

CASL TECH NOTES

Consortium for Advanced Simulation of Light Water Reactors

October 2015
Volume 3, Issue 1



VERA Training Workshops held

In April, CASL delivered its first formal "Quick-Start" training at the Advances in Nuclear Fuel Management (ANFM) American Nuclear Society topical meeting. The ANFM topical is a standing meeting that provides a forum for addressing a broad spectrum of front-end nuclear fuel management activities within the context of reactor physics and fuel cycle economics. The meeting has traditionally had a strong utility presence. This inaugural Quick-Start training was extremely successful, with 15 diverse participants.

The hands-on tutorials used with the training are based on CASL's Watts Bar Unit 1 simulations. They sequentially increase in complexity, moving from a 2D fuel rod to a fully detailed 3D reactor core. The progression allows students to quickly understand the basic layout of the code input.

CASL's deployment program includes both Quick-Start training aimed at getting experienced engineers up and running as quickly as possible and a week-long training workshop that provides a deeper explanation of the methods behind the consortium's Virtual Environment for Reactor Applications (VERA). In June, CASL utilized the Quick-Start tutorials again at its annual summer student workshop, with 28 students participating in the event. The class took advantage of the Oak Ridge Leadership Computing Facility's (OLCF's) world-class Titan supercomputer to run the tutorials as part of this year's workshop, which was taught by ORNL's Andrew Godfrey and Robert Salko. Mike Doster, CASL's Education Director and North Carolina State University nuclear engineering (p.7)

About Tech Notes

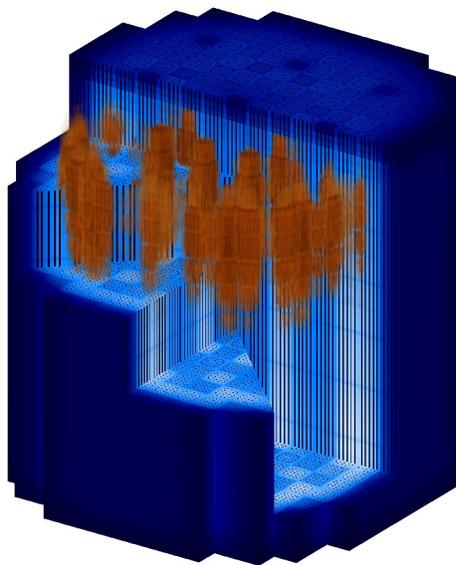
CASL Tech Notes are produced by CASL's technical staff to spotlight areas of particular technical interest and to discuss CASL science and engineering innovation, accomplishments, activities, and plans. Tech Notes is produced on a quarterly basis.

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CIPS Simulation Capability Implemented in VERA

During FY15, CASL significantly advanced VERA's capability to model the CRUD Challenge Problem to predict the occurrence of CRUD Induced Power Shift (CIPS). VERA has been modified to include the space and time dependent deposition of CRUD onto the fuel, along with boron capture and its effects on local rod power and thermal hydraulic conditions. Early in CASL's program, coolant chemistry subcomponents (MAMBA and MAMBA-BDM) were developed to describe local CRUD deposition.



Since then the coolant chemistry subcomponents have been integrated within VERA's subchannel thermal-hydraulics and neutronics subcomponents. Most recently all three subcomponents have been coupled within VERA, allowing VERA to simulate multiple cycles of operation to simulate CIPS. Figure 1 illustrates a VERA-predicted CRUD thickness distribution using 3-physics coupling.

VERA's chemistry component, MAMBA, is used to simulate CRUD growth in the radial direction (1D) above a specified surface area of a fuel rod. (p.10)

Figure 1 CRUD predictions using VERA's coolant chemistry code coupled with sub-channel thermal-hydraulics and neutronics [image courtesy Ben Collins (ORNL)]

Watts Bar Operating Cycles Simulated to Present

Among the most important accomplishments during CASL Phase 1 is the development and deployment of CASL's Virtual Environment for Reactor Applications (VERA), a high-fidelity, multi-physics engineering tool that utilizes modest high-performance computing (HPC) systems and engineering-scale clusters to simultaneously simulate the local fuel rod neutronics and coolant channel thermal-hydraulics over the life of the reactor. VERA has the potential to predict core performance with higher fidelity than is currently afforded by existing industrial codes, and can perform analyses relating to common evolutions of operating commercial pressurized water reactors (PWRs), including startup testing, power escalation, fuel cycle depletion, and fuel assembly discharge, reinsert, and shuffling. To demonstrate VERA's capability, CASL has, in the past, simulated Watts Bar unit 1 (WBN-1). In his most recent installment of (p.4)

Departure from Nucleate Boiling (DNB) Multi-Physics Approach & Applications using VERA

Departure from nucleate boiling (DNB) serves as a critical parameter in nuclear power plant operational and safety analysis. It occurs when a fuel rod clad surface is overheated due to the formation of a local vapor layer on the waterside surface, causing a dramatic reduction in heat transfer capability. DNB is a complex phenomenon that has been experimentally and analytically investigated over the past several decades. Its complexity is inherent in the multi-scale and multi-physics processes (fluid flow, heat transfer, material and surface effects) that govern its occurrence. Simulation is further complicated by the geometric complexity of the fuel assembly design, variability of operating power profiles, and scarcity of open and microscopic experimental test data.

Although DNB is generally associated with local and microscopic vapor formation during overpower conditions (subcooled boiling), liquid film dryout can also occur during some high coolant temperature and low flow accident scenarios. Because of the diverse nature of the physics involved and the importance of the phenomenon, CASL's work on DNB is by nature extremely collaborative, bringing together experts in DNB phenomenology, modeling and simulation, experimental methods & data, and validation and uncertainty quantification (VUQ) methods.

Industry predictions of DNB are currently based on empirical correlations derived from small scale rod bundle tests that simulate each unique fuel assembly design. With the data in hand, a subchannel thermal-hydraulic code is applied to calculate the local fluid conditions in the rod bundle for each test point and these local fluid conditions are then used to develop an empirical DNB correlation. Commercial PWRs must apply regulatory-approved DNB correlations as part of the plant safety analysis.

CASL's coupled multi-physics approach currently utilizes two primary tools: Computational Fluid Dynamics (CFD) is used to provide design-specific turbulent mixing data and subchannel analysis is used for practical application (full reactor core) simulations using CFD-generated results for refinement of the local fluid turbulence. An example of the approach is provided within CASL-I-2014-0119-000 to analyze a postulated PWR main steamline break (MSLB) event initiated at the hot zero power (HZP) with all coolant pumps continuing in operation (i.e., the high flow case).

During a postulated PWR main steamline break (SLB) event initiated from the hot zero power (HZP) condition, the increased steam flow rate from the broken steam pipe on one of the steam generators would result in a significant reduction in the primary coolant temperature and an increase in the reactor core average power and the peak fuel rod power, thus imposing a challenge to the Departure from Nucleate Boiling (DNB) criterion. As required in a PWR safety analysis, the most reactive shutdown control rod assembly is assumed to be stuck in its withdrawn position. A return to power following a steam line rupture is problematic mainly because of the high power peaking factors that exist as a result of the postulated stuck control rod. The core is ultimately shut down by the boric acid injection delivered by the safety injection system.

Westinghouse researcher Yixing Sung is leading CASL's effort to model DNB performance with coupled multiphysics. For this initial demonstration, the team used a five step approach to model the WBN-1 core:

- 1) Deplete the core to the end of cycle 1 and create a restart point for HZP conditions using VERA;
- 2) Generate a reactor system state point with Westinghouse's version of RETRAN from the HZP MSLB transient calculation for use as core boundary conditions;

- 3) Generate the core inlet temperature distribution using CFD (in this case, CD-adapco's STAR-CCM+ was used);
- 4) With VERA's coupled neutronics/T-H capability, predict the quasi-steady state core response (e.g., pin-by-pin power and local fluid conditions in each subchannel); and
- 5) Using the results from 4), calculate the DNB Ratio (DNBR) with VERA's CTF subchannel code.

For this analysis, the RETRAN-generated boundary conditions included:

- ◆ 20% of rated power
- ◆ 421°F inlet average; -37/+10°F variation across the distribution
- ◆ 460 psi system pressure
- ◆ Full core geometry (all 193 assemblies)
- ◆ 0 ppm soluble boron concentration
- ◆ All control rods inserted with one rod stuck in the withdrawn position.

First, the CFD-predicted local temperature and flow rates at the lower core inlet were generated for use as boundary conditions for downstream analysis. Although during the event the low temperature coolant is injected from one cold leg, a cold stream is predicted between the injection cold leg and the adjacent cold leg due to swirling of the flow. Also, the CFD solution exhibits an oscillatory behavior that is attributed to both physical and numerical causes; strong vortex flow in the lower plenum induces a non-uniform pressure upstream and the multi-hole geometry of the lower core plate tends to promote manometer effects numerically. Therefore, a search for bounding cases was conducted. The search was concluded when the flow rate and temperature at the monitored location repeated themselves during iteration and for this simulation the values are considered pseudo-global extremes.

For depletion calculations, a quarter-core model was used in VERA using coupled neutronics/T-H to end of cycle (EOC) 1 at 441 Effective Full Power Days (EFPD), at which point quarter-core model was expanded into a full-core model for the SLB scenario and a restart file was created. The restart state point was set to the limiting DNBR conditions as determined by RETRAN, and the CFD-predicted inlet temperature and mass flow rate distributions were input to VERA. (p.3)

Table 1 Comparison of Hot Channel Parameters for High-Flow SLB Sensitivity Study

Parameter	Uniform Inlet Flow	Non-uniform Inlet Flow	Inlet Temp. Distribution T_MIN	Inlet Temp. Distribution T_MAX
Max. Pin Linear Power (W/cm)	257.0	243.3	232.8	264.9
Max Clad Temp (°C)	274.1	269.9	267.2	276.4
Max Fuel Temp (°C)	1016.6	958.2	906.0	1051.2
MDNBR	10.5	10.5	11.7	10.2
CHF (W/m ²)	8474.0	8274.8	8472.3	8474.6
Heat Flux (W/m ²)	805.1	787.1	724.3	827.3
Eq. Quality	-0.061	-0.067	-0.078	-0.059
Mass Flux (kg/m ² /s)	4462.9	5473.5	4413.4	4410.6

DNB ... continued from page 2

The rupture of a steam line in one of the four primary coolant loops resulted in a highly asymmetric vessel inlet coolant temperature and an asymmetric core power distribution. Because the most reactive control rod was assumed to be stuck outside the core in the same region of the vessel affected by the loop with the steamline break, high power peaking factors occurred in and around the assembly with the stuck rod. Also, because this analysis assumed that offsite power was available, the core flow rate was relatively large at 20% of the nominal. Figure 2 shows the calculated pin power distribution at 45.8 cm from the bottom of the core, along with the full core power distribution and predicted coolant temperature distribution. As illustrated by the figure, the core power distribution was highly asymmetric; the high power assemblies were clustered in and around the stuck control rod location. The hot channel factor was calculated to be ~7.02 with a bottom peaked axial power profile.

Because the axial power was bottom peaked, cross-flow from the surrounding channels into the hot channel appeared to occur only in the first 50 cm of the channel, after which the axial flow either stayed the same or slowly decreased. The enthalpy rise in the hot channel was not rapid, and as a result, the liquid reached saturation temperatures only after 70 cm from the top of the active fuel. Figure 2 shows the 3D liquid temperature distribution, demonstrating the enthalpy rise in high powered regions (i.e., channels surrounding the assembly with the stuck rod). The locations of the cold regions are consistent with the inlet temperature distribution.

A sensitivity calculation was performed to evaluate the impact of the CFD-predicted inlet flow distribution. For a uniformly distributed inlet flow, the effects of inlet turbulence begin to dissipate within the first 122 cm of core entry due to mixing with high flow rates. Although the hot channels are the same for the uniform and non-uniform cases, the axial profiles and hot rods differ due to the higher flow in the non-uniform case. However, the rod temperatures in the non-uniform case quickly drop below those predicted in the uniform case at higher elevations due to larger cross-flow mixing. The equilibrium quality is small in both cases. Boiling starts later in the non-uniform inlet flow case due to larger mixing. The maximum heat flux, hence the margin to DNB failure in terms of minimum DNBR (MDNBR), occurs at the same axial elevation in both cases.

The effect of different inlet temperature distributions with a uniform inlet flow distribution was also evaluated by comparing hot channel conditions. Table 1 summarizes the results from the two inlet temperature distribution cases (T_MIN and T_MAX), as well as the original uniform and non-uniform inlet flow cases. Results indicate that a higher inlet temperature in the stuck rod assembly yields slightly more limiting results in terms of fuel and clad temperatures, heat flux, and DNBR.

The DNBR was calculated using VERA CTF's default correlation (Biasi). At each iteration of the coupled code calculation, CTF performs a series of pseudo-transient calculations until convergence is achieved on mass and energy balances. Calculated moderator temperature, density and fuel temperatures are exchanged with VERA's neutronics subcomponent to calculate a power distribution. Iterations between the two codes continue

until convergence is achieved on the coolant temperature and density.

These simulations required approximately 20 neutronics/T-H iterations for global convergence, with a total wall-clock time of ~6.5 hours each on the OLCF Titan computers. The neutronics model used 58 axial mesh regions. Flux calculations used a 47-energy group library. Transport sweeps were performed on 1,243x12=14,906 Titan processors. To accommodate the full core model at restart, 1,243x16= 19,888 processors were allocated for memory. The T-H model included 56,288 subchannels, 112,064 gaps and 55,777 rods that were solved in parallel on 193 cores.

Planned future work includes:

- Complete testing and application of the VERA CTF W-3 correlation for DNBR calculation;
- Perform CFD simulations of the vessel inlet distributions and VERA simulations of the core response for the HZP SLB case without offsite power (low flow case);
- Compare the DNBR margins between the high and low flow cases and determine the limiting DNB case;
- Develop an approach to verification, validation and uncertainty quantification (VVUQ) of the code solutions and predictions for the purpose of the limiting case selection

For more information, see CASL-EC-2015-0173-000.

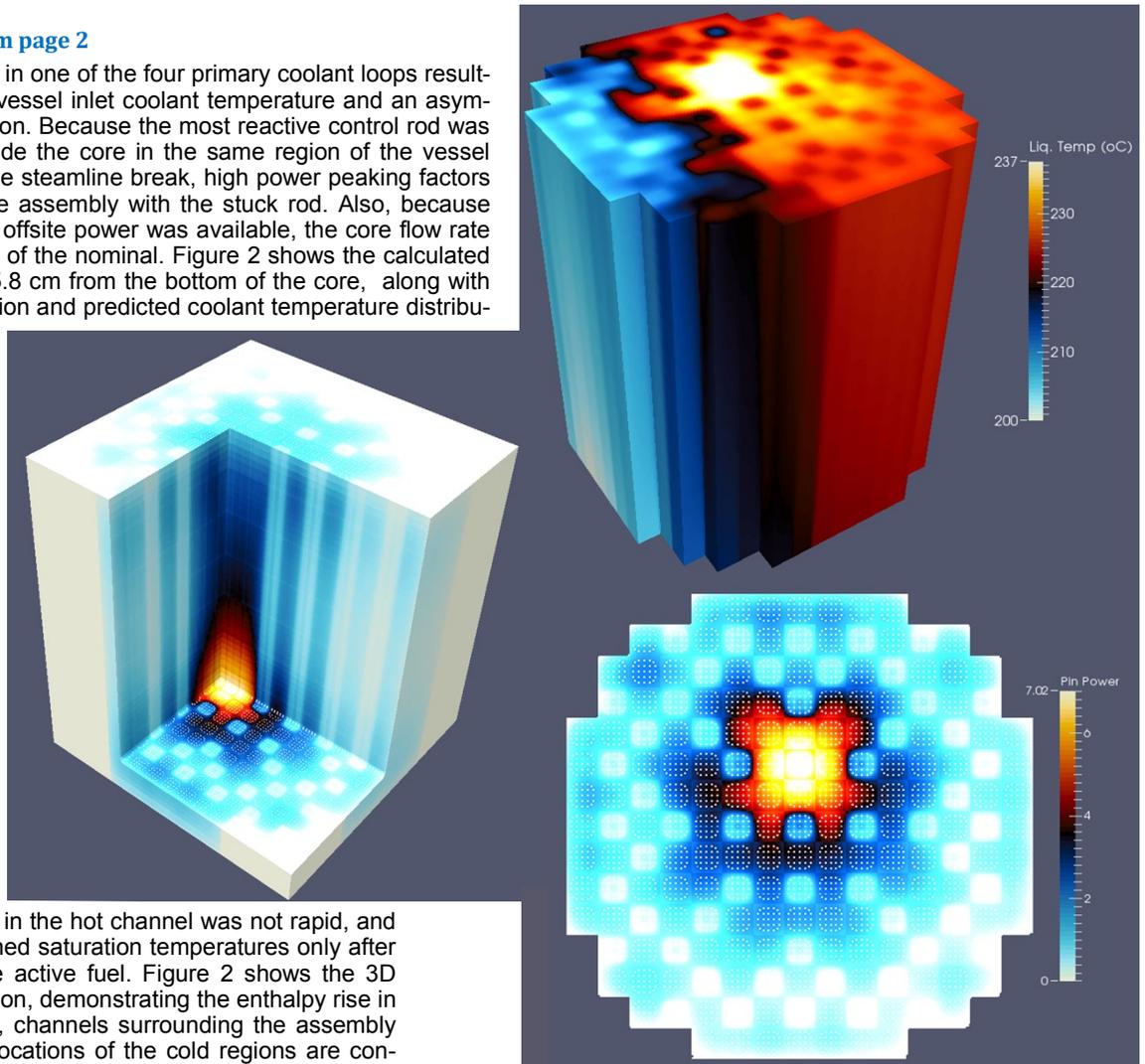


Figure 2 [top] 3-D Coolant Temperature Distribution ; [left] Whole-Core Pin Power Distribution; [bottom] Pin Power Distribution at z=+45.8cm

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Watts Bar Operating Cycles Simulated to Present ... (continued from p. 1)

these important benchmark problems, CASL researcher Andrew Godfrey utilized the VERA core simulator's new shuffle capability to bring its WBN-1 predictions up to the current cycle. These predictions lay the groundwork for follow-up demonstrations of Challenge Problem capabilities; for example, initial CRUD prediction capability was demonstrated using WBN-1 cycle 7's CRUD event as a validation opportunity.

The WBN-1 VERA models are based on the reactor and fuel specifications provided by TVA and Westinghouse. 193 Westinghouse 17x17 nuclear fuel assemblies are operated on 18-month cycles in the 4-loop Westinghouse reactor core. Burnable absorbers are used to control the power distribution in the fresh fuel. Additionally, WBN-1 has participated in the U.S. Department of Energy's Tritium Production Program, with many Tritium-Producing Burnable Absorber Rods (TPBAR) included in most cycles.

Many of the WBN-1 fuel cycles had distinguishing characteristics, including:

- Cycle 1 used Pyrex burnable absorber rods; also cycle 1's power history 1 was more complicated than others due to frequent periods of low power operation or shutdowns.
- Cycle 2 began the use of IFBA/WABA poison types and included TPBAR LTAs.
- Cycle 3 began the use of annular blanket pellets for the fuel rods containing IFBA.
- Cycle 4 implemented a 1.4% mid-cycle power uprate.
- Cycle 6 transitioned to a slightly different fuel design with IFM grids and began the batch inclusion of TPBARs.
- Cycle 7 experienced CIPS.
- Cycle 11 significantly increased the number of TPBARs and had no WABAs.
- Cycle 12 changed the control rod design and also had no WABAs.

A 53 axial level model was chosen in the fuel for the edits and thermal-hydraulic coupling to resolve each spacer grid (approximately three inch mesh in between grids). For parallelization, complete spatial decomposition was performed by axial plane and by fuel assembly, resulting in 59 axial planes (3 for the top reflector and 3 for the bottom) and 73 radial nodes, requiring a total of 4307 processors for the calculation. The number of processors could be reduced to as few as 472, requiring less than 4 GB/core of memory; however, this would increase the runtime by approximately a factor of ten.

WBN-1 utilizes both in-core and ex-core instruments to monitor the neutron flux in the reactor. The in-core detectors are moveable fission chambers that are used to perform core surveillance activities and ex-core calibration at prescribed intervals ranging from one to three months. The signals returned from these detectors are aligned and processed into "flux maps" that are compared to predicted power distributions. The flux maps are also an excellent source of validation data for reactor physics applications.

Each cycle depletion was run using quarter-core rotational symmetry, even though a few of the cycles were not symmetric. For these cases it is assumed that the effect on the core power distribution is small and the asymmetric assemblies, being low power and on the core periphery, are not significant for core reactivity or flux mapping. Every power maneuver and shutdown performed in each cycle was not simulated; depletion is performed by burnup at representative conditions. Comparison points (boron and flux maps) are made at HFP conditions at sufficient intervals (~1 week) following maneuvers that that the plant is considered to be close to equilibrium isotopics and depletion is performed using equilibrium xenon.

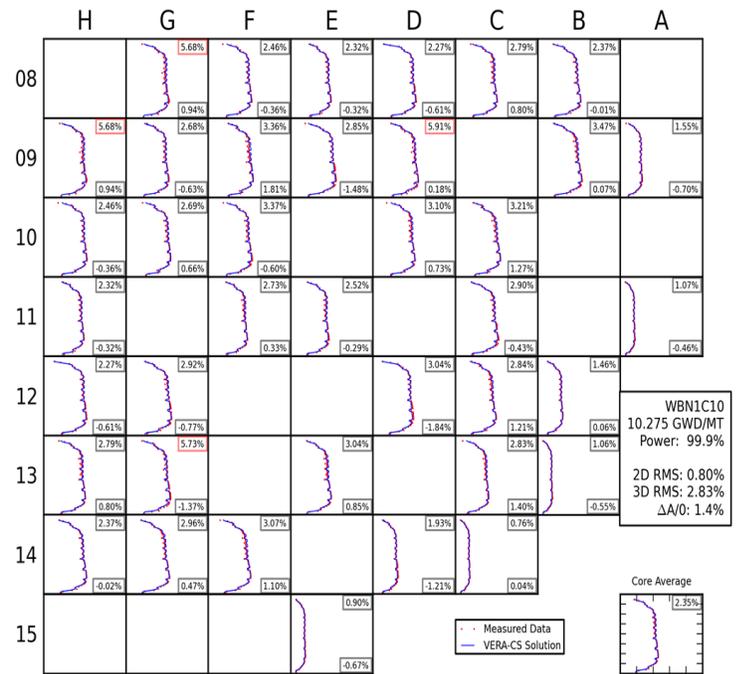


Figure 3 Hot Full Power Flux Map Comparisons of VERA predictions to WBN-1 Measurements, cycle 10.

The following parameters were calculated with VERA and compared with TVA-provided measured WBN-1 data:

- Beginning-of-cycle (BOC) criticality of the reactor;
- BOC hot-zero-power (HZIP) control bank reactivity worth (CBW);
- BOC HZIP isothermal temperature coefficient (ITC);
- Hot-full-power (HFP) critical boron letdown over the entire fuel cycle; and
- HFP in-core instrument response distributions (flux maps).

Table 4 provides a comparison summary of the measured versus VERA-predicted results, and include over 400 critical boron measurement and 183 HFP measured flux map comparisons (an example flux map comparison is shown in Figure 3). The majority of the results look very good, especially given that this is the first application of VERA on a multi-cycle scale. A few outliers exist and may require further investigation to rule out possible issues with the methods. The VERA calculations were performed on the INL Falcon HPC resource, and the average fuel cycle depletion required approximately 21 hours on 4307 cores, or 88,000 cpu-hours. The total cpu resource utilization over all cycles was 1.06 million cpu-hours. For the 440 state-points calculated (~37 per cycle), the average runtime of a single statepoint was 35.9 minutes, and the average number of iterations between MPACT and CTF was 11.1. In total, 4899 fully coupled iterations were successfully performed and fully converged. For more information, see CASL-U-2015-0206-000.

Table 4 Comparison of VERA Results with WBN-1 Measurements

Measurement	Sample Size	Mean ± 1 sigma	Runtime per Cycle
BOC HZIP Critical Boron	12	-9 ± 24 ppm	1.75 hours
BOC HZIP Bank Worth	76	1.2 ± 4.3%	3.33 hours
BOC HZIP ITC	11	-0.8 ± 0.7 pcm/°F	0.75 hours
HFP Boron Letdown	384	-24 ± 19 ppm	21.9 hours
HFP Flux Maps - Radial - Total	165	1.9 ± 0.3% RMS 3.7 ± 0.4% RMS	--

ITM/DNS for High Volume Fraction Bubbly Flow Regimes: Simulations for Closure Development

An essential part of developing a closed form set of equations (closures) for prediction of two-phase flow with computational fluid dynamics (CFD) is understanding how the bubbles generated by boiling interact. An accurate prediction of moderator and fuel performance once boiling has begun is needed to simulate CASL Challenge Problems related to boiling water reactors (BWRs), departure from nucleate boiling (DNB) behavior in pressurized water reactors (PWRs), loss of coolant accidents (LOCAs), and other scenarios where two-phase flow is present. NCSU researchers Fang and Bolotnov and UND researchers Lu and Tryggvason are breaking new ground in developing insights to this complex flow phenomena.

Previous direct numerical simulation (DNS) studies of multiphase flows have been in excellent agreement with experimentally based correlations. Bubbly flows (as opposed to boiling flows) lend themselves relatively well to small scale direct numerical simulations. They are therefore a natural starting point for investigations using DNS data to build closure models for the large scale flow fields within a nuclear reactor.

When implemented in CFD, DNS solves the Navier–Stokes equations numerically without the use of a turbulence model; this requires that the whole range of spatial and temporal scales of the turbulence must be resolved. One key to the DNS of multiphase flows is the accurate prediction of the phenomena taking place at the interface separating the phases—that is, at the surface of the bubbles. Use of direct interface tracking methods (ITM) uses a set of single-phase conservation equations, known as the one-fluid formulation, where the differences in material properties and surface tension are accounted for by solving a convection equation. Thus, DNS with ITM provides researchers with a small scale analytical method to examine two-phase flow dynamics.

To examine the merging and breakup of bubbles in churn-turbulent gas-liquid flows, the CASL thermal-hydraulics team has conducted a series of simulations of bubbles in a channel containing turbulent flow using a Front Tracking code (FTC3D) and a Level Set based code (PHASTA). The bubble interfaces separating the gas and the liquid is shown in Figure 4 for five different points in time for four variants of surface tension.

As the bubbles move through the flow, the nearly spherical high surface tension bubbles tend to move to the channel wall, leading to rapid coalescence, and re-introduction to the free stream as the bubble reaches a critical size. Thus, when the surface tension is sufficiently high, the bubbles continuously merge to form larger and larger bubbles, until most of the gas is coalesced into one large bubble. As the bubbles in the high surface

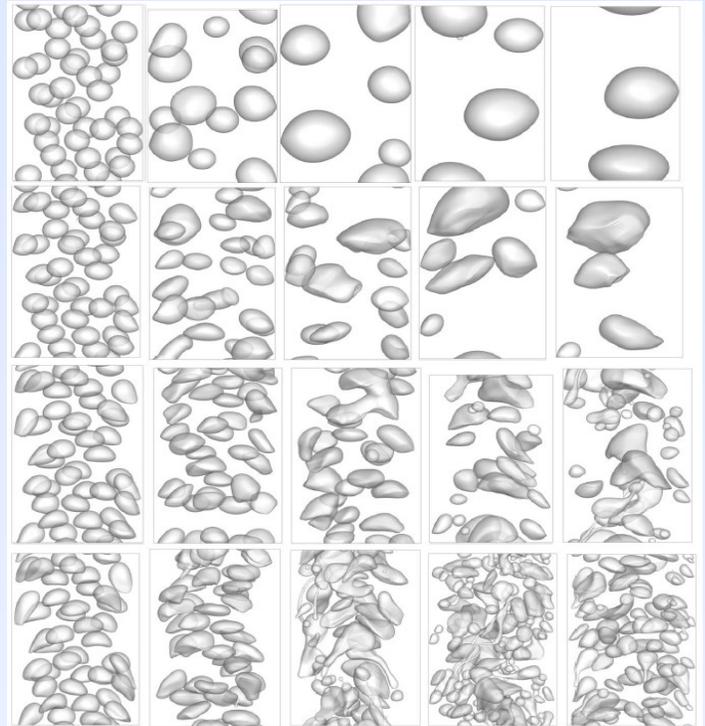


Figure 4 DNS IMS for five variants of surface tension at the same void fraction: (a) 0.08 (b) 0.01 (c) 0.004 (d) 0.002. The frames have been selected to illustrate how the flow evolves and are not evenly spaced in time.

tension case coalesce they move to the center of the channel and since the bubble becomes ellipsoidal, it tends to block the channel and thus slow down the flow.

For lower surface tension bubbles, initially the bubbles merge into larger bubbles, but as they are deformed they also start to break up. The more deformable, low surface tension bubbles are not pushed to the wall. Because the lower surface tension bubbles are more deformable, the larger coalesced bubbles create less of a flow blockage than high tension bubbles.

For intermediate surface tension, the behavior is significantly more complex and includes the formation of long gas filaments. The study collected a wide variety of calculated parameters, including average void fraction, average vertical velocity, streaming stresses, lateral gas flux, volumetric flow rates, average wall shear stress, total interface area, projected (p.6)

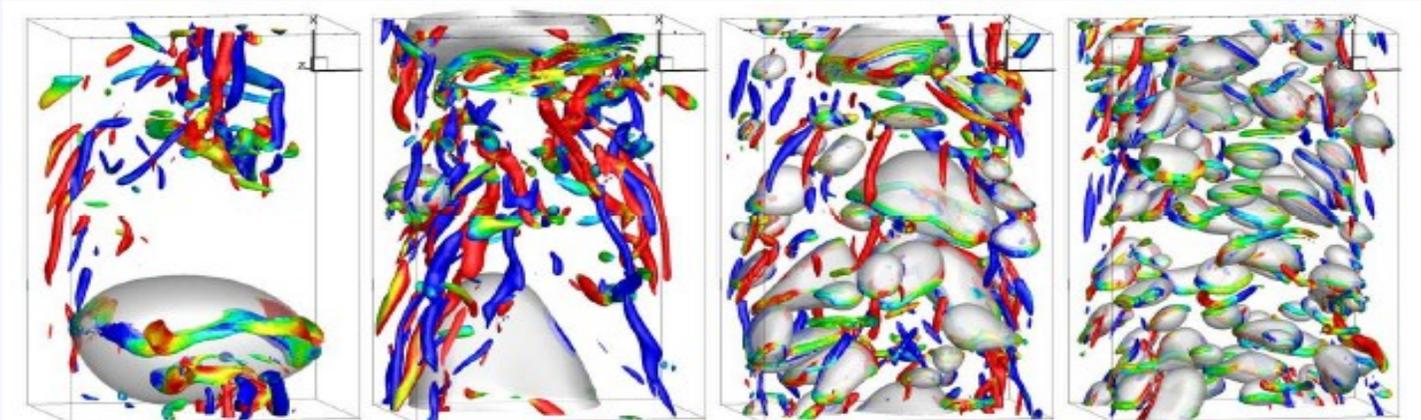


Figure 5 Bubbles with vertical structures observed late in the simulation for Figure 4 cases (a), (b), (c) and (d).

ITM/DNS for High Volume Fraction Bubbly Flow ... (continued from p. 5)

surface area, etc, for various points in time in the simulation.

An example of the vorticity field is shown in Figure 5 at a time point late in the simulation, after the bubbles have coalesced (and broken up, in the lower surface tension cases); red and blue indicate vortices aligned with the flow, with rotation of the opposite sign, and green/yellowish vortices are perpendicular to the flow. While the initial velocity field of the simulation was turbulent, the bubble motion appears to quickly change the structure of the turbulence in major ways.

Next, the research team created a single PWR subchannel domain for simulation. Both single-phase and two-phase turbulence were simulated for Reynolds numbers (Re) of 29,079 (53.8 million cell mesh, RE01) and 80,774 (1.11 billion cell mesh, RE02). The two cases were compared to investigate the influence of PWR geometry on the turbulent flow structures. Since the mesh size requirement for DNS decreases exponentially as Reynolds number increases, 80,774 was chosen to approach realistic PWR conditions while managing the computational resources required. Table 2 provides a listing of the model parameters for both cases.

Table 2 Modeling Parameters for the PWR Subchannel Cases

Case	RE01	RE02	
Domain sizes (mm)	40.5x12.6x12.6		
Rod radius (mm)	4.57		
Reynolds number resolved (Re_b)	29,079	80,774	
Bulk resolution (mm)	8.11×10^{-2}	3.25×10^{-2}	
Thickness of first B. L. ($y^+=1$) (mm)	8.11×10^{-3}	3.25×10^{-3}	
Number of boundary Layers	13	13	
Number of points	9,249,506	186,825,949	
Number of elements	53,837,248	1,111,168,768	
Number of computing cores used	8,192	131,072	
Element per core	6,572	8,478	

Case	RE01	RE02	Realistic PWR condition
Liquid/Gas Viscosities (Pa-s)	8.585×10^{-2} ; 1.965×10^{-1}		
Liquid/Gas Densities (kg/m ³)	712.22; 46.17		
Mean velocity (m/s)	0.27	0.75	4.62
Reynolds number (Re_b)	29,079	80,774	452,500

Periodic boundary conditions are utilized to represent a much longer domain than is computationally feasible in the DNS with ITM approach. A single-phase turbulent velocity profile is first generated by placing a sphere blockage region at the domain center to create fluctuations. When large turbulence structures are observed the spherical barrier is removed. When the single phase turbulence achieved statistically steady state flow conditions, bubbles were introduced and the bubble motion and deformation were resolved using level-set interface tracking method. For this study, considering both computational cost and results reliability, 17 bubbles were used for the RE01 case and 262 bubbles for RE02. The bubble distribution and turbulence for RE02's 262 bubbles are shown in Figure 6 (the direction of mean flow is from left to right).

Both single- and two-phase subchannel simulations were performed at the Leadership Computing Facility (ALCF) located at the Argonne National Laboratory. The simulation results were visualized using the open-source software, ParaView. The void fraction and gas-liquid velocity profile from the two phase RE01

case are shown in Figure 7. In the region where the void fraction is higher than 0, the corresponding gas velocity is observed to be larger than liquid velocity because the bubbles are accelerated by the buoyancy force in the subchannel. When two-phase flows achieve statistically steady state conditions, the drag coefficient can be estimated based on the bubbly buoyancy force and bubble terminal velocity. Assuming steady state conditions and approximating the bubble relative velocity obtains a drag coefficient is close to the expected value.

Further evaluations of the data and additional simulations are planned in 2016:

- ◆ Examine the importance of the coalescence criteria and its influence on the statistics of the flow in more detail;
- ◆ Benchmark the results between the front-tracking and level-set methods;
- ◆ Extend the simple two-fluid model to turbulent flow with bubbles of different sizes and topology changes, and assess the relationship of the closure terms to average quantities and summary variables for the unresolved quantities.
- ◆ Develop partitioning methods to recognize the correlated behavior of different bubbles and test at scale.

In future CASL plans to apply a functional form of correlations distilled from these studies to be used in CFD and subchannel flow modeling. For more information, see L3:THM.CLS.P11.01. It is notable that this work received the International Data Corporation (IDC) HPC Innovation Excellence Award (November 2014).

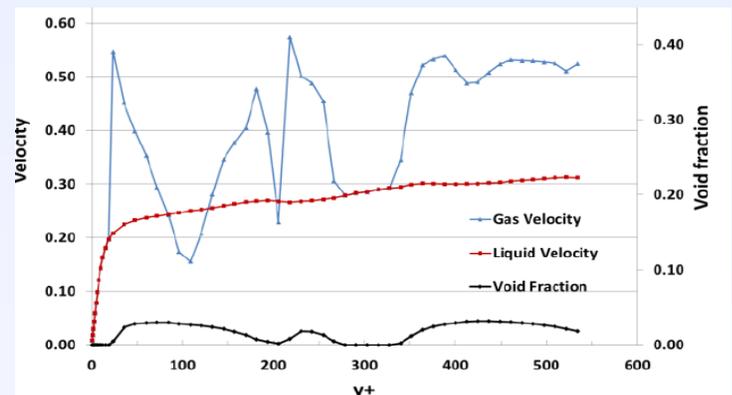


Figure 7 Void fraction and gas-liquid velocity profile from two-phase conditions, RE01

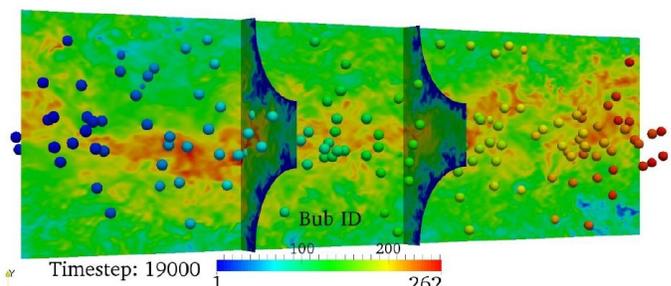


Figure 6 Distribution of 262 bubbles in the turbulent flow

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EPRI Test Stand Demonstrates CASL Fuel Performance Modeling Capabilities

A strategic element for the deployment of the Virtual Environment for Reactor Applications (VERA) is a CASL Test Stand. Test Stands are intended to provide key stakeholders with an opportunity to work with VERA at an early stage development on applications that are of mutual interest to both the Test Stand sponsor and CASL. Test Stands generate essential user feedback that can be used to enhance both VERA's technical capabilities and CASL's deployment and support processes.

Brenden Mervin at the Electric Power Research Institute (EPRI) recently concluded a Test Stand that was focused on evaluating VERA's BISON-CASL fuel performance capabilities. EPRI stepped through a series of 7 single rod 2D axis-symmetric models and compared VERA's results with results from EPRI's Falcon fuel performance code. The difficulty level increased with each step in the series, beginning with a simple reactor power up followed by steady-state operation and ending with an axially-varying power history with multiple power ramps. The simulations modeled a generic pressurized water reactor (PWR) fuel rod as well as a fuel rod from the Watts Bar Unit 1 reactor.

In general there was good agreement between the results from VERA and Falcon in the calculated trends for temperature, displacement, and hoop stress. However, there were differences in the magnitude predicted. For example, Figure 8 displays a hoop stress comparison for a generic PWR fuel rod during the down power following steady-state operation with a second cycle restart. It can be observed for this case that VERA predicts less stress relaxation during the down power as well as during the first step in power ascension for the second-cycle restart; VERA predicts more stress relaxation during the final hold period after the second cycle power ramp is complete; VERA predicts less

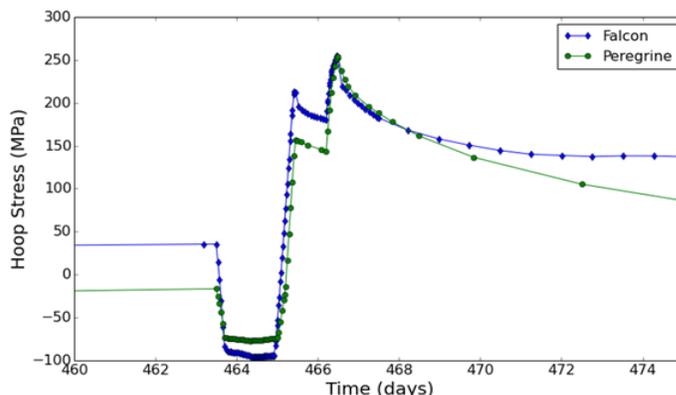


Figure 8 Comparison of cladding inside surface hoop stress taken at a point along the axial centerline of the active fuel region

stress buildup during the first step increase during the second-cycle power ramp; and VERA predicts more stress buildup during the second step increase of the second-cycle power ramp.

Since VERA's fuel performance capability is still under extensive active development, the initial results are promising and suggest with a good degree of confidence that the code will provide a significantly advanced fuel performance analysis capability, particularly when utilizing its 3D geometry model. As the capability matures, CASL will perform more benchmarking and validation activities and this study will be repeated.

In addition to evaluations of the prediction capabilities of VERA, the opportunity to enhance several CASL processes related to deployment and user support were identified. These enhancements have been incorporated into CASL systems and are anticipated to improve the effectiveness of CASL deployments for both future Test Stands and other applications.

More information on the EPRI Test Stand, including a detailed review of the prediction results obtained and recommendations to CASL, can be obtained from CASL-U-2014-0121-000a.

VERA Training Workshops Held ... (continued from p. 1)

professor, noted that [during the workshop] “the students have the opportunity to submit a big scientific problem on a world-class machine, allowing them to do problems they would never be able to do elsewhere.”

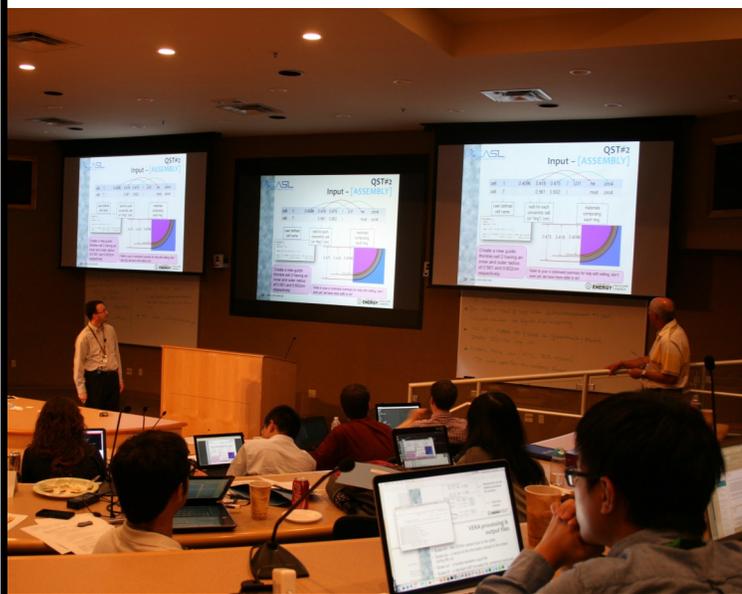
In the future, CASL plans to refine and expand its Quick-Start training, offering more advanced tutorials addressing several of the CASL Challenge Problems. Also, there are plans to devel-



op modules for a CASL Institute that will offer a certificate of completion. Finally, CASL is in the process of developing academic modules for classroom use of VERA. The initial modules are expected to be available late in 2016. For more information see CASL-U-2015-0118-000 and CASL-U-2015-0118-001.

Above: Bob Salko (ORNL) coaches participants running Quick-Start VERA Simulations at the ANS ANFM Topical Meeting .

Left: Andrew Godfrey (ORNL) provides set up information and background on commercial power reactors for students participating in the CASL student summer workshop.



Verification and Validation Supporting VERA Neutronics Code

As CASL produces its VERA software each physics capability must be tested, verified, and validated (V&V). The overarching objective of code verification is to establish that a computational model implemented in a code accurately represents the developer's conceptual representation of the physics, while validation refers to the process of determining the degree to which a computational model provides an accurate representation of the real world. Researchers on CASL's Radiation Transport Methods (RTM) team has implemented a rigorous V&V program for it's MOC capability as implemented in the MPACT code.

CASL's verification activities encompass both the source code and the code solution, providing comprehensive software testing and evaluation of the numerical error in the solution. Unit testing is used to isolate small bites of source code to determine whether they are fit for use. In contrast, regression testing seeks to uncover bugs in existing functional areas of the code after changes have been made to the source. RTM's practice is to create unit tests for all functions and methods while the code itself is being written; unit testing accelerates the process of finding and correcting bugs by allowing the location of the fault or failure to be easily traced. One of the challenges of writing the unit tests is the difficulty of setting up realistic tests with relevant initial conditions such that the part of the application being tested behaves like part of the complete system. If these initial conditions are not set correctly, the test will not be exercising the code in a realistic context, which diminishes the value and accuracy of unit test results.

Since unit testing only examines the functionality of the units themselves, it is recognized that unit testing will not catch every error in the program. Specifically, unit testing does not catch integration errors or broader system-level errors. Therefore, RTM also incorporates regression testing as a part of its verification process. Regression tests are a series of tests that are repeated as the code development progresses. The results are compared against previously recorded outputs to ensure that new features and enhancements do not alter the reproducibility of existing features. The best practice used in MPACT is that when a bug is located and fixed, a test is recorded that exposes the bug and the test is rerun regularly after subsequent changes to the program.

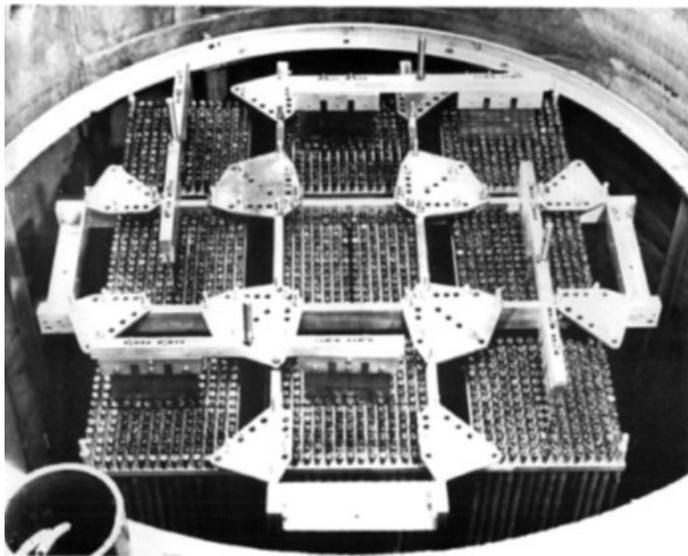


Figure 9 Babcock and Wilcox critical experiment facility. The experiments reported by the facility are used in the validation of VERA's MOC neutronics code.

A summary of some of the key capabilities tested during verification include:

- **Geometry**
 - ◇ Cylindrical, Quarter, Rectangular and Generalized cylinder pin geometries
 - ◇ Inserts
 - ◇ Control rod (+ rod movement)
 - ◇ Baffle/Reflector
 - ◇ Upper/lower nozzle, core plate, reflector
 - ◇ Multiple assemblies/modules
 - ◇ Symmetry
 - ◇ Grids
 - ◇ Detectors
- **Transport Solvers**
 - ◇ P0 and Pn 2D MOC
 - ◇ P0 and Pn 2D-1D with SP3 (and NEM)
- **Other Solvers**
 - ◇ Depletion (native and Origen)
 - ◇ Search (boron, rod)
 - ◇ Multistate
 - ◇ CMFD (Multilevel, MGNode, 1Gsweep)
 - ◇ Feedback (internal and CTF)
 - ◇ Eq Xe/Sm
 - ◇ XS Shielding (Subgroup vs ESSM)
 - ◇ Cusping treatment
- **Parallel**
 - ◇ MPI (space, angle, space+angle), explicit file
 - ◇ OpenMP (threading)

Another principal motivation of CASL's verification activities is the evaluation of the numerical error in the solutions produced by the code. Initially, this was focused on mesh convergence studies; however, a more comprehensive and thorough verification has been planned based on the Method of Manufactured Solutions (MMS). The essential concept behind MMS is, rather than solving a specified problem with prescribed boundary and initial conditions, to specify the solution (Manufactured Solution) and substitute the solution into the governing equation/neutron transport equation. This results in an extra analytical source (Manufactured Source). The boundary and initial conditions can be obtained by evaluating the manufactured solution at the boundary and at initial time. This set of boundary and initial conditions, together with the manufactured source have "manufactured" a problem from which the exact analytical solution is known. By comparing the numerical solution from the solver with the manufactured analytical solution and observing the expected rate of convergence in the successive grid refinements, the numerical solution can be verified.

Additionally, verification of VERA's code solution is being accomplished through comparisons with calculated quantities on fine scales from continuous energy (CE) Monte Carlo methods, including 3D core pin-by-pin fission rates at operating conditions, intra-pin distributions of fission and capture rates, reactivity and pin power distributions of depleted fuel, and support for other capabilities such as gamma transport and thick radial core support structure effects.

For validation, the goal is to identify those tests which will increase confidence in the quantitative predictive capability for practical reactor applications; thus, it is important to compare VERA's predictions to measured reactor data in addition to experimental data. A comprehensive validation plan was developed for VERA's core simulator capability (p.9)

Verification and Validation ... (continued from p. 8)

(coupled MOC and subchannel thermal-hydraulics), with the primary validation sources identified as:

- 1) Measured data from experiments with small critical nuclear reactors. This includes critical conditions, fuel rod fission rate distributions, control rod or burnable poison worths, and isothermal temperature coefficients.
- 2) Measured data from operating commercial nuclear power plants. This includes critical soluble boron concentrations, beginning-of-cycle (BOC) physics parameters such as control rod worths and temperature coefficients, and measured fission rate responses from in-core instrumentation.
- 3) Measured isotopics in fuel after being irradiated in a nuclear power plant. This includes gamma scans of ^{137}Cs activity, burnup based on ^{148}Nd concentrations, and full radiochemical assays (RCA) of the major actinides and fission products.

During the first phase of CASL, progress has been made in each of these areas, with the exception of fuel deple-

tion / measured isotopics in item 3. The comprehensive validation matrix developed within CASL-U-2014-0185-000 lists the required code capabilities, features, and the application range with the proposed benchmarking activities. Although it is unlikely that CASL can complete all of the validation activities listed, the matrix provides guidance towards prioritizing validation activities to ensure that sufficient effort is performed across the full range of capabilities and features for VERA's core simulator. Similar matrices for VERA's other capabilities are under development.

CASL-U-2015-0143-000 describes a series of benchmark calculations performed by University of Michigan and Oak Ridge National Lab researchers using VERA's MOC radiation transport code, MPACT, to validate its results against the B&W-1484 [4] and B&W-1810 [5] benchmark experiments. 18 of the 44 critical configurations were examined in depth. For the B&W-1484 cases, agreement was within 200 pcm of the measured eigenvalue for cases using P_2 scattering. For the B&W-1810 cases, the root-mean-squared value was 77 pcm for and 208 pcm for P_2 and TCP0 scattering, respectively, with a maximum discrepancy of 112 pcm and 261 pcm for P_2 and TCP0 scattering, respectively. The fission rate comparisons, which were available for four of the 1810 cores, yielded RMS comparisons between 0.47% and 0.76% with maximum errors between 1.27% and 2.11%.

CASL-U-2015-0076-000 describes the modeling of the Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS) [6] using VERA. The BEAVRS benchmark provides two cycles' worth of operational history, including power levels and boron concentrations. Figure 10 illustrates VERA's shuffle feature with the pin exposures mapped from the end of cycle 1 to the beginning of cycle 2. Figure 11 provides a graph of the VERA-predicted critical boron concentration against that measured in the BEAVRS experiments. In addition, flux maps are provided at several points during each operating cycle. Comparisons with VERA predictions show reasonable agreement, with a 2D RMS error of 2.7%. BEAVRS cycle 1 critical boron concentration compared well with VERA predictions, and flux map comparisons were consistent with measured trends.

More information on VERA neutronics code verification and validation activities are available in CASL-U-2014-0185-000, CASL-U-2015-0234-000, CASL-U-2015-0143-000, and CASL-U-2015-0076-000.

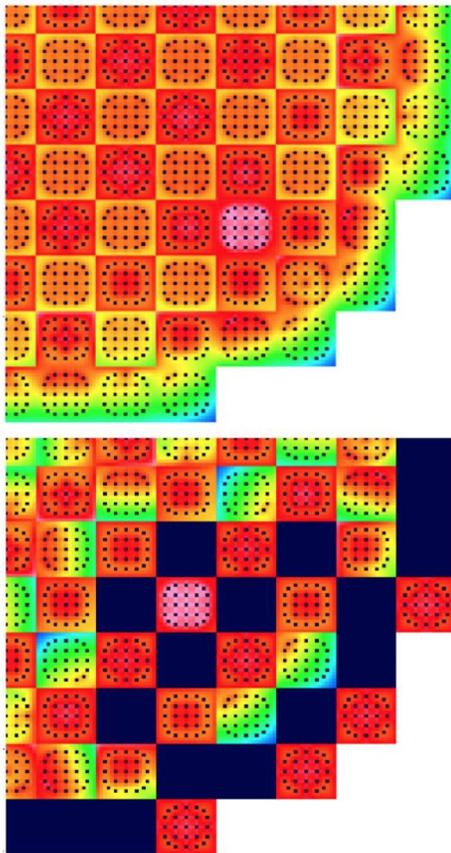


Figure 10 Pin Exposure at End of BEAVRS Cycle 1 (top) and Beginning of Cycle 2 (bottom)

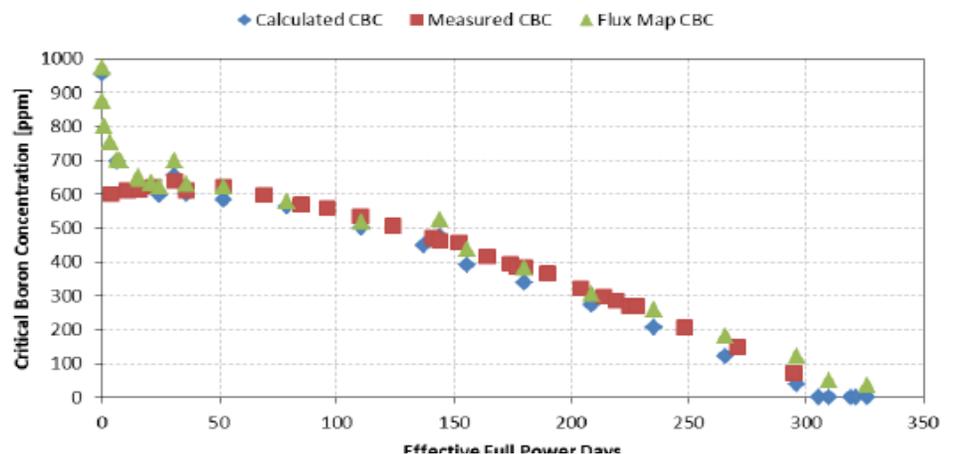


Figure 11 Calculated versus Measured Critical Boron Concentration as a function of effective full power days for BEAVRS cycle 1

References cited in this article include:

- [4] M. N. Baldwin and G. S. Hoovler, "Critical Experiments Supporting Close Proximity Water Storage of Power Reactor Fuel," Tech. Rep. BAW-1484-1, The Babcock & Wilcox Company, 1978.
- [5] L. W. Newman, W. A. Wittkopf, W. G. Pettus, M. N. Baldwin, H. A. Hassan, V. O. Uotinen, J. D. Connell, and P. S. Campbell, "Urania Gadolinia: Nuclear Model Development and Critical Experiment Benchmark," Tech. Rep. BAW-1810, The Babcock & Wilcox Company, 1984
- [6] N. Hoerlik, B. Herman, B. Forget, and K. Smith. "Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS)," v1.0.1 Proc. Int. Conf. Mathematics and Computational Methods Applied to Nuc. Sci. & Eng., Sun Valley, Idaho (2013).

For a full listing of relevant references, please see the CASL reports cited.

CIPS Simulation Capability Implemented in VERA... (continued from p. 1)

The primary physics and chemistry associated with CRUD formation currently treated in VERA include:

- ♦ Solving for the radial temperature drop across the CRUD layer, while accounting for localized heat sinks due to internal (chimney) boiling within the CRUD layer;
- ♦ Prediction of CRUD growth which is governed by the time evolving coolant concentration of particulates, surface erosion due to fluid flow, the cladding temperature, and the sub-cooled nucleate boiling rate on the cladding surface;
- ♦ Time evolving coolant chemistry at the CRUD surface and inside the pores of the CRUD;
- ♦ Mass transport of soluble boric acid into the interior of the CRUD due to boiling induced Darcy flow;
- ♦ Modeling the diffusion of soluble boric acid inside the CRUD due to the flow induced concentration gradients within the CRUD layer;
- ♦ Mass evaporation in the form of steam vapor due to internal (chimney) boiling with the CRUD layer; and
- ♦ Boron hideout (i.e., the precipitation of soluble boric acid into solid lithium tetraborate) within the CRUD layer.

The time dependent coolant chemistry is supplied by the calling routine and consists of the following parameters:

- ♦ Boron concentration;
- ♦ Lithium;
- ♦ nickel ferrite (particulate);
- ♦ nickel (soluble);
- ♦ iron (soluble);
- ♦ dissolved hydrogen;
- ♦ core coolant pressure;
- ♦ coolant inlet temperature;
- ♦ local bulk coolant temperature above the cladding surface element;
- ♦ surface area of the given cladding surface element;
- ♦ surface heat flux at the cladding surface element;
- ♦ temperature of the cladding surface element;
- ♦ turbulent kinetic energy in the fluid element above the cladding surface element;
- ♦ outer radius of the fuel rod.

Each of the physical processes have a direct feedback to the others, e.g., a locally high power causes higher surface temperatures which cause a larger local steaming rate, causing more CRUD deposition, which in turn suppresses the power. The coupling approach using in VERA, with the parameters exchanged, is shown in Figure 12.

To model the CRUD in the neutronics calculation, a representation of the CRUD layer must be included in the neutronics simulation mesh. In order to prevent the need to modify the simulation mesh as the CRUD grows, a fixed concentric mesh was generated on the surface of the fuel and the predicted CRUD was homogenized onto the mesh using volume homogenization. To understand how sensitive the results were to the degree of homogenization of the CRUD, parametric studies were completed for the expected range of CRUD thickness. In all cases, the effect on the meshing was considered minimal. Extreme CRUD cases show the most sensitivity but it is considered comparable to the error introduced by other meshing choices. The results of the sensitivity studies suggested that a single 150-200 micron thick region can provide sufficient accuracy to simulate the CRUD layer in the neutronics calculations. Thus, when the CRUD mass is transferred from the chemistry calculation into the neutronics calculation, it is homogenized into the fixed CRUD mesh layer.

The outputs from the chemistry component include CRUD thickness, the effective thermal resistance of the CRUD layer, the boron mass surface density, the mass evaporation flux, and the CRUD mass surface density. (p.11)

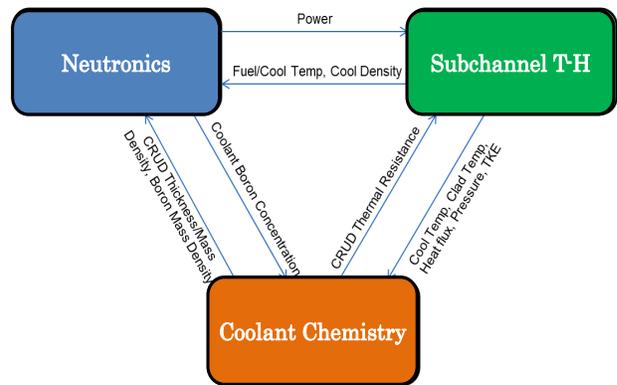


Figure 12 VERA Coupling Interfaces for CRUD/CIPS Predictions.

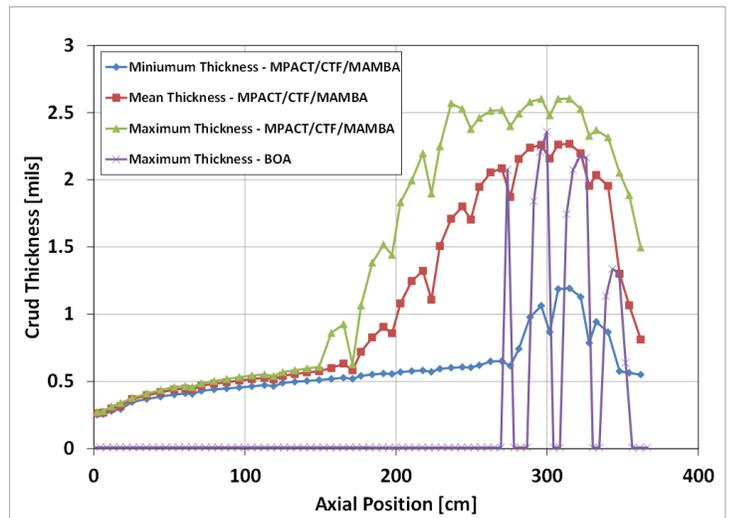


Figure 13 WBN Cycle 7 Comparison of VERA-predicted CRUD thickness with Industry code predictions for core location F-10. at 16.29 GWd/

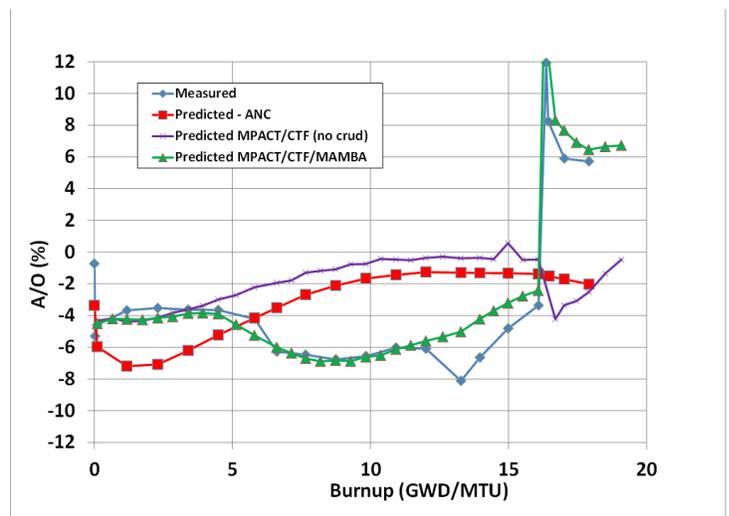


Figure 14 Watts Bar Cycle 7 predictions with VERA with and without CRUD feedback compared with plant measurements.

CIPS Capability Implemented in VERA ... (continued from p. 10)

To demonstrate the application of the methodology and VERA multi-physics, researchers Jeff Secker (Westinghouse), Ben Collins (ORNL), Brian Kendrick (LANL) and Bob Salko (ORNL) simulated Watts Bar cycles 5, 6, and 7. Cycle 7 was known to have significant CRUD deposits and experienced CIPS. It should be noted that there was a long mid-cycle outage at ~16 GWd/mtU which removed boron from the CRUD layer. To compensate for this strong power shift upwards, the plant was operated with several control rods inserted. Cycle 5 did not have CIPS indications while cycle 6 may have had some mild CIPS indications, although much less than cycle 7.

The VERA-predicted axial offset during cycle 7 with and without the CRUD included is shown in Figure 14, along with Watts Bar measured data. The core locations with the largest boron deposition in the CRUD and resulting CIPS effects were correctly identified and were also consistent with predictions using the industry CRUD/chemistry code, BOA, developed by Westinghouse and EPRI, as illustrated in Figure 13. VERA did predict mild CIPS for cycles 5 and 6, but to a much lesser extent than cycle 7. Figure 15 shows the distribution of CRUD mass and thickness predicted across the reactor core for cycle 7.

The simulation was run on 4307 cores on the INL Falcon compute cluster and took 16 hours and 34 minutes to complete which is comparable to the same case without CRUD.

This initial application of VERA on the CIPS challenge problem indicated a need to further adjust some of the chemistry inputs to improve the code fidelity when coupled. These adjustments were made and resulted in good agreement between measured

and predicted core axial offset behavior for WBN-1 cycle 7, as shown in Figure 14. However, there is still room for improvement; while the boron mass and maximum CRUD thickness predictions are good, the CRUD mass is greatly over-predicted compared to estimates from plant observations. The predicted core CRUD mass is in the range of 200-400 pounds, while the actual CRUD mass estimated in plants that have experienced CIPS is more likely in the 20-60 pound range. VERA deposits CRUD at all axial locations on the rod, although the thickest predictions are in the upper spans of the core, consistent with plant observations. Actual plant observations suggest there is little CRUD deposited in the lower half of the fuel assembly.

Future development work includes:

- ◆ A corrosion product mass balance capability must be added to allow modeling of the CRUD sources;
- ◆ Further comparisons are needed to validate the fidelity of the chemistry subgrid model;
- ◆ CRUD shuffling from one cycle to the next is required, along with the ability to remove a portion of the CRUD present at end of cycle to simulate the effects of shutdown chemistry or ultra-sonic cleaning;
- ◆ B10 depletion of the boron in the CRUD;
- ◆ Extension of the modeling to other plant cycle that experienced CIPS as well as those that didn't experience CIPS to validate the model predictions.

For more information see CASL-U-2015-0166-000 and CASL-I-2015-0318-000.

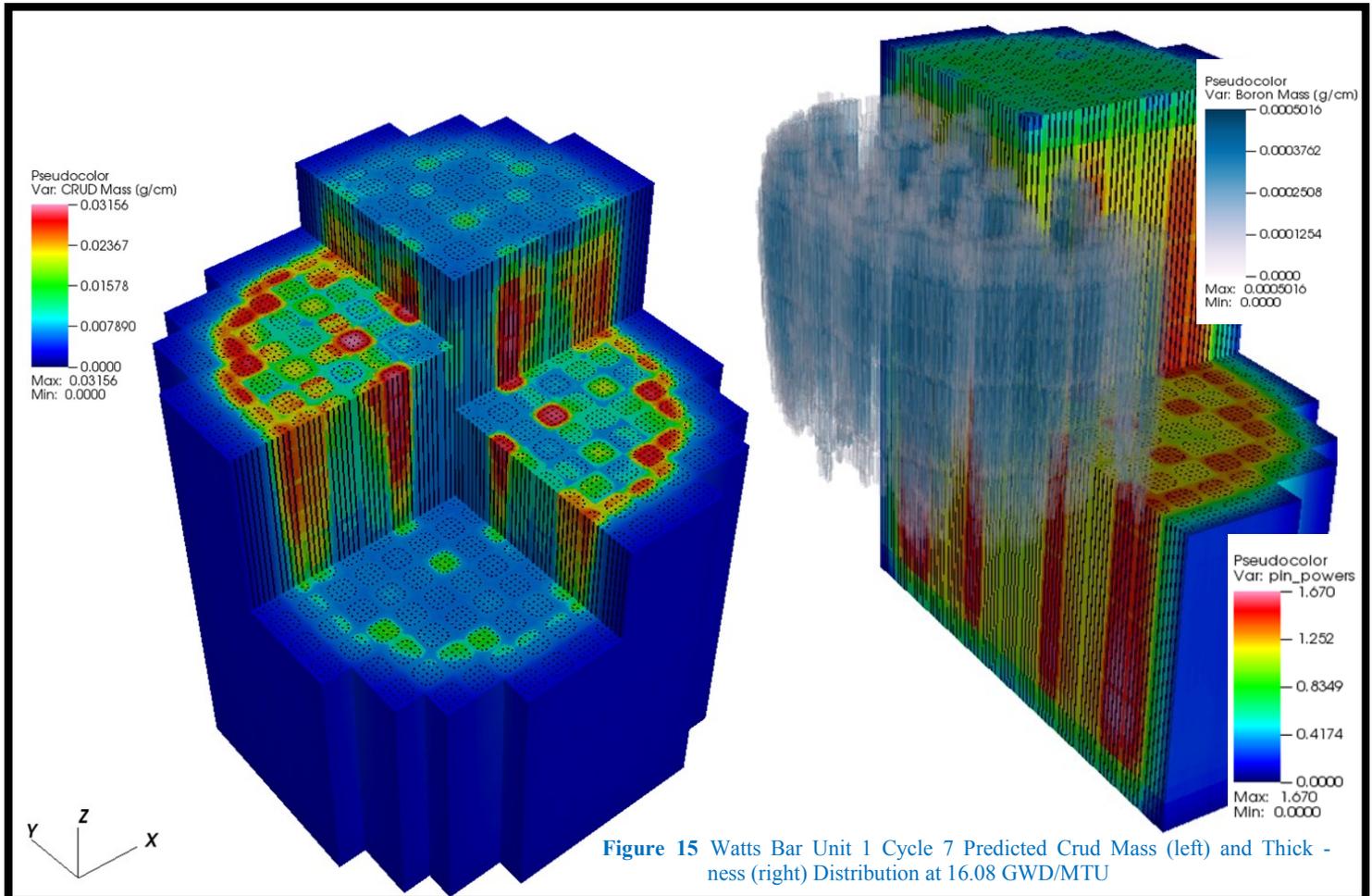


Figure 15 Watts Bar Unit 1 Cycle 7 Predicted Crud Mass (left) and Thickness (right) Distribution at 16.08 GWd/MTU

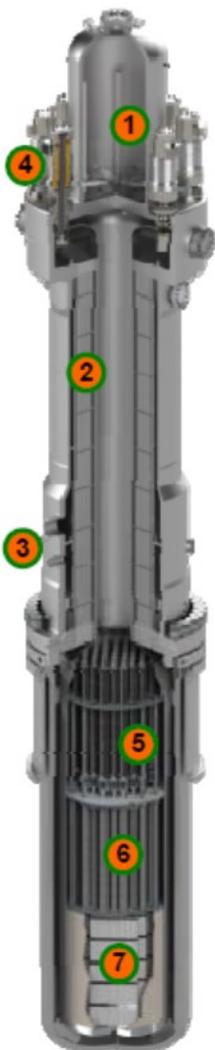
Illustration of VERA Capability to Model a Typical SMR

Small modular reactors (SMRs) such as the one illustrated in Figure 17 are being considered by the commercial nuclear power industry as an option for more distributed generation and for replacement of older fossil fuel generating facilities. SMRs are more compact than operating pressurized water reactors (PWRs), producing from 50 MWe to 200 MWe as compared to 1000 MWe or higher for their full-sized cousins, and are offered as “expandable” units; that is, their modular design allows the utility to add more units progressively at the same site.

Over the past year, TVA, UT-K, ORNL and B&W researchers completed several simulations of a typical integral PWR SMR using VERA. The work included development of fuel assembly lattice designs, core cycle designs, and control rod management simulations, progressing from simple 2D lattice calculations to a single 3D fuel assembly and finally to full core 3D simulations with control rod bank moves. The work exercised a majority of the VERA core simulator components.

The primary objective of the study was to establish a viable fuel design (<5% U235 enrichment) and core loading pattern that could reach the goal cycle length of 1400 EFPDs (Kenner, CASL-U-2014-0069-000). The initial simulations provided input to fuel economics studies as well.

Current PWRs typically operate throughout the entire cycle with almost all rods out (ARO), using soluble boron in the coolant for reactivity control. Conversely, boiling water reactors (BWRs) typically maneuver their control blades as often as every 2 GWd/mtU burnup (about 36 EFPD), with as many as 20 rod maneuvers in a 2-year cycle. The control rod maneuvers are used for gross adjustments and feed water flow rate is used for fine adjustments.



1. **Pressurizer**
2. **Once-Through Steam Generator**
3. **Feedwater Inlet / Steam Outlet**
4. **Reactor Coolant Pumps**
5. **Electro-Hydraulic CRDMs**
6. **Upper Internals**
7. **Reactor Core**

Figure 17 Illustration of a typical iPWR

©Babcock&Wilcox Company mPower

Flow control works for BWRs because the void reactivity coefficient is strong and a change in flow directly impacts the core average quality. PWRs are not designed to operate with substantial voids, so the sensitivity of

reactivity to flow will be much less. Thus, the option of controlling reactivity through flow isn't expected to be as useful for the iPWR. Therefore, although the iPWR SMR is essentially a short pressurized water reactor, for designs that do not utilize soluble boron it is envisioned that core power will be managed through manipulation of the control rods in a way that is more similar to current BWRs. It is likely that the iPWR SMR will need to maneuver the control rods as frequently as a typical BWR, with approximately 40 rod maneuvers over a 4-year cycle.

Since the initial VERA studies did not include control rod maneuvering, an additional set of simulations was completed to consider the effect of the control rods on cycle length while demonstrating VERA's capabilities for modeling control rod management. For simplicity, the VERA illustration assumed that rod maneuvers would be completed every 150 EFPD. The final maneuver at 1200 EFPD was assumed to be ARO. No other adjustments to the operating parameters (e.g., core coolant inlet temperature) were made for the study, although a single case was run to illustrate that VERA can handle changes to other operating conditions with rod moves throughout the cycle.

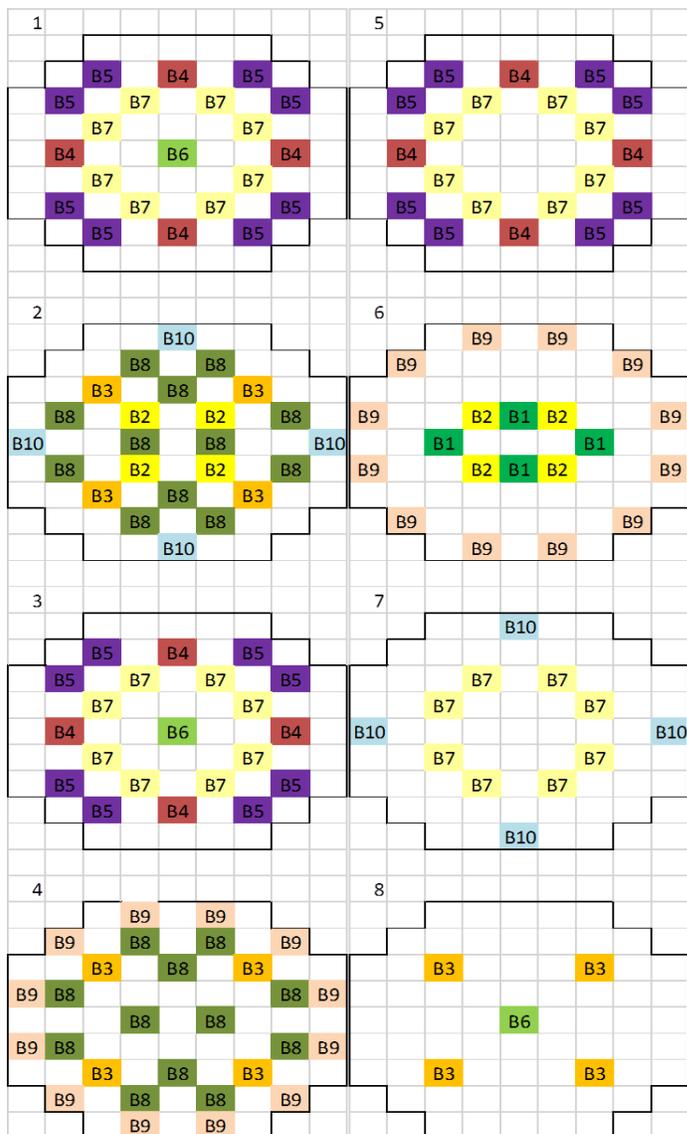


Figure 16 Proposed Ten-Bank Control Rod Management Scheme Rod Bank Move Sequence and Insertion Depth.

Move	EFPD	Bank	Steps
1	0	4	15
		5	15
		6	15
		7	15
2	150	2	20
		3	20
		8	0
		10	20
3	300	4	0
		5	0
		6	0
		7	0
4	450	3	0
		8	0
		9	0
		4	30
5	600	5	30
		7	50
		2	0
6	750	1	60
		9	0
		7	50
		10	50
7	900	3	50
		6	50
		2	0
8	1050	3	50
		6	50
		ARO	228
9	1200	ARO	228

Rods not shown are fully withdrawn

Modeling a Typical SMR... (continued from p. 13)

Since the proposed commercial iPWR reactors have control components in almost every fuel assembly, there are many combinations of “banks” possible. The 10-bank scheme used was formulated based on BWR plant schemes. The banks were assumed to be operated using a “deep/shallow” management approach, meaning that when possible a rod bank is either fully withdrawn or is inserted to greater than 60% depth. No bank is inserted for two consecutive maneuvers.

The goal for the simulation was to achieve a core average multiplication factor of 1.000 ± 0.003 over each 150 EFPD segment for a 1400 EFPD cycle length. Power peaking was compared against typical acceptance criteria ($F\Delta H < 1.55$, $FQ < 2.4$, and average assembly power < 1.45). The 10-bank control rod moves were iteratively simulated to arrive at a combination of banks and insertion depths that provided a core reactivity near the target. First, VERA was used to determine the hot excess reactivity for the core design with all rods out (ARO) and then the worth of each of the control rod banks was calculated using VERA. Using this information, the required control rod bank insertion depth was estimated and iterative VERA simulations were completed to arrive at the critical control rod bank positions.

Figure 16 provides the move sequence and insertion depths arrived at using VERA for the 10-bank scheme where 228 steps denotes full withdrawal. The predicted core power and coolant temperature distribution are shown for the maximum power peaking during the cycle at 150 EFPD. Unfortunately, the combination of assembly lattice, core loading pattern, and control rod management did not arrive at a successful solution, as the cycle length fell short of the targeted 1400 EFPD cycle and the power peaking exceeded the acceptance criteria.

However, the work did successfully illustrate VERA’s capability to model this type of SMR. VERA’s fuel shuffling functionality was not exercised, since the iPWR SMR features a once-through cycle. The VERA method of characteristics (MOC) neutronics subcomponent was used to predict power and reactivity with control rod maneuvering, both with and without thermal-hydraulic feedback. The problem was scaled from 35 to 3815 CPU cores, effectively demonstrating the solution time with respect to computing capacity. Computer clusters at Oak Ridge National Laboratory, Idaho National Laboratory and Tennessee Valley Authority were used.

The work also underlines the need for additional VERA tools to search for critical control rod insertion depth. The recommended search capability will be extremely useful for not only this application, but also for BWRs as CASL develops BWR capability in Phase 2.

For more information, see CASL-U-2015-0041-000R and CASL-U-2014-0069-001.

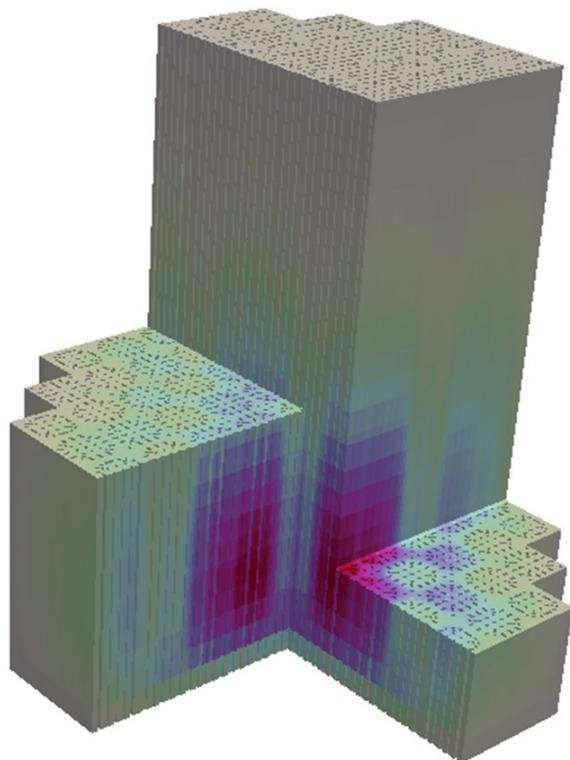
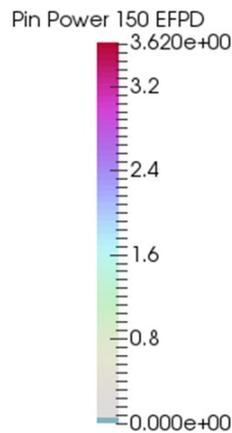
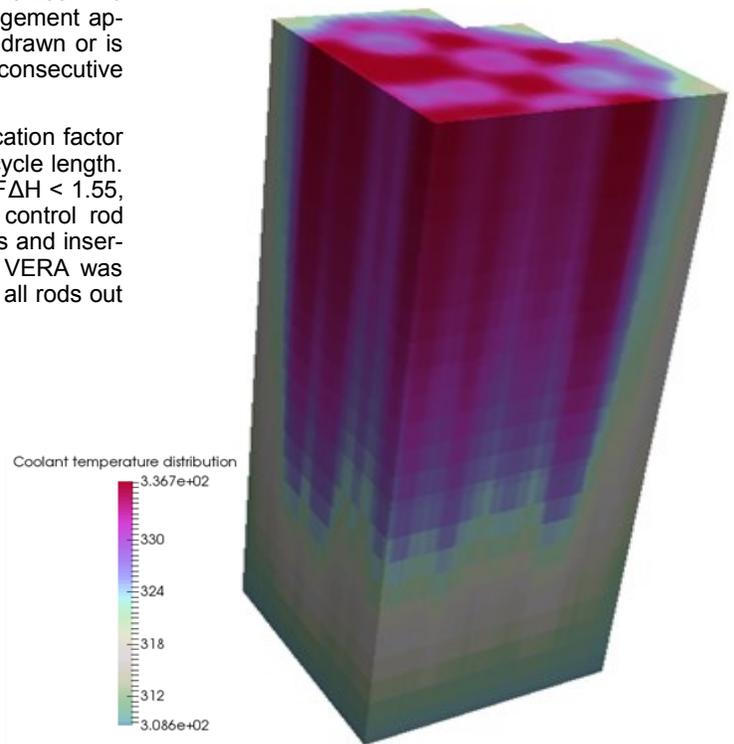


Figure 18 Results for a Ten-Bank Control Rod Management Scheme for a Typical iPWR SMR; Core Power Distribution at 150 EFPD [right]; Coolant Temperature Distribution [above].



CASL's Chief Scientist, Paul Turinsky

“Don't Confuse Symmetry with Balance.”

- Tom Robbins, from *Even Cowgirls Get the Blues*

In this issue of CASL TechNotes one will recognize the maturing of CASL as the consortium's effort shifts from the development of modeling and simulation (ModSim) capabilities of several single physics areas to multi-physics coupling, validation, and demonstrations. It is these later activities that CASL has worked towards as the terminal goal of addressing the CASL challenge problems and delivering

the technology for use by industry. It isn't that work on individual physics ModSim has ceased (as is evident in the article on ITM/DNS in this issue), but rather that CASL's ModSim capabilities have matured to a level that allows for feasible, and necessary, implementation of the individual physics within the VERA framework.

This shift in CASL's activities is reflected in CASL's revised organizational structure. The focus area that had been developing V&V, UQ and data assimilation (VUQ) has merged with the focus area that tested and applied the software (AMA) to create the Validation and Modeling Applications (VMA) focus area. Also, a new focus area has been implemented to facilitate the broad deployment of CASL technology (Technology Deployment and Outreach (TDO) focus area). These two teams are tasked with taking the ModSim capabilities developed by the Hub and applying them to problems of interest to industry.

The expansion of the Hub's activities has also made resource allocation more challenging, where improvements in fundamental modeling are competing with the necessary applications and deployment activities. CASL has elected to validate and apply its ModSim capabilities as early as possible through Challenge Problem demonstrations and industry Test Stands, knowing that the software is far from a commercially-polished shrink-wrapped software package. The early exposure of VERA to users has provided CASL's developers with a very efficient method to sort out what is working and what is not working, which then sheds light on the allocation of additional resources to address so identified needs.

Also, CASL's Science Council has not been shy about its advice on shifting emphasis from ModSim development to ModSim V&V and testing/applications in an industrial setting. The council wisely recognizes that in less than five years the building blocks for a post-CASL entity will have to have been established to ensure the technology is sustainable. Of course some additional resource allocation would ease the transition, but reality is as it is.

All that said, the CASL team has struggled with balance—when to research this or pursue that; what is the right time to implement coupling between two codes; or when should we get feedback from users without turning them off with an immature code? We try to ensure progress is made across the project, resulting in a multitude of research topics in diverse directions and at opposing scales, I am confident that CASL has achieved the right balance and that its ongoing performance and legacy will validate the Energy Innovation Hub concept.

VERA Software Releases in 2015

In April 2015, CASL released version 3.3 of the Virtual Environment for Reactor Applications (VERA), followed by the first release of the VERA-EDU package in September. The releases included selected computational tools and supporting infrastructure for standalone and coupled simulations. The infrastructure components provide a common user input capability and integrated physics with data transfer and coupled-physics iterative solution algorithms.

VERA3.3 and VERA-EDU include capability for 2D lattice, 2D and 3D core neutronics problems for pressurized water reactor geometries that can be used to calculate criticality and fission rate distributions by pin for input fuel compositions. Integrated cross section capabilities are included that provide problem-specific cross sections for the problems defined. Subchannel thermal-hydraulics capability is provided that allows analyses for single and multiple fuel assemblies. The fuel rod performance capability includes 1D, 2D, and 3D fuel rod temperature, fuel rod internal pressure, free gas volume, clad integrity indicators, and fuel rod waterside diameter. These capabilities allow simulation of power cycling, fuel conditioning and deconditioning, high burnup performance, power uprate scoping studies, and accident performance simulations. VERA3.3 also includes coupled physics capabilities provided for MOC radiation transport + subchannel thermal-hydraulics (2-physics 2-way) and MOC radiation transport + subchannel thermal-hydraulics + axisymmetric 2D R-Z fuel rod modeling (3 physics 2-way). VERA3.3 is intended to be used for testing and evaluation. Testing within CASL has focused specifically on Westinghouse four-loop reactor geometries and conditions with example problems included in the distribution. VERA-EDU has been released to specific organizations for development of the academic modules and is expected to be ready for general release late in 2016.

VERA System Requirements: Linux platforms, including CentOS 6.6, Ubuntu 14.04.1, SUSE Linux Enterprise Server 11 SP3, Fedora 21, and CrayOS, with functioning gcc, g++ and gfortran compilers and X11 libraries are supported. A computer having a least 32 cores is required to run standalone cases; coupled cases require a machine having at least as many computing cores as fuel assemblies to be simulated in the reactor core, considering symmetry. Detailed system software and third party library requirements are provided in the VERA Installation guide.

For more information, see www.CASL.gov/VERA.shtml

About CASL

CASL is a DOE Energy Innovation Hub focused on modeling & simulation of Commercial Light Water Reactors. CASL connects fundamental research and technology development through an integrated partnership of government, academia and industry that extends across the nuclear energy enterprise. Learn more at www.casl.gov.



Acknowledgments

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