NQA-1 compliant program. A successful external audit of VERA (exclusive of BISON), at ORNL, was performed in August 2019 with a subsequent successful audit of BISON at INL occurring in February 2020.

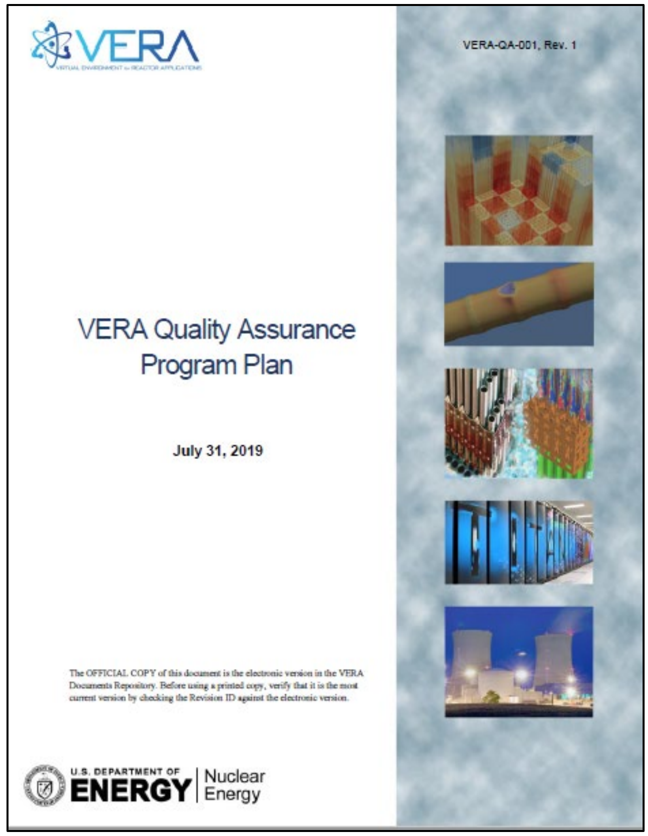

Figure 1. VERA Quality Assurance Program Plan

COUPLING OF VERA WITH NRC CODES

Additional activities under Task 1 focused on the coupling VERA and native NRC codes. This included coupling VERA to NRC's fuel performance code FAST and NRC's systems analysis code TRACE. These activities are aligned with the ability to model advanced fuel concepts for confirmatory analyses. Milestones include:

- Couple and demonstrate interoperability of VERA with the NRC's fuel performance code, FAST, and
- Develop a coupling interface for VERA to NRC's systems code TRACE, for transient analysis.

The coupling of VERA & FAST was achieved by refactoring CTF, a subchannel thermal-hydraulic solver, and extending the fuel solver base class to allow for general coupling of any external fuel performance code. The coupling of FAST leverages work that was performed for the development of CRAB (i.e., Task 4), which has recently been extended to include the coupling of FAST and TRACE.

The VERA/FAST coupling has successfully been demonstrated for one-way coupling with the ability to execute all fuel rods in parallel within a VERA quarter core model. This entailed approximately 14,000 FAST individual fuel rod calculations with the results available to be viewed in VERAView. The one-way VERA/FAST coupling is currently available within VERA and accessible to the NRC. Additionally, VERAView has been provided separately to NRC under open source that can be used a visualization tool.

The two-way coupling of VERA and FAST has been performed for a single fuel rod as a demonstration, but additional support beyond a single fuel rod is pending and awaiting the completion of the FAST and TRACE coupling for multiple fuel rods.

The VERA and TRACE coupling was performed via VERA's sub-channel thermal-hydraulic code CTF. This was achieved using a non-overlapping domain, with boundary conditions exchanged for each code at the core inlet and outlet locations in an explicit coupling as shown in Figure 3 (Wysocki, et. al 2019).

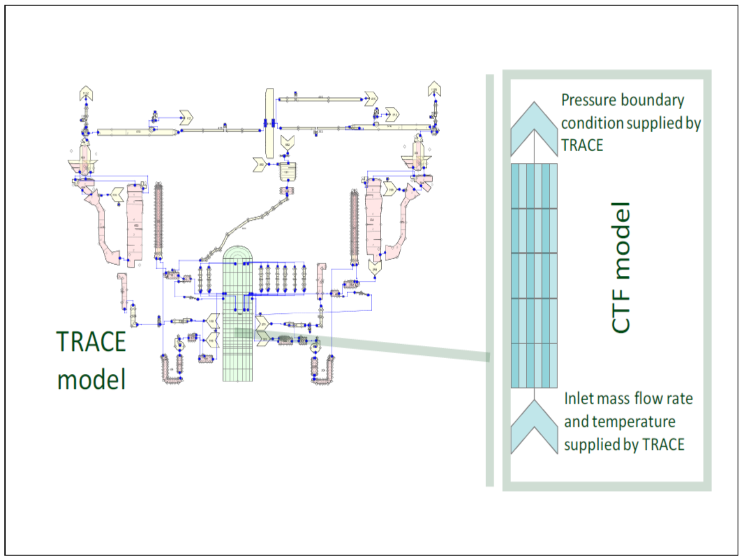

Figure 2. TRACE and CTF coupling scheme

In this coupling scheme, CTF models the details of the core while TRACE models the balance of the system. The use of the TRACE's Exterior Code Interface (ECI) library, available as part of TRACE version 5, was incorporated as part of the CTF build. ECI provides a generic interface for exposing solution variables required by TRACE and CTF, as well as enabling the communication between codes. The integration of CTF and TRACE provides pin-by-pin resolution of core parameters in response to system changes. Additional work remaining is validation for a range of transients in consideration of solution robustness and numerical stability and, if necessary, implement an implicit/semi-explicit coupling scheme.

TASK 2. ADVANCED FUEL MATERIALS MODELS DEVELOPMENT, UQ AND DOCUMENTATION

Task 2 focused on the development of advanced materials models which included advanced fuel forms such as U_3Si_2 and Cr-doped fuel and advanced claddings such as Cr-coated zirconium alloys and FeCrAl claddings.

Advanced fuels and claddings, under loss of active cooling, are sometimes characterized by:

1) Improved reaction kinetics with steam (lower oxidation rates, decreased heat of oxidation, reduced hydrogen embrittlement, and reduced hydrogen production).

2) Improved fuel properties (lower fuel temperatures, high fuel melt temperatures, reduced cladding internal oxidation, and reduced fuel relocation/dispersion).

3) Improved cladding properties (resilience to fracture, geometric stability, resistance to thermal shock, high clad melt temperature, and minimal fuel-clad interactions; and

4) Enhanced retention of gaseous and solid/liquid fission products.

These detailed models, developed by CASL, have been provided to the NRC, in a series of reports that will allow the NRC a greater understanding of BISON and potentially allowing the incorporation these models into NRC's developed codes (e.g., FAST).

These efforts for advanced fuel claddings are summarized in the report "ATF material model development and validation for priority cladding concepts" (Gamble, 2019). This report describes the material property models and their implementation in BISON. Concepts included within this report are existing Zirconium-based cladding, chromium-coated claddings, and FeCrAl-based claddings. Also included in this report are sensitivity and uncertainty analyses for different cladding material relative to burst pressure behavior under LOCA conditions.

The development efforts for advanced fuel forms are summarized in the report "ATF material model development and validation for priority fuel concepts" (Gamble, 2019). This report describes the material property models and implementation in BISON, for fuel concepts of Cr_2O_3-doped UO_2 fuel and Uranium Silicide (U_3Si_2).

Both reports provided the NRC with material properties that were used to evaluate new advanced concepts within the NRC's material property library.

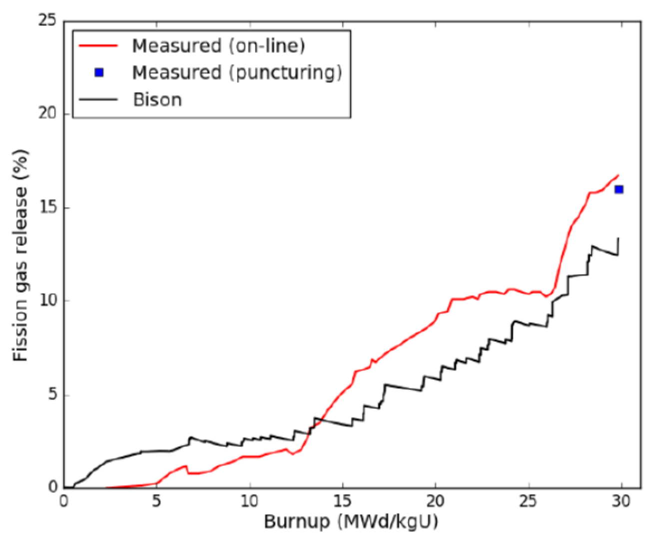

Figure 3. BISON Predicted Fission Gas Release for Cr-doped UO2 fuel (Halden)

Validation of the Cr_2O_3-doped fuel was performed against integral fuel rod data from Halden which included measured fuel centerline temperature, internal rod pressure and fission gas release (Figure 4). For U_3Si_2, validation was performed to recent PIE data for the ATF-13 R4 and ATF-15 R6 rodlets irradiated in the ATR at INL. These experiments investigated low-burnup behavior of U_3Si_2 with respect to axial elongation of the fuel stack, clad outer diameter, and fission gas release. Sensitivity and uncertainty analyses were performed with respect to fission gas release and fuel elongation for both fuel forms. It is noted that much of fuel form development is supported by lower length scale modeling as described in the reports "Mesoscale Material Model Development for priority fuel concepts (doped-UO_2 and U_3Si_2)" (Aagesen, et. al., 2019), "Modeling fission gas release from doped oxide nuclear fuel" (Cooper, et. al., 2019), and "Fission gas and creep in uranium silicide fuel" (Cooper, et. al., 2019).

TASK 3. GENERATION OF BENCHMARK PROGRESSION PROBLEMS FOR ADVANCED FUEL RELOADS

Task 3 focused on the development of VERA models loaded with various advanced technologies such as uranium silicide fuel forms (Davidson, et. al. 2019), High-Assay, Low-enriched Uranium (HALEU), and FeCrAl cladding (Novellino and Jessee 2019). These models serve as a high-fidelity, high-resolution reference solution to identify limitations in the two-step neutronics analysis employed by NRC, typically used in the calculation of key core parameters, such as reactor pin power distribution.

The traditional two-step method is widely deployed throughout the nuclear industry. This methodology is based on a series of single fuel assembly lattice physics calculations (performed in 2-D). A series of these lattice physics calculations are performed, representing different fuel types in the core, all of which are used to generate nuclear cross section tables as a function of different states such as fuel burnup and feedback parameters (e.g., fuel temperature, moderator density, etc.). These tables are then used as input to a 3-D core calculation based on nodal diffusion with reconstruction methods for the pin power.

In contrast, VERA solves the neutron transport equation directly without the approximations associated with the two-step method. Figure 5 displays a comparison between VERA and the two-step process for Watts Bar 1, Cycle 14 power distribution at beginning of cycle. Evident is the higher resolution detail of the VERA solution as compared with the coarse-mesh nodal solution.

One key outcome from Task 3 was identifying where these high-fidelity VERA solutions could be used to improve the existing 2-step process used at the NRC. One area identified was the use of VERA for the generation of nodal nuclear cross section data. This would supplement the lattice physics calculations, during generating the cross-section tables. More specifically, VERA is being assessed for use in generating cross-sections for the interface regions between peripheral fuel, baffles, and the reflector regions. All these regions are used in determining the core leakage, which influences the determination of the radial power profile.

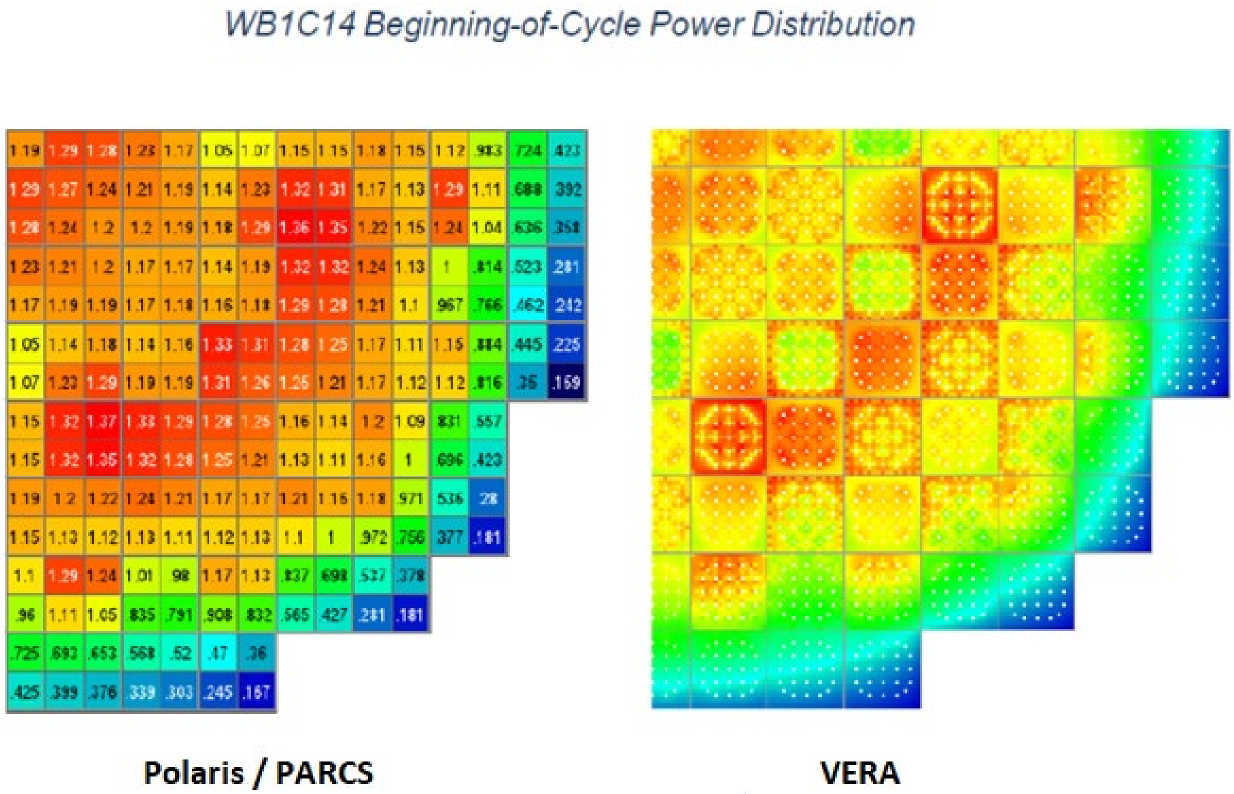

Figure 4. Quarter-core VERA Comparison to Polaris/PARCS (Two-step method)

TASK 4.CRAB DEVELOPMENT

The Comprehensive Reactor Analysis Bundle (CRAB) is the framework adopted by NRC for the coupling NRC codes with DOE codes for purposes of performing confirmatory analysis, primarily for advanced, non-LWR reactors. CRAB is based on the use of the MOOSE framework which allows for coupling via the MOOSE multiapps capability that was developed under the NEAMS program. The use of MOOSE multiapps enables non-MOOSE based codes, such as the NRC codes FAST and TRACE, to be integrated with DOE developed software.

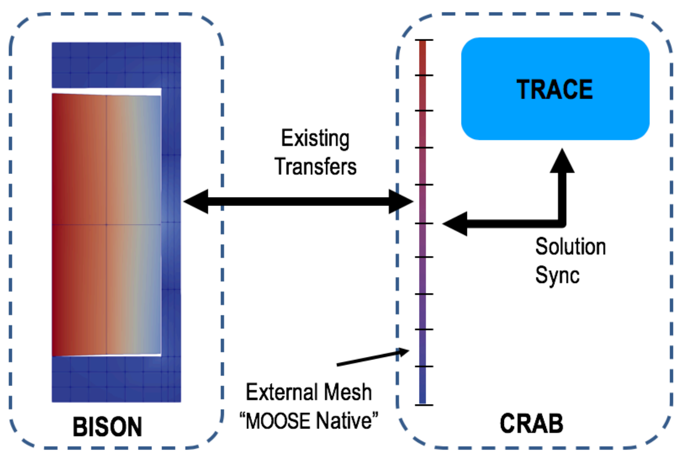

Figure 5. TRACE and BISON coupling scheme

The first CRAB application was demonstrated with coupling DOE's fuel performance code BISON with NRC's systems code TRACE, as shown in Figure 6. This was performed with the goal to demonstrate the MOOSE multi-apps approach for the coupling of independent codes. Working closely with the NRC, the focus was on mapping data transfers between codes, the preservation of conserved quantities based on differing code discretization schemes, and numerical stability of the transient time stepping scheme.

Code validation for the TRACE and BISON coupling was successfully performed through direct comparison from the LOFT L2-5 experiments. The LOFT L2-5 experiments simulated a Loss of Coolant Accident (LOCA) for commercial PWRs (Gardner, et. al. 2019). LOCA was one of the challenge problems within the CASL program for which significant advancements have been made. Significant progress has been made in the areas of thermo-mechanical response of both the fuel and cladding, modeling phenomena such as high-temperature steam oxidation, crystallographic phase transformation, high-temperature creep, and cladding oxidation energy deposition (Williamson, et. al. 2019). The validation to the LOFT experiments complement existing LOCA validation within BISON that include separate effects ballooning and burst experiments as well as integral rod validation tests.

CRAB continues to be actively developed under the NEAMS program for continued integration of DOE and NRC codes for the analysis of advanced non-LWRs.

TASK 5. ESTABLISHMENT OF CFD TWO-PHASE FLOW CAPABILITIES AT NRC

The focus of Task 5 was to establish a CFD test stand for the NRC. The test stand would help develop insight in the area of two-phase flow modeling using STAR-CCM+, a commercial CFD code. Improvements to two-phase flow modeling was achieved with the CASL developed two-phase closure models (Feng, et. al., 2019). The goal of Task 5 was to build confidence in the two-phase flow CFD methods generated by CASL, while focusing on accuracy, robustness, and scalability in prediction of the critical heat flux.

Working with NRC, CFD models are being exercised for purposes of validation against experiments for parameters such as void distributions (Liu and Bankoff, 1993), boiling predictions (Bartolomei & Chanturitya) and fuel bundle applications (Rod Bundle Heat Transfer Test facility). In addition, experiments were performed to characterize the behavior of two-phase flow phenomena (i.e., boiling critical heat flux) for oxidized and chromium-coated Zircaloy-4 surfaces (Seong, et. al. 2019).

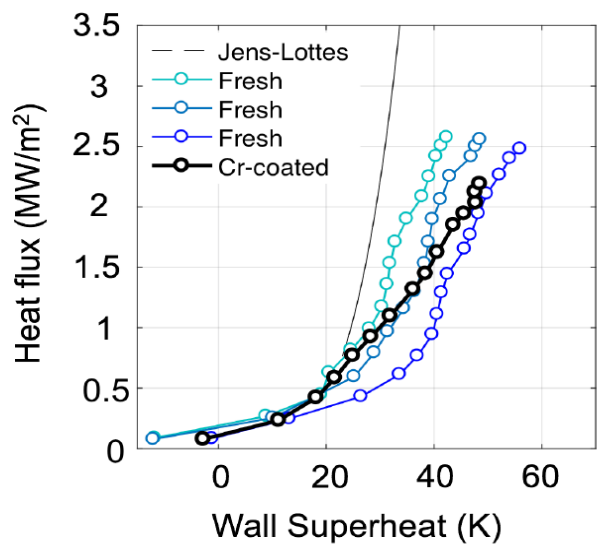

Figure 6. Clad Surface Heat Flux (Zr-4, Cr-coated Zr-4)

This work has direct application to advanced technologies such as coated claddings. Task 5 focused on examining the behavior of cladding surfaces under two-phase flow conditions. Varying surface wettability (i.e. contact angle), 2-D surface profile and roughness were investigated in Task 5.

Coated claddings were found to be more hydrophobic than unoxidized Zircaloy-4 with a larger contact angle and a slight lower roughness. Initial results, shown in Figure 7, displays the cladding surface heat flux as a function of wall superheat, up to the point of critical heat flux. Three samples of fresh zircaloy-4 (3 samples of unoxidized cladding) and one Cr-coated test sample were utilized. As expected, the CHF for the Cr-coated surface is reduced, warranting additional analyses.

TASK 6. REPORT ON THE INDUSTRY APPLICATION OF VERA FOR PWR RELOAD DESIGN

Task 6 focused on benchmarking VERA against nuclear operating fleet measured data and showcased an industry application of VERA for a reactivity insertion accident and DNB design basis events. Task 6 is to provide the NRC with an evaluation of VERA from an industry's perspective, in terms of accuracy, uncertainties, and its potential use in future licensing submittals.

VERA core models were benchmarked against measured data, which included low power physics testing parameters (i.e., critical boron, rod worth, isothermal temperature coefficients) and at-power core reactivity evolution through cycle and periodic flux mapping.

All calculations were performed by Westinghouse and include a range of reactor fuel designs and representative cycle lengths of operating PWRs. Representative designs include 2-loop, 3-loop, and 4-loop reactor designs; various fuel rod designs such as IFBA, WABA, Gadolinia, and Pyrex burnable absorbers, and various assembly designs of 14x14 through 17x17 fuel lattices. In total, 24 cycles of results were analyzed with excellent comparisons with measured data (Mangham, et. al. 2019).

For the control rod reactivity insertion accident (RIA), two reactors were analyzed – the AP1000 Cycle 1 core and Farley Unit 1, Cycle 27 (Kucukoybaci 2020). The analyses included assessment of peak fuel and clad temperatures, linear heat rate, and the maximum liquid temperature which is used in the calculation of DNB as a function of time (Figure 8).

High fidelity, high-resolution VERA simulations were also performed for several NUREG-0800 Chapter 15 transients and accidents such as reactivity-initiated events and several DNB limited licensing events including main steam line

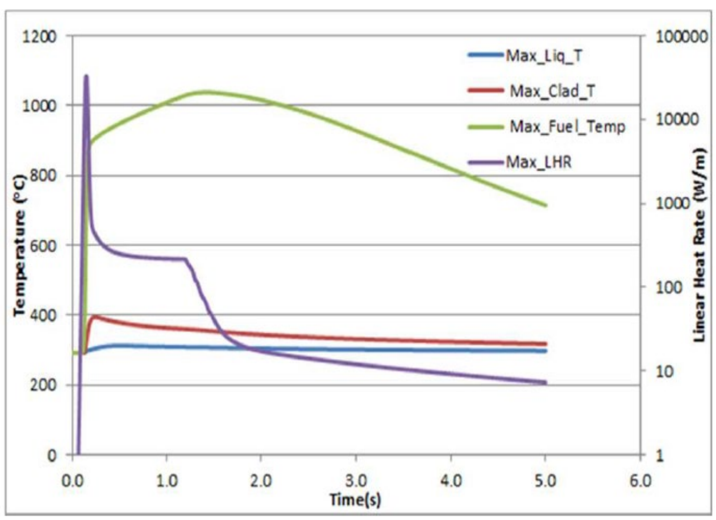

Figure 7. AP1000 reactor core temperatures and linear heat rate for HZP RIA

break and complete loss of flow (Sung, et. al. 2020).

TASK 7. VERA EX-CORE CAPABILITY DEVELOPMENT AND NRC COLLABORATION

The focus of Task 7 was on further developing the coupled VERA-Shift ex-core capability, while engaging with NRC on current development and future capabilities. Task 7 was added as a result of discussion with NRC during a status meeting in April 2019 at NRC headquarters. The scope of this work included improvements to the Shift hybrid approach (CADIS) for variance reduction (especially in regions beyond the beltline), linking of Shift to the Grizzly code for material component damage assessment, and benchmark and validation of VERA-Shift.

The CASL report "Demonstration of Comprehensive Ex-Vessel Fluence Capability" (Davidson, et. al. 2019) summarizes the recent developments of VERA-Shift and describes several benchmark activities for VERA-Shift 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.

Detailed fluence analysis was also performed using measured coupon data from Davis-Besse Cycle 6 (Smith, 2020). 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. Figure 9 displays the Shift calculated to measured reaction rates for the measured quantities. 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
$^{238}U(n,f)^{137}Cs$	0.9671
$^{238}U(n,f)^{137}Cs$	1.0050
$^{237}Np(n,f)^{137}Cs$	0.9815
$^{237}Np(n,f)^{137}Cs$	1.0010
$^{58}Ni(n,p)^{58}Co$	1.0300
$^{58}Ni(n,p)^{58}Co$	1.0340
$^{54}Fe(n,p)^{54}Mn$	1.0440
$^{54}Fe(n,p)^{54}Mn$	1.0500
Average =	**1.014**

Figure 8. Shift Reaction Rates Comparison (Davis-Besse, Cycle 6)

CONCLUSIONS AND FUTURE WORK

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

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. The linkages have been performed with VERA, leveraging the ECI library or through direct calls. This work has leveraged the data 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.

CRAB coupling based on MOOSE multi-apps was successfully demonstrated for BISON and TRACE. Follow-on work with coupling of FAST and TRACE via the CRAB coupling is ongoing. Ongoing work for two-way coupling of FAST and VERA for whole-core, pin-by-pin analysis is dependent upon this work in CRAB being completed.

ACKNOWLEDGMENTS

This research was supported by the Consortium for Advanced Simulation of Light Water Reactors (www.casl.gov), an Energy Innovation Hub (http://www.energy.gov/hubs) for Modeling and Simulation of Nuclear Reactors under US Department of Energy Contract No. DE-AC05-00OR22725.

An award of computer time was provided by the Advanced Scientific Computing Research (ASCR) Leadership Computing Challenge (ALCC) Program. This research used resources of the Oak Ridge Leadership Computing Facility at ORNL, which is supported by the Office of Science of the US Department of Energy under Contract No. DE-AC05-00OR22725.

This research made use of the resources of the High-Performance Computing Center at INL, which is supported by the Office of Nuclear Energy of the US Department of Energy under Contract No. DE-AC07-05ID14517.

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