CASL TechNotes

Consortium for Advanced Simulation of Light Water Reactors

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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** will be produced on a quarterly basis.*

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2D Lattice Physics Problems Simulated with MPACT

The term "lattice physics" refers to the simulation of detailed neutron interactions at the fuel rod level for one or more arrays of fuel rods. Current commercial LWR core reload design tools utilize two-dimensional (2D) lattice physics calculations as the first step in a two-step approach; they provide a set of representative parameters to a three-dimensional (3D) nodal diffusion code that enables reconstruction of the core reactivity and pin power distribution. In order to eliminate some of the approximations entailed by this two-step approach, CASL is integrating the lattice physics simulation with the 3D core-level solution thereby allowing a more direct approach and a higher degree of fidelity in the modeling of heterogeneous core configurations.

The MPACT (Michigan Parallel Characteristics based Transport) code, currently under development by the University of Michigan for CASL, will integrate a 2D lattice physics Method of Characteristics (MOC) methodology with a 3D core-level solution to provide the capability for detailed neutronics core analysis. By directly integrating these two-levels of physics MPACT can enable streamlined steady-state eigenvalue calculations for high-fidelity full-core LWR analysis with neutron flux and power distribution information at the sub-pin level.

CASL's AMA focus area recently completed initial testing of MPACT against reference results from Monte Carlo simulations and in-house industry codes. AMA compared the lattice eigenvalues and normalized fission rate densities to solutions generated by two independent continuous energy (CE) Monte Carlo particle transport codes, KENO-VI and MCNP5 for a 2D hot zero power (HZP) beginning of life (BOL) lattice. **(p.2)**

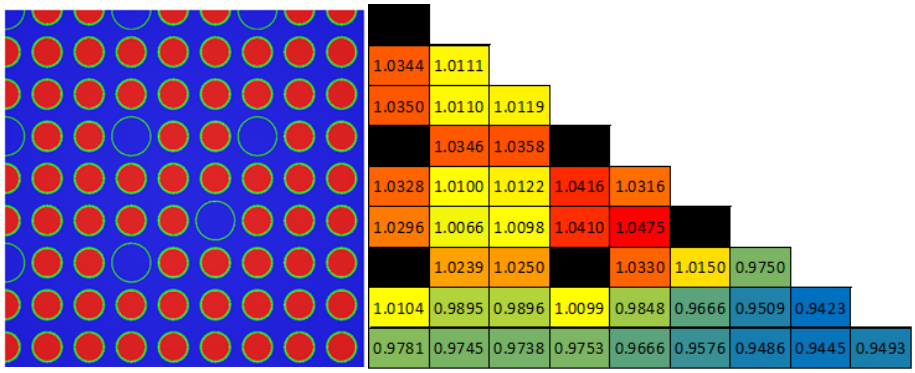

Figure 1 MPACT Power Distribution Results: No poisons, Moderator and fuel at 600K, 3.1wt% Enrichment (Case 2B)

Collaboration on GTRF Forcing Input

A team of CASL scientists from Los Alamos National Laboratory and Westinghouse Electric Corporation (WEC) collaborated on an assessment of calculation approaches for forcing inputs to grid-to-rod fretting (GTRF) using Hydra-TH, Star-CCM+ ,and WEC's proprietary VITRAN (VIbration TRansient Analysis – Nonlinear) code. A series of computational fluid dynamics simulations were completed and the calculated flow field rod excitation forces were applied as input to evaluate the sensitivity of the fuel-rod assembly dynamics to the turbulent fluid forces.

CFD-calculated Forces

A series of isothermal turbulent flow calculations were carried out by Mark Christon, Jozsef Bakosi and Lori Pritchett-Sheats of LANL on both 3x3 and 5x5 rod bundle geometries.

The turbulence models assessed in the study included implicit large-eddy simulation (ILES), Reynolds-averaged Navier-Stokes (RANS) models (e.g., the Spalart-Allmaras model), and detached-eddy simulation (DES), a blended LES/RANS method. Details on the turbulence models used are described in the Hydra-TH Theory Manual (LA-UR-12-23181).

For the study, the flowing water was specified at 394.2 K (942.0 kg/m^3 and 2.32x10^{-4} kg/m/s) with an inlet velocity of 5 m/s axially, with no cross-flow applied. A physical duration of 1.0 second was selected for the simulations. Time-averaged statistics were collected beginning at 0.2 sec, after the turbulent flow reached a statistically stationary state (fluctuation around a clearly defined mean). **(p.4)**

Coming in our next issue of TechNotes*: CASL's Education Program and Summer Workshop*

Analysis of 2D Lattice. . . (continued from p. 1)

In addition, an analysis of a 2D 3x3 multi-assembly problem was performed and the control rod reactivity worth was evaluated. In each of these cases MPACT was shown to provide solutions that are in excellent agreement with the reference solutions. Figures 1 to 5 provide some examples of the results obtained with MPACT, and Table 1 lists some of the rod worth calculation results.

Comparisons were also made against the Westinghouse in-house lattice physics code PARAGON. The PARAGON code has been extensively validated and correlated against measurements of U.S. and world-wide commercial PWRs and against critical experiments, and it is indicative of the current industry state of the art. The MPACT results were also in good agreement with the reference PARAGON solutions. These comparisons are important to understanding the use of MPACT in an industrial framework, especially when moving to the more complex geometries pertaining actual core designs, and the results are useful in identifying possible refinements for the CASL team.

Application and testing of MPACT v1.0 on several lattice physics problems encompassing a wide range of fuel temperatures, integral and discrete burnable absorbers, control rods, and multi-assembly controlled configurations has indicated that MPACT is capable of solving 2D lattice problems under a variety of fuels and compositions. The study also provided some important data points on code runtime, and a summary of some of the observations is provided in Table 2 for different cross-section groupings.

The MPACT testing required extensive collaboration between ORNL Researcher Andrew Godfrey, Westinghouse Reactor Physicist Fausto Franceschini, University of Michigan Researcher Ben Collins, VERA Product Integrator Scott Palmtag, and ORNL CASL Intern Julie Stout (Summer and Fall '12). The comprehensive study leveraged the CASL Team's close relationships and complementary areas of expertise, allowing the exchange of key information and feedback among the team members which is required to produce a CASL product with such broad applicability.

For more information, see CASL-U-2012-0172-000.

Table 1 Rod Worth Calculation Results

	KENO-VI CE	MPACT	MPACT Relative Error
Rod Worth ENDF/B-VI	-2715	-2662	-1.9%
Rod Worth ENDF/B-VII	-2691	-2635	-2.1%

Table 2 Example MPACT Runtime Performance

		ENDF/B-VII ORNL 60g Subgroup		B-VII ORNL 60g ESSM	
Case	Cores	Ray Spacing (cm)	Time (mm:ss)	Ray Spacing (cm)	Time (mm:ss)
2B	8	0.05	4:11	0.05	3:00
2M	8	0.004	35:50	0.004	22:33
2K	8	0.05	4:23	0.05	3:13
2P	8	0.05	4:24	0.05	3:21

The MPACT (Michigan Parallel Characteristics based Transport) code is being developed for CASL under the leadership of Ben Collins, Brendan Kochunas, and Tom Downar at the University of Michigan.

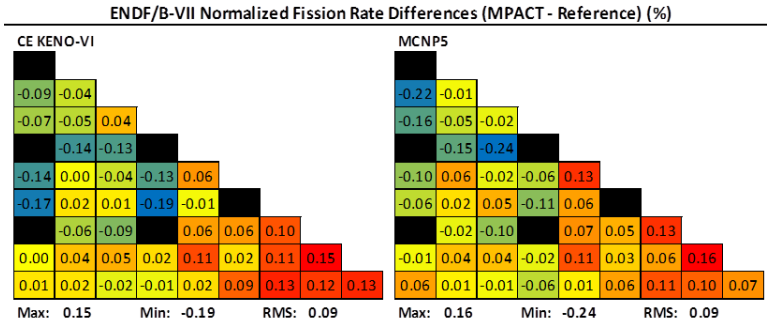

Figure 2 Normalized Fission Rate Differences: MPACT vs. KENO-VII and MCNP5, No poisons, Moderator and fuel at 600K, 3.1wt% Enrichment (Case 2B)

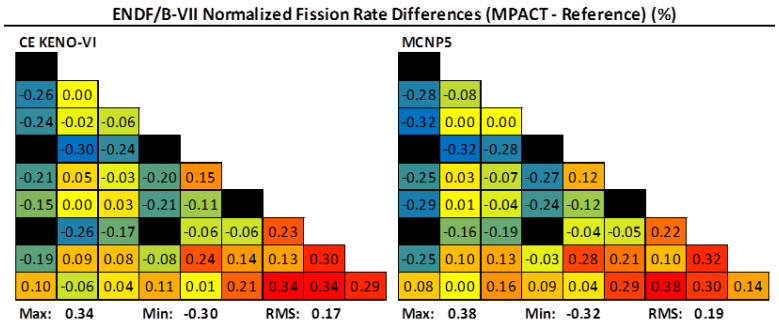

Figure 3 Normalized Fission Rate Differences: MPACT vs. KENO-VII and MCNP5, 128 IFBA Rods, Moderator and fuel at 600K, 3.1wt% Enrichment (Case 2M)

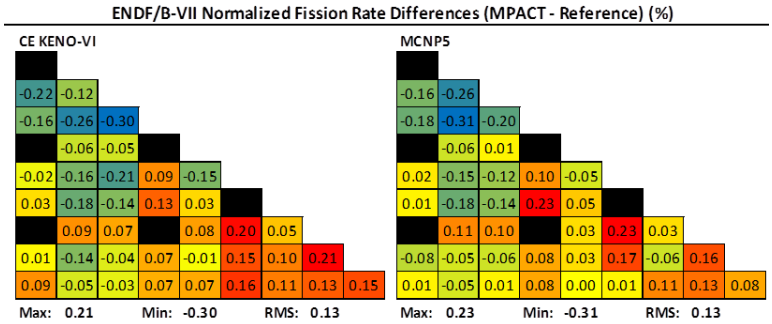

Figure 4 Normalized Fission Rate Differences: MPACT vs. KENO-VII and MCNP5, Zoned Enrichment (3.6 and 3.1wt%), Moderator and fuel at 600K (Case 2K)

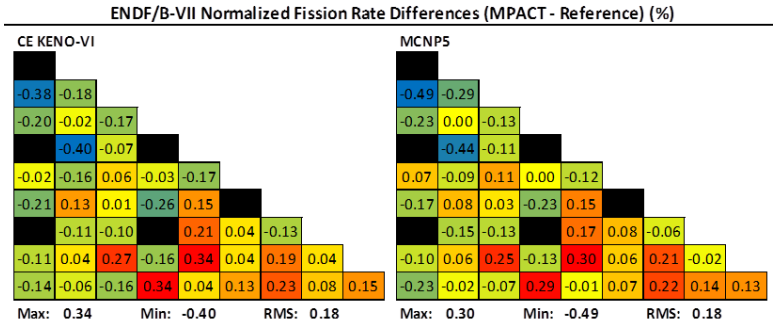

Figure 5 Normalized Fission Rate Differences, MPACT vs. KENO-VII and MCNP5, 24 Gadolinia Rods, Moderator and fuel at 600K, 3.1wt% Enrichment (Case 2P)

Westinghouse Implementing a CASL Test Stand

On February 7, Westinghouse engineers met with CASL researchers to discuss the deployment of a test stand on Westinghouse's Cranberry Township, PA, computer cluster. Test Stands are targeted deployments of the CASL VERA, ideally on the User's computational platform, for application testing by CASL Partner Users. The Test Stands will be used to study specific challenge problems, and to demonstrate and apply CASL's ModSim capabilities.

MPACT Development Lead Ben Collins (U-Mich) discusses the expected VERA radiation transport capabilities that will be available in time for the WEC Test Stand scheduled for June, 2013.

The workshop, hosted by Bob Oelrich, Manager of Westinghouse Methods Development, was attended by several Westinghouse engineers who provided insight to potential industrial uses of VERA. AMA Focus Area Deputy and Westinghouse R&D Manager Zeses Karoutas discussed Westinghouse's vision for applications of VERA, noting that VERA is expected to provide Westinghouse with insights and a more mechanistic understanding of reactor and fuel performance. Fausto Franceschini (Westinghouse R&D) discussed the possibility of applying VERA to the simulation of Westinghouse advanced reactor designs, the AP1000™ and the Westinghouse small modular reactor (SMR). Larry Mayhue (Westinghouse PWR Core Methods) discussed application of the higher fidelity codes within VERA to benchmark industry reactor physics codes, and Greg Fisher (Westinghouse Radiation Engineering and Analysis) discussed the potential for utilizing VERA in shielding applications.

Westinghouse Fellow Engineer Larry Mayhue

The initial installation of VERA on the Westinghouse computer cluster is undergoing, with some lead time allowed to prepare for the more formal test stand deployment and simulations beginning in Summer 2013.

Each of the CASL industry partners are expected to host a test stand. EPRI's test stand may be deployed in Fall '13, as the new EPRI computer cluster becomes available, and TVA's test stand is anticipated for Spring 2014. As the maturity level of the VERA capability is advanced, users outside of the CASL Consortium partnership may host test stands as well. The deployment of Test Stands is expected to allow for User feedback on usability and effectiveness, generate expert Users of the technology at the industrial level, and expand the validated range of the technology.

Pilot Project on Fibrous Debris Effects

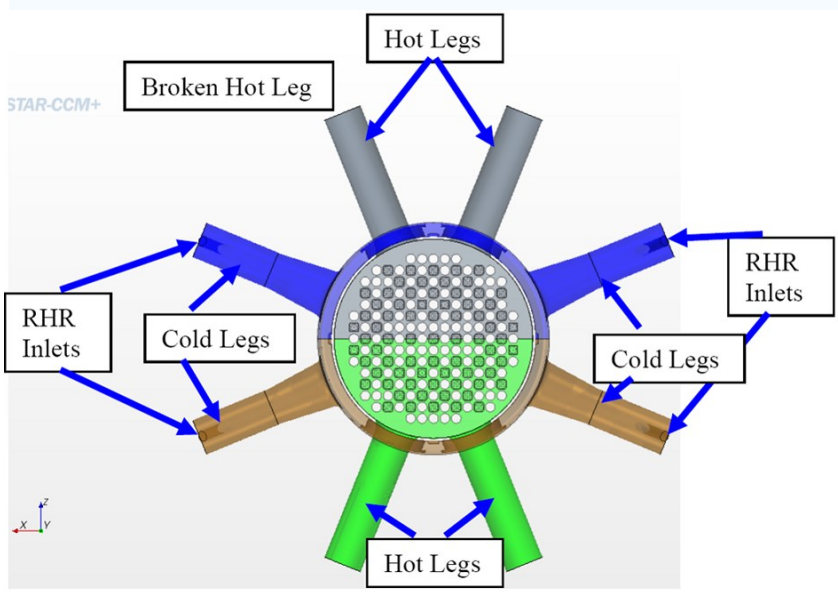

Figure 6 A Horizontal Cross-section of a 4-loop PWR showing the Hot and Cold Leg Configurations, along with the RHR Inlets

Pressurized water reactor (PWR) containment buildings are designed both to contain radioactive material releases and to facilitate core cooling in the event of a loss-of-coolant-accident (LOCA). Reactor core cooling following the LOCA may utilize water discharged from the LOCA pipe break and containment spray. This water is collected in a sump and is recirculated through the emergency core cooling system (ECCS) and the containment spray system (CSS). Although the sump contains several screens to remove any debris in the water, it is possible that fibrous debris from reactor insulation or other sources could be present in the recirculated water. Concerns have been raised about the potential for the debris to affect long term core cooling during the LOCA event.

Nuclear fuel assemblies (FA) are equipped with bottom nozzle filters designed to trap debris prior to entry into the active fuel region. Industry tests have demonstrated that, when present, fibrous debris collects at the bottom nozzle or at the lowest spacer grid, causing higher resistance to the coolant flow. The redistribution of flow and effect of the blockage on the fuel temperatures due to the postulated scenario and presence of the fibrous debris is not fully understood.

In order to demonstrate some of CASL's simulation capabilities on a high-performance computing system, the Advanced Modeling and Applications (AMA) team piloted a full core simulation of a 4-loop Westinghouse NSSS with postulated fibrous debris (p.7)

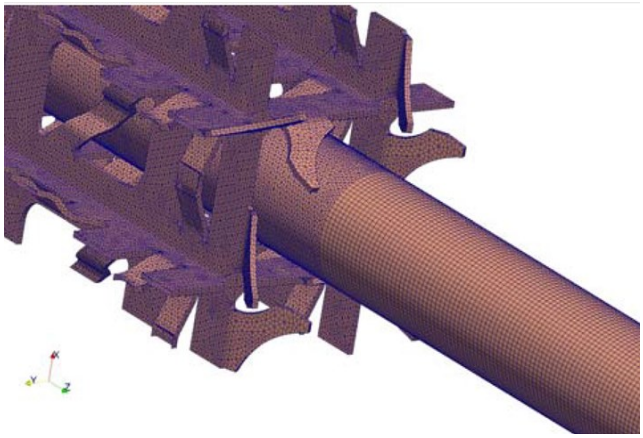

Figure 7 The element distribution shown in this 3M Cubit mesh of the fuel rod and spacer surfaces was demonstrated to be too coarse for the GTRF application

Figure 7 provides an illustration of the 3M cell Cubit mesh.

All calculations were performed in a time-accurate way using the neutrally dissipative second-order trapezoidal rule time-integrator. A fixed CFL condition was used for all calculations in conjunction with implicit second-order treatment of the advective and diffusive terms.

> ***Courant–Friedrichs–Lewy condition*** *(CFL condition) is a necessary condition for convergence when solving certain partial differential equations using explicit time-marching schemes.*

Various statistics of the fluctuating flow field were analyzed and compared to data from computations carried out by Westinghouse using Star-CCM+ and from experiments at Texas A&M University. The available results showed good agreement with both simulations and experiments. Comparing different approaches to compute turbulent flows, the team concluded that low-order RANS models do not appear to be appropriate to provide time-accurate pressure force fluctuations at the resolution required for the GTRF problem.

Results from Hydra-TH and STAR-CCM+ are in reasonable agreement, and show that the mixing vanes are the main source of turbulence that generates the excitation forces on the fuel rod. The excitation forces decay along the span downstream of the spacer grid. The Hydra-TH results with 14 million cells are relatively close to the STAR-CCM+ results with 48 million cells. Results from both Hydra-TH and STAR-CCM+ show the force in the X-component is slightly lower than the Z-component.

VITRAN Calculations

WEC engineer Roger Lu used the CFD-calculated RMS forces as inputs to the WEC VITRAN code. VITRAN is a specialized code developed by Westinghouse to simulate flow-induced vibration and fretting wear of a fuel rod (see CASL-I-2012-0135-000 for a more detailed description of the code). The non-linear dynamic VITRAN model includes a single fuel rod and its associated grid supports (represented as springs and gaps), as shown in Figure 8, and calculates the rod frequency response and motion, the support impact forces (normal and friction forces), the sliding and sticking distances and the work rates based. Inputs to the code include the hydraulic excitation forcing function (the power spectral density, or PSD) and the power history of the fuel rod to calculate of rod-to-grid gaps, cladding creep-down, spring relaxation, and grid lateral growth. The model uses the normal work rate to calculate the rod wear rates and the scar depths using empirical wear coefficients. High flow velocity and turbulence imposes stochastic and fluctuating pressure (force) on the fuel rod surface and induces fuel rod vibration. The PSD is used to describe the fluctuating pressure. Experimentally measuring the PSD and the related correlation length on the fuel rod surface is very difficult, and it recent years, due to the significant increase in computing capability, CFD has been introduced to calculate PSD using numerical techniques. In this study, the hydraulic forcing functions were supplied by the Hydra-TH and STAR-CCM+ calculations.

The VITRAN model includes six spacer grids. For these calculations, the input and boundary conditions were applied consistent with the VIPER loop test used for comparison. All grid cells were assumed to have zero preload and zero gap. The VITRAN results show that (p.9)

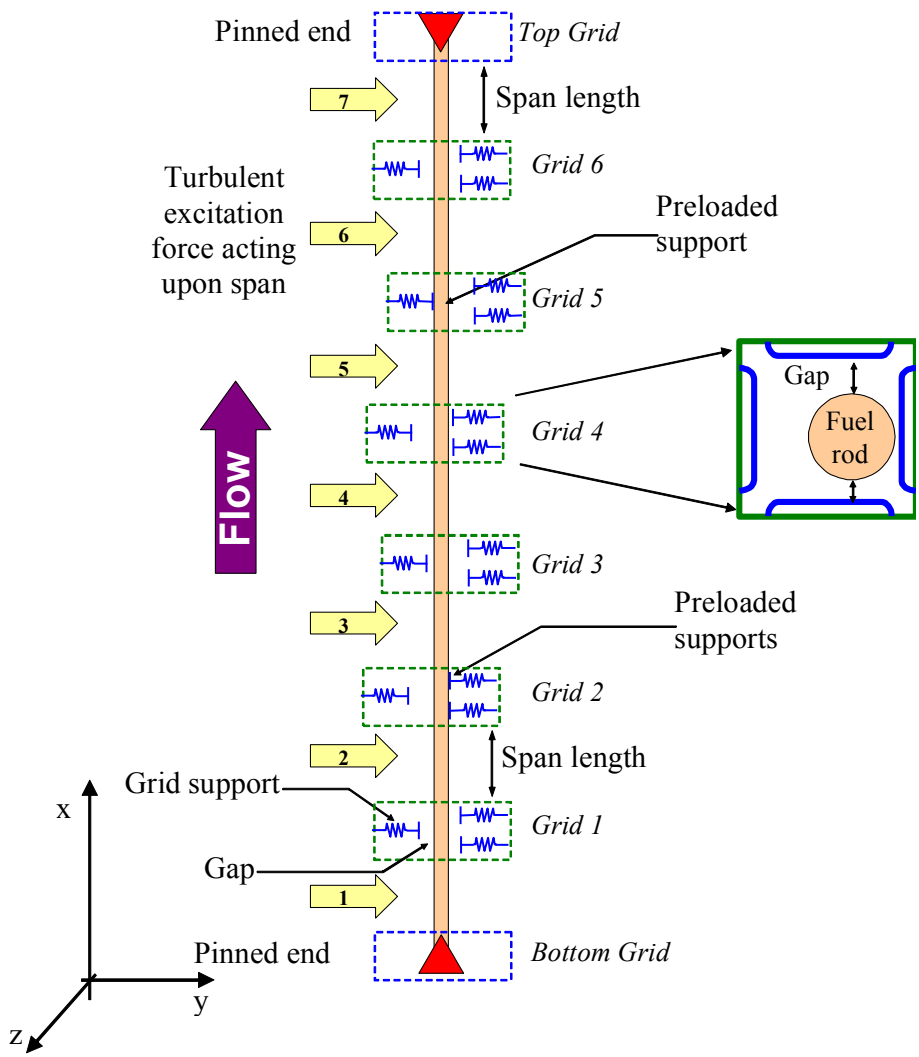

Figure 8 VITRAN Model Schematic

Product Integrators

Gregg Swindlehurst, RIA and LOCA CPI

Jeff Secker, CRUD CPI

Nam Dinh, VPI

In 2012, CASL established the Challenge Problem Integrator (CPI) role. The first year of CASL development highlighted the need for subject matter expert champions to set expectations, development paths, and define success for each of the Challenge Problems (CPs). Because the CPs include diverse coupled physics applications that cut across CASL's Focus Areas, the CPIs have responsibility for driving the development of critical applications, products, and outcomes that traverse the Focus Area boundaries.

Each of the CPIs are currently preparing a Charter and an Implementation Plan for their Challenge Problem. These documents are expected to help guide the development process, allow for targeted synergistic application development, and provide a definition of success for the CASL team. CRUD CPI Jeff Secker (WEC) has already established the CRUD CP Charter and Implementation Plan, and the CASL development team has made significant progress toward providing a higher fidelity CRUD ModSim tool for industry use. The draft Charters and Implementation Plans for active CPs (CRUD, PCI, GTRF) are expected by the end of April, with other CPs to follow.

The CPIs also provide a focal point for the CASL development team to jointly deliver CASL solutions and ModSim applications. The CPIs work with the Focus Area teams to set and define milestones, to complete certain milestones as appropriate, and to review milestones for which they are the customer. While CPIs do not specifically have budget authority, they do influence the Focus Area budgets through the milestone planning process. As CASL continues to evolve, CPIs will be established (or retired) as areas for application are identified.

Each of the CPIs have extensive experience within their subject CP. Gregg Swindlehurst (GS Nuclear Consulting, LLC) has more than 34 years of experience in safety analysis and reload design methodologies, and provided a leadership role in the development of Duke Energy's in-house codes and methods, including the development of RELAP5 and GOTHIC. He has worked extensively with the EPRI RETRAN and VIPRE codes. Jeff Secker (WEC) has worked for Westinghouse for 33 years in the areas of core design, advanced fuel development, advanced fuel management and CRUD modeling and methods. Robert Montgomery currently manages the Nuclear Energy Sector at PNNL. He has more than 20 years of experience in the modeling, analysis, and evaluation of nuclear fuel rod, assembly and structural material behavior under normal operation, transient conditions, and in a defective state and has participated in developing several nuclear fuel rod analysis codes, including the EPRI FALCON code. Yixing Sung (WEC) specializes in the field of PWR reactor core thermal-hydraulics, including code and methods development. He has more than 20 years of experience with new plant and fuel designs, power uprates, and reactor core reloads.

In addition to the CPIs, the CASL project has also established the roles of Validation Data Integrator (VDI) and the Core Simulator Integrator (CSI). As the VDI, Professor Nam Dinh (NCSU) works with the appropriate Focus Areas to establish verification and validation data availability and needs, at both the single-physics and multi-physics levels. Nam has more than 20 years of academic, R&D and engineering experience in nuclear reactor experimentation, modeling, simulation and validation. The CASL Core Simulator Integrator, Dr. Scott Palmtag (Core Physics, Inc.), coordinates the development, verification and validation of the VERA core simulator capability (see Tech Notes Vol.1 Iss.1). Scott has over 15 years of experience developing BWR and PWR core simulators.

Zeses Karoutas is the overall product integrator and is the deputy lead for the AMA focus area in CASL. He will oversee solutions to the challenge problems and guide the product integrators. Zeses currently works in Westinghouse as the Manager of the PWR Fuel Technology group and has about 34 years experience in the areas of thermal hydraulic analysis and testing, advanced fuel development and DNB testing and correlation development.

Rob Montgomery, PCI CPI

Scott Palmtag, CSI

Yixing Sung, DNB CPI

Zeses Karoutas, CPI Lead

VUQ Spans Focus Areas to Facilitate Industry Implementation of CASL Technology

Coupled industry legacy code applications have provided important insights for the nuclear community and results from CASL's VERA are expected to provide additional insights. VERA is envisioned as a more mechanistic coupled treatment of the physical processes at a higher fidelity than current industry codes. The mission to validate the advanced models and methods developed for VERA is central to industry implementation of the CASL modsim predictive capability. Per outgoing VUQ Focus Area Lead Jim Stewart, "VUQ is essential for achieving science-based predictive M&S capabilities for the CASL virtual reactor. The VUQ process guides the CASL R&D investments, leads to best-estimate predictions with reduced uncertainties, and aids in designing future experiments." Per outgoing Focus Area Lead Jim Stewart, "VUQ is essential for achieving science-based predictions with reduced uncertainties, and aids in designing future. VUQ Focus Area Lead Vince Mousseau and Deputy Brian Williams will re-emphasize the application of VUQ at the challenge problem level. Vince noted that industry acceptance of many CASL tools will be predicated on VUQ demonstrations.

The VERA validation is being expanded to effectively apply available data. As a rule, complex multi-physics applications require an exponentially complex calibration and validation. A potentially higher-fidelity modsim approach and result can be overshadowed by the multiplicative uncertainty of the system. A VUQ objective is to cross-cut the large, multi-faceted, and evolving body of information related to the available validation database, legacy modeling findings, and CASL's modsim approach and results. Then, VUQ aims to provide a systematic and, in some instances quantitative, delineation and ranking of gaps and issues related to the information.

VUQ has also established a process to identify and assess candidates for validation of VERA: a top-down process is applied to identify a range of possible experiments and plant measurements of potential interest that can supplement the existing information, and a bottom-up approach is used to more extensively evaluate and apply existing validation information. Potential paths for upgrading experimental methods and measurement techniques have been explored, and VUQ is currently in the process of collecting Product Integrator input on validation of Challenge Problem solutions before making recommendations on supplementary experimental studies.

A Case Study on CRUD Modeling

In addition to collecting and understanding the available validation database, VUQ recently provided insights and a better understanding of reactor performance through parametric sensitivity studies using the VERA component *DAKOTA*. A study of two Westinghouse-designed four-loop pressurized water reactors (PWRs) [designated Plant A and Plant B] assessed the influence of thermal-hydraulic parameters on mass evaporation rate (a predictor for crud formation) using quarter core models, ranking their relative importance, while uncertainty quantification (UQ) assessed the mean and variance with respect to input parameter uncertainties.

For Plant A, the three sensitivity analysis (SA) techniques applied consistently ranked temperature as the most influential parameter and pressure as second. Temperature exhibited a positive correlation while pressure was negatively correlated. The sensitivity analysis for Plant B better demonstrates the power of these screening techniques. The lead coefficient of the Dittus-Bolter correlation for boiling and the exponent of the partial boiling model were identified as crucial model form parameters and the four operating parameters were again identified as significant parameters. However, the remaining model form parameters (due to be calibrated) had comparably little effect.

In the uncertainty quantification studies, both Latin Hypercube Sampling (LHS) and Polynomial Chaos Expansion (PCE) techniques yielded similar estimates for the response means and standard deviations. (In some scenarios, PCE could provide considerable cost savings over Monte Carlo methods to obtain similar results, though for high dimensional parameter spaces sampling may prove more effective). Considerable Plant B variability is likely attributable to model form parameters and future studies should consider performing forward propagation of uncertainty. Simulation results indicate considerable variation in both mean and standard deviation of the CRUD deposition rate throughout the reactor quarter core.

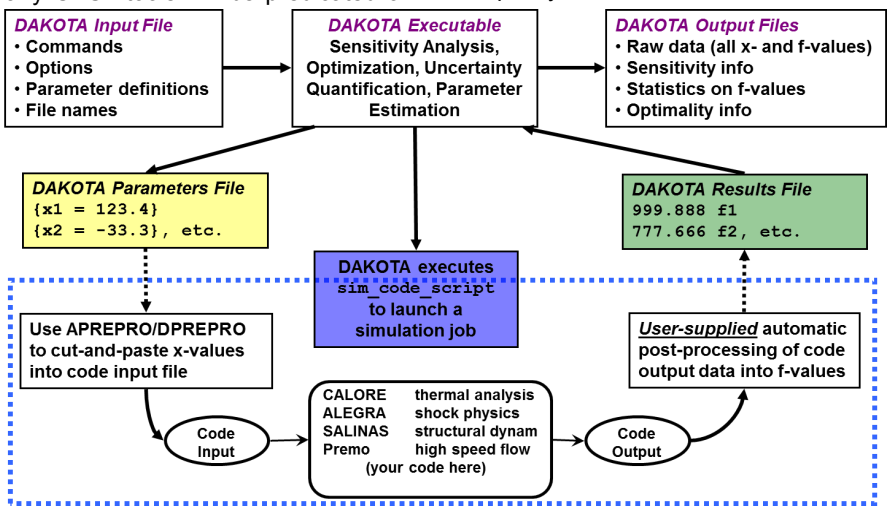

Figure 9 Loose coupling of DAKOTA to a generic application

The studies were not exhaustive, but they do provide an illustration of the powerful capabilities of DAKOTA and the workflow processes implemented by VUQ. These will be used with other VERA multi-physics applications for evaluating challenge problems as they are available. More information is available in VUQ.VVDA.P4.02, VUQ.VVDA.Y1-1.02, and VUQ.Y1.03.

A Tool with Wide Applications

DAKOTA is a freely available, SNL-developed software package for sensitivity analysis, optimization, uncertainty quantification, and calibration with black-box computational models. To perform optimization, uncertainty quantification, or sensitivity analysis in a loose-coupled or "black-box" mode, DAKOTA iteratively writes parameter files, invokes a script to run the computational model, and collects resulting responses from a results file. This overall execution process is depicted in Figure 9. DAKOTA provides a flexible, extensible interface to any analysis code, includes both established and research algorithms designed to handle challenges with science and engineering models and manages parallelism for concurrent simulations. DAKOTA strategies support mixed deterministic/probabilistic analyses and other hybrid algorithms. You can read more about DAKOTA in SAND2001-3796.

Fibrous Debris Effects Pilot. . . (continued from p. 3)

following a LOCA event. The work was led by Westinghouse Engineering Fellow Dr. Jin Yan, in close collaboration with CD-Adapco's Robert Brewster, and utilized CD-Adapco's commercial computational fluid dynamics (CFD) application STAR-CCM+ (version 7.04.006). Dr. Yan noted, "The CFD results will give more details of flow and temperature fields of coolant and solids in the reactor core under complicated transient accidental conditions than have not been available previously."

The simulation leveraged an existing computational mesh constructed by the AMA team for the reactor and fuel. The CFD simulation includes a full 360-degree model of the reactor vessel, including the cold and hot legs, as shown in Figure 6. The upper head of the reactor was not included in the model to reduce computing cost and a solid wall was placed at the boundary instead. The geometries of the reactor internals were meshed in great detail, except for the spacer grids, which were represented by porous media. The mesh of the reactor core was built in Prostar and the remaining regions of the reactor vessel were meshed using the STAR-CCM+ polyhedral mesher; the total cell count was over 1 billion mesh cells. A typical mesh in the core region is depicted in Figure 10. The various meshes were assembled on the Westinghouse large memory workstation into a single domain connected through interfaces. The simulation was executed on Westinghouse computer clusters and the INL Fission computer. Post-processing was done on the Westinghouse large memory workstation.

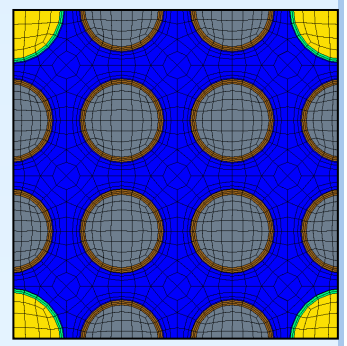

Figure 10 A typical mesh (horizontal cross-sectional view) in the core region

The fibrous debris was modeled as a gradual time-dependent pressure drop increase across the bottom nozzle region of each fuel assembly as the fibrous debris accumulates and was assumed to accumulate uniformly across the reactor core. The core decay heat (formulated based on NS-RAT-DS-85-026) was applied to each fuel rod in the model using a power density table that was generated based on typical core conditions (calculated using Westinghouse's ANC neutronics code). Normalized axial power shapes were applied, with the fuel rod axial power shape determined based on its core nodal location and relative radial rod power.

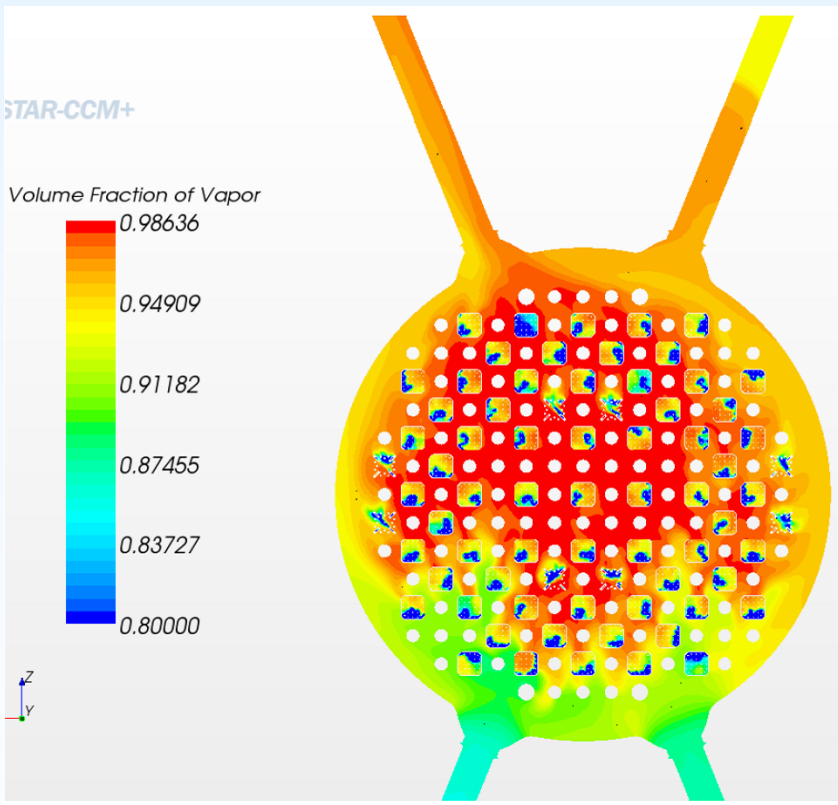

Figure 11 Cross-section of the reactor core with the volume fraction of vapor at 94 seconds into the LOCA event (there is some liquid remaining in the guide tube assemblies at this moment).

The transient simulation was started 18 minutes after the postulated hot leg break LOCA. All of the coolant and all solid structures (including the fuel) were initialized at the RHR cooling temperature of 190ºF at the beginning of the simulated transient. A constant mass flow rate of 91.482 kg/s and temperature at 190°F was applied at each RHR inlet. One of the hot legs was assumed to be at 0 psi (relative to atmospheric pressure) as the outlet boundary condition; the rest of the hot legs were closed. Phase change was simulated with using a Volume of Fluid (VOF) model. The entire flow domain was assumed to be filled with liquid water initially.

The volume of liquid coolant present in the core and its depletion is a key parameter indicating whether fuel assemblies are uncovered during accidents. The simulation provided an indication of the collapsed liquid level in the core and the mass flow rate through the broken hot leg, indicating that the liquid mass flow increases substantially when boiling starts and quickly reduces in inventory. The water level in the core decreased sharply at the beginning of boiling and then slowly decreased as the liquid boiled off. The liquid inventory was depleted almost the same rate in all quadrants when boiling started. However, shortly after the onset of boiling, the quadrant closest to the broken hot leg depleted at a higher rate than the other quadrants, suggesting convection of entrained steam toward the broken loop. Steam continued to accumulate more rapidly in the broken loop quadrant until vapor began to discharge at the exit (break) after approximately 40 seconds. Figure 11 provides a cross-section of the reactor core with the volume fraction of vapor at 94 seconds into the LOCA event.

The maximum pellet and clad waterside surface temperatures increased rapidly in the first 15 s (due to decay heat application). Once the clad reached the saturation temperature and boiling started, the temperature increase rate slowed down, and the pellet centerline temperature responded about 20 seconds later. Figures 14 and 15 graph clad outer surface temperatures and fuel rod centerline temperatures, respectively, at various elevations as a function of LOCA event time.

Table 3 Run Time information for the Fibrous Debris CFD Simulation

Physical Time (s)	94
Total Solver CPU Time (s	8576077312.0
Total Solver Elapsed Time (s)	4766887.0
Average CPU Time per Iteration (s)	9.48

An interesting finding uncovered by the simulation is the **(p.10)**

CASL Metrics Development

Like most projects, CASL must measure and track the strategic areas of its operation and research and this is accomplished by implementing corresponding strategic metrics. CASL Project Manager Jeff Banta noted that there are many benefits of establishing specific performance metrics, including:

- Improving the management and delivery of CASL products and services.
- Improving internal and external communications between CASL and its stakeholders.
- Emphasizing a "results-oriented" culture driving timely and accurate deliverables.
- Justifying projects and their costs.
- Demonstrating the accountability and stewardship of taxpayer resources.

- **Metrics will be used to track progress toward achieving strategic objectives**
  - Data collection methods are in place
  - Initial evaluation complete and updates scheduled for end of PoR 6 and 7
  - Corrective actions will be based on metric trends

To ensure the metrics are both valuable and value-adding, CASL metrics adhere to an established philosophy known as *SMART*: specific, measureable, achievable, realistic, and time-bound.

CASL will be measuring both operations and outcome level metrics. Examples of operations level metrics include total number of milestones for the PoR, milestones delivered on schedule, and number of students engaged with CASL. Outcome level metrics measure progress towards achieving the goals and objectives set forth in the CASL Program Plan using tools such as PCMM and include items such as number of CPs under investigation, effectiveness of the CPs to drive solutions development, and understanding perceived impact of the development results. There are also several metrics related to the VOCC Laboratory, including lab up-time and utilization.

Performance measurement is mandated by the Government Performance and Results Act (GPRA) of 1993 and the Government Performance & Results Modernization Act of 2010 (signed into Law Jan 2011) and is central to other legislation and Administration initiatives.

Table 4 provides a summary of a few of the proposed metrics. Data collection will occur on regular basis as needed to support the metrics.

Table 4 Proposed CASL Metrics for PoR 6 and 7

Strategic Outcome	Proposed Metric
Address design, operational, and safety challenges for LWRs	⇒ Number of CPs under investigation ⇒ Maturity of CP solutions
Develop and effectively apply modern virtual reactor technology	⇒ PCMM assessments of VERA on progression problems and CPs
Engage nuclear community through modeling and simulation	⇒ Number of VERA licenses granted ⇒ IC and User group activity/ membership ⇒ Faculty, graduate, postdoctoral researchers utilizing/evolving VERA
Deploy new partnership and collaboration paradigms	⇒ VOCC Lab availability/utilization ⇒ Virtual collaboration attributable to VOCC technology

VERA Snapshot 3.0

VERA, the Virtual Environment for Reactor Applications, provides CASL's ModSim technology and consists of integrating and interfacing software together with a suite of physics components adapted and/or refactored to simulate relevant physical phenomena, often in a coupled manner. VERA also includes the software development environment and computational infrastructure needed for these components to be effectively used. Development of VERA is central to the CASL objective to "apply existing modeling and simulation capabilities and develop advanced capabilities to create a usable environment for predictive simulation of light water reactors."

The Virtual Reactor Integration (VRI) focus area periodically produces "snapshots" of VERA. These snapshots contain the most recent tested VERA configurations and are used by the CASL team to test capabilities and make progress on Challenge Problems. Less frequently, the snapshot is released externally to CASL (a "formal" VERA release). The most recent snapshot, 3.0, is described in CASL Milestone report VRI.P6.04 (available on the CASL SharePoint site).

An essential part of VERA application development includes an automated continuous-integration build and test system based on TriBITS lifecycle model (SAND2012-0561). CASL's implemented development system includes a stringent set of nightly regression tests to ensure that the application's capabilities have not been compromised during the development process, and that coupled applications perform as expected. Without such a system to continuously build and test integrated applications, experience has shown that application capabilities can erode due to changes in interfaces and functionality, portability problems, build system changes, etc. Applications that are continuously built and tested deliver fewer defects and allow for frequent (daily if necessary) snapshots.

The VERA 3.0 Snapshot report provides a summary status of each of the VERA applications, along with a graphical summary of VERA's progression over the CASL project lifetime. VERA 3.0 includes, as standalone applications:

- Cobra-TF
- Common input module
- DAKOTA
- DTK
- Drekar
- Hydra-TH
- Insilico (Denovo)
- LIME
- Mamba2.0
- Moose
- MPACT
- Peregrine
- Relap5-3D
- SCALE/XSPROC

Coupled component applications included in VERA 3.0 are:

- DAKOTA/Cobra-TF,
- Insilico/Cobra-TF,
- and Insilico/Drekar.

CASL-developed legacy (proprietary limited distribution) capabilities outside of VERA include ANC9.5, VIPRE-W, DAKOTA/VIPRE-W, ANC9.5/VIPRE-W, ANC9.5/VIPRE-W/BOA.

Each component in Vera 3.0 is accessible from the CASL-VRI git software repository to those who have the proper access permissions. The system provides the following features: automated revision control and tracking, enforcement of IP protection, and accessibility of the applications for CASL staff.

Collaboration on GTRF . . . (continued from p. 4)

the CFD modeling methodologies used by Hydra-TH and STAR-CCM+, while different, produce comparable RMS forces. Both codes show very good agreement. However, it would be desirable to perform additional computations with Hydra-TH using higher resolution meshes to test the sensitivity of the RMS forces. Less than 2% difference in the wear work-rate was observed between the cases run with Hydra-TH loads and STAR-CCM+ loads.

Why Large-Eddy Simulation?

From the engineering viewpoint the most useful information that can be obtained from simulations of turbulent flows are *statistical* and *integrated quantities* derived from the fluctuating flow field. Examples of statistics are the mean velocity, the root-mean-square (RMS) pressure, and the turbulent kinetic energy spectrum. Examples of integrated quantities are the mean drag or mean lift on an airplane wing or the PSD distribution of the fluctuating forces that load the fuel rods in a pressurized water nuclear reactor. The current engineering practice for the GTRF problem is to compute turbulent flow solving the RANS equations augmented by a turbulence model. RANS models directly compute the statistics by solving for only the mean field values and, depending on the model, the second moments. For example, the κ-ε model is a popular way to approximate the effects of fluctuations on the mean velocity. However, it is important to appreciate that the main goal of the κ-ε model is to provide closure for mean velocity via the time scale ~k/ε . Consequently, one can expect a statistically meaningful description of the mean but less so of the fluctuations, e.g., k or ε, themselves, only their effect on the mean. If the second moments, e.g., the fluctuation about the mean, are also important, a model with a higher level of description is required. Figure 12 provides an illustration of the results obtained for the ILES, DES and RANS models.

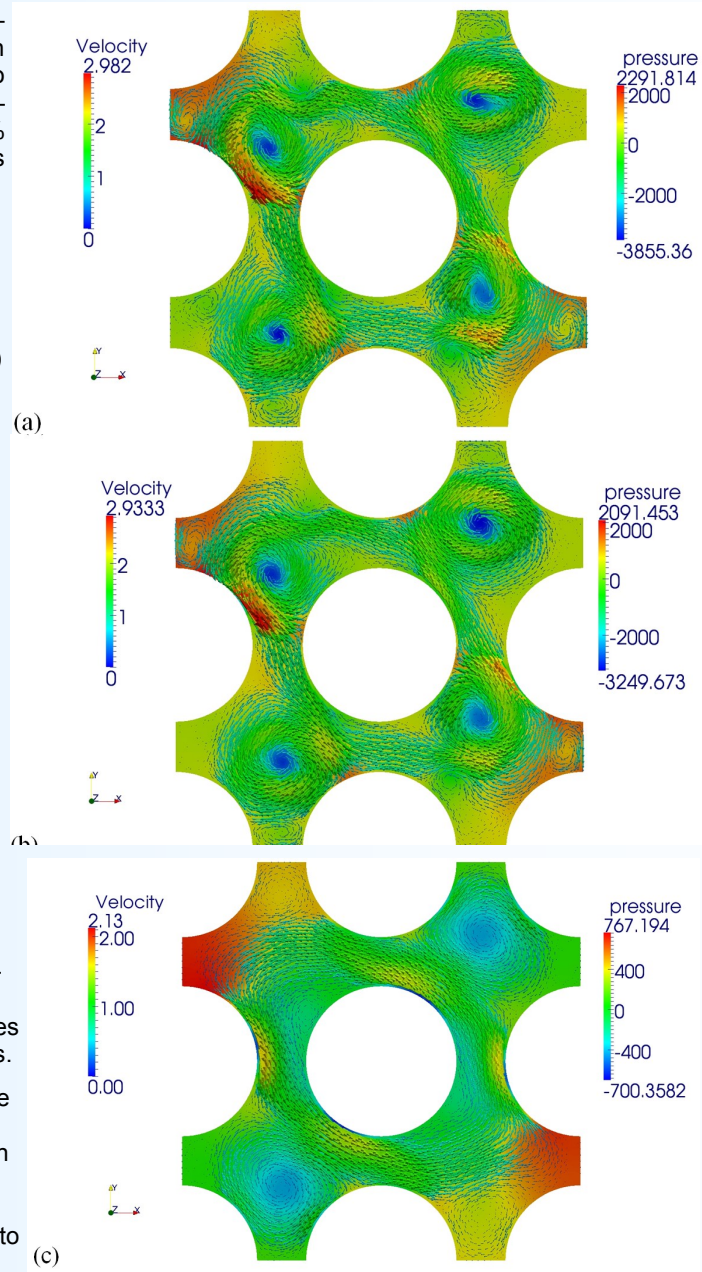

Figure 12 Snapshots of instantaneous velocity and pressure on cut-plane for the 3M mesh at t = 1.0 second for (a) the ILES, (b) detached-eddy simulation, and (c) Spalart-Allmaras RANS models

Mesh-related Findings

Numeca's Hexpress/Hybrid mesh generator, a.k.a., "Spider", was used for the first time to generate hybrid meshes for the GTRF problem. A method for quantitative assessment of complex unstructured meshes with no-slip walls was developed and used to assess a series of meshes generated for the GTRF problem by two mesh generators.

Arguably the most important quantity for coupling to a structural code is the fluctuations of the pressure force loading the rod. The RMS forces were calculated on a series of 3 meshes with increasing mesh resolution. Using the same algorithm and code, the team found that the predicted RMS forces, integrated for the whole rod, an order of magnitude larger using the higher-quality Spider meshes compared to Cubit meshes. The rod force distributions computed with Hydra-TH and STAR-CCM+ are quite comparable, albeit using relatively coarse meshes with Hydra.

Study Conclusions

The study concluded that the displacement, acceleration and wear work-rates computed with VITRAN indicate there is little sensitivity to using RMS forces computed with Hydra-TH or STAR-CCM+ as input. The RMS force comparison indicated that the CFD methods used by Hydra-TH and STARCCM+, although different, predict transient forces that show very good agreement, and the mixing vanes result in significant turbulent mixing which generates the unsteady excitation forces on fuel rod. The excitation forces generated by mixing vanes decay along the span downstream the grid. The study additionally noted that a minimum mesh resolution of approximately 7 to 14 million cells is required to achieve RMS pressures that are of reasonable fidelity for the subsequent VITRAN calculations.

For more information, see CASL-I-2012-0165-000.

Corrections and Clarifications

The TechNotes article "Progress in THM Development" neglected to mention Professor Tom Downar and Assistant Research Scientist Ben Collins in the list of University of Michigan-based research team members involved in a sensitivity, verification and validation study of STAR-CD, STAR-CCM+ and Nphase boiling models. Our apologies!

Fibrous Debris Effects Pilot (continued from p. 7)

appearance of a strong circulating flow in the bypass channel providing enhanced core cooling for some time. The vector plot near the core inlet in Figure 13 shows the high speed jets through the holes on the lower former plates. This downward flow is attributed to greater hydrostatic pressure in the core bypass region relative to the fuel assemblies as boiling progresses in the core. A coincident increase in upward flow in the fuel assemblies is also suggested by the cladding temperature trends of Figure 14. The outer clad temperatures are shown to decrease at the lower elevations as subcooled liquid from the inlet plenum penetrates further upward in the assembly with the onset of boiling at higher elevations. These results demonstrate the important capability of the CFD analysis to resolve the influence of debris accumulation on the redistribution of flow and heat transfer in the core.

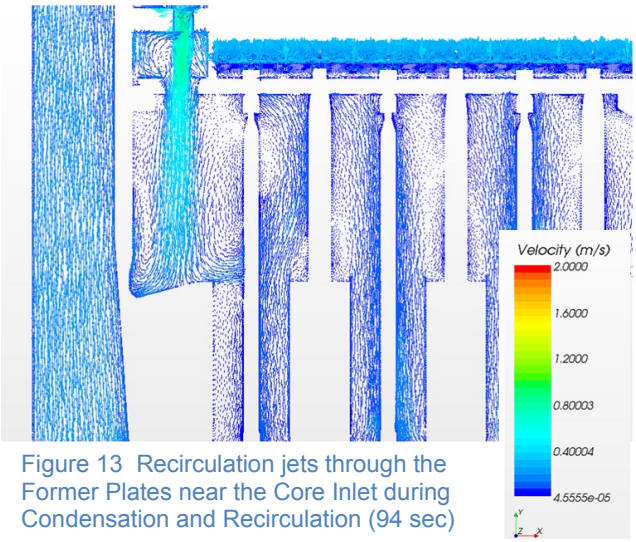

Figure 13 Recirculation jets through the Former Plates near the Core Inlet during Condensation and Recirculation (94 sec)

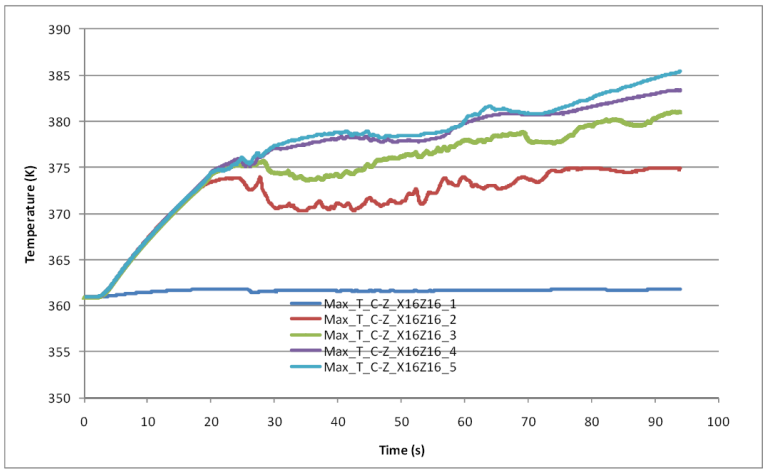

Figure 14 Cladding Outer Surface Temperature of Rod X16Z16 at various Elevations

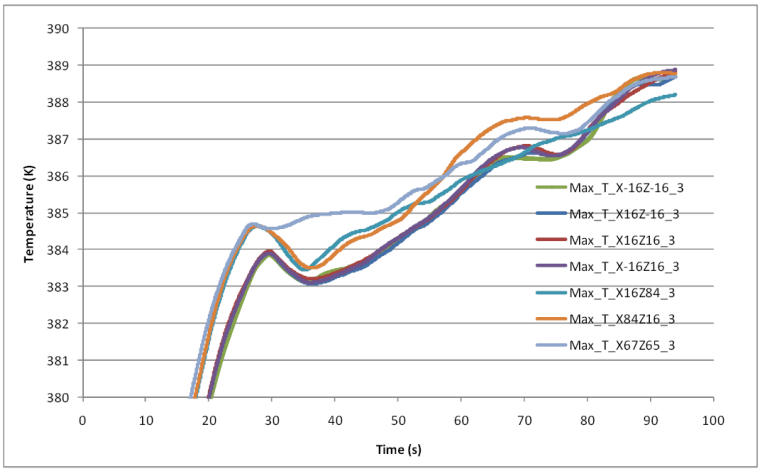

Figure 15 Fuel Centerline Temperature of Rod X16Z16 at various Elevations

The large model size and computational requirements associated with this model provided valuable experience in identifying logistics-related issues. This computationally demanding simulation was run on 4800 cores to ensure memory use during execution did not exceed available capacity on any core. No scaling test was done as part of this initiative. The associated run statistics, provided in Table 3, illustrate the execution time. At the termination of the run, only half of the decay heat was transferred out of the vessel through boiling (vapor generation), clearly indicating longer simulations are necessary to reach peak fuel temperatures.

A more expeditious and realistic simulation could be achieved by applying a more representative initial temperature condition to the fuel rods. However, this simulation demonstrated that a CFD model can provide insights of fluid flow and temperature distribution under such complex situations. Eric Volpenhein of CD-Adapco noted, "It is a remarkable demonstration of the ability to explore and quantify the redistribution of flow and heat transfer throughout the reactor core in unintended circumstances using contemporary modeling & simulation through CASL. The opportunity to contribute to a reliable and appropriate response to the long standing interest in fibrous debris is immense."

More details on the model and simulation are provided in CASL-I-2013-0029-000.

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.

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