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Nuclear Science User Facilities High Performance Computing: FY2019 Operations and Accomplishments Report

Eric T Whiting, Stephanie J Parker

March 2020

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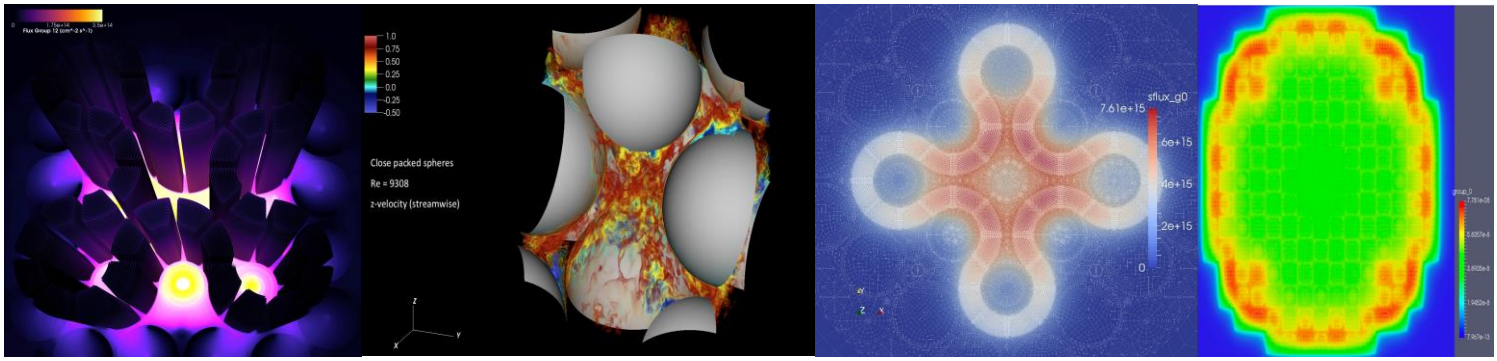
Idaho National Laboratory



Nuclear Science User Facilities High Performance Computing: FY2019 Operations and Accomplishments Report

March 2020

Prepared by:
Stephanie J. Parker, Tami Grimmett, Simon M. Pimblott, J. Rory Kennedy & Eric Whiting

Purpose

This report highlights a subset of projects that were completed in FY 2019 by researchers using Idaho National Laboratory's High-Performance Computing (HPC) resources.

Funding

This research made use Idaho National Laboratory computing resources which are supported by the Office of Nuclear Energy of the U.S. Department of Energy and the Nuclear Science User Facilities under Contract No. DE-AC07-05ID14517.

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Executive Summary

Idaho National Laboratory (INL), as supported by DOE-NE through the NSUF, provides supercomputer systems, data storage, network connectivity, system management, cybersecurity, user support, data analytics, modeling and simulation codes, and visualization resources to the extended DOE-NE user community, including users at university, in industry, and government laboratories to enable a wide range of research and development and mission supporting activities. The provision of high-performance computing (HPC) capabilities is a key enabler of collaboration and of innovation in nuclear energy systems research and technology development and implementation to support the mission and objectives of DOE-NE.

In FY 2019, INL enhanced its HPC capabilities with the opening of the Collaborative Computing Center, which includes data center space for up to 197 computer equipment racks. INL's Falcon supercomputer has been consistently oversubscribed since installation in 2014. In early FY 2019, a 20,160 core, 1.0 Petaflop Dell system, called Lemhi, was installed. This machine was key in supporting the Consortium for Advanced Simulation of Light Water Reactors (CASL) as well as DOE-NE programs such as the VERA user group training and MAMBA calibration. In addition, in August 2019, a contract award for a $19.2M computer with a performance rating of 5.6 Petaflops from 99,792 compute cores with GPU capabilities adding an additional 0.56 Petaflops of compute capability.

During FY 2019, the INL HPC capabilities were utilized by 425 users from INL, the NRC and DOE and 68 other institutions including 35 universities and 22 industry partners. HPC job scheduling policies give priority to DOE-NE programs such as NSUF, CASL, NEAMS, GAIN, NEUP, FCT, and LWRS with access by Idaho university students and faculty at a lower priority. Due to the deployment of the Lemhi system, 326 million core-hours of compute time were delivered in FY 2019, an increase of 75 million core-hours over FY 2018. Delivery exceeded the operational goal of 80% utilization (315 million core-hours). The average oversubscription of Falcon was 2.3× (meaning the average wait queue for the year was 79,654 processor cores) while the average oversubscription of Lemhi was 1.7× (average wait queue ~ 33,352 processor cores).

A wide range of studies utilizing INL HPC capabilities were undertaken in FY 2019 and contributed summaries of 31 of those studies are presented in this report. A large portion of HPC use was geared towards either molecular dynamics (MD), density functional theory (DFT), or computational fluid dynamics (CFD) based studies. In addition, a number of computational analyses intended to demonstrate reactor improvement/modification ideas were performed as well as a series of targeted computational studies on topics important to nuclear and other energy systems.

The subset of projects presented in this report gives a clear indication of the high value and strong utilization of the INL HPC capabilities supported by the NSUF on behalf of DOE-NE. Though most of the projects focus on the challenges facing nuclear energy, the breadth of scope of the investigations supported is a clear indication of the multidisciplinary nature of the INL HPC capability.

Introduction

Idaho National Laboratory's (INL) High Performance Computing (HPC) resources provide scientific computing capabilities for INL and the Department of Energy Office of Nuclear Energy's (DOE-NE) efforts in advanced modeling and simulation. This includes supercomputer systems, data storage, network connectivity, system management, cybersecurity, user support, data analytics, modeling and simulations codes, and visualization resources for the extended DOE-NE user community, including users at universities, in industry, and government laboratories. Scientific computing enables a wide range of research activities, such as the performance of materials in harsh environments (including the effects of irradiation and high temperatures), performance of existing light-water and advanced nuclear reactors, modeling of geomechanical changes in subsurface flow, and multiscale analysis of nuclear fuel performance.

The Nuclear Science User Facilities (NSUF) program combines access to nuclear science research and development (R&D) capabilities and scientific expertise with exceptional ideas provided by external contributors (universities, laboratories, and industry). These collaborations define the cutting edge of nuclear technology research and stimulate cooperative research between user groups conducting basic and applied research. INL's HPC support is a key enabler of this collaboration and opens the door to nuclear energy innovations.

INL recognizes the importance of HPC in all areas of science and as such is strongly committed to growing our capabilities and enhancing our ability to support DOE-NE's computational science programs. The envisioned future-state requires a transformational application of scientific computing. The establishment of the Advanced Scientific Computing (ASC) division, the construction of the Collaborative Computing Center (C3), and the recent installation of the Sawtooth HPC system are important steps in this transformation.

Advanced Scientific Computing

INL's Scientific Computing Strategy from 2018 highlighted the establishment of the ASC division within the Nuclear Science and Technology mission organization. Accordingly, INL's High Performance Computing operations and support organization, along with the computational frameworks department, was moved to the Nuclear Science and Technology Directorate under ASC in September 2018. A full-time ASC director was appointed in June 2019. The Scientific Computing Strategy highlighted INL's strengths and opportunities. The 2030 vision for Scientific Computing included the following statement:

> "Due to the high potential of rapid and transformational breakthroughs in the science and engineering of materials and systems from developments in the field of scientific computing, it is essential that INL implements a visionary strategy that expands our computational research capabilities through investments in scientific computing capacity, development and validation of innovative modeling tools, and expansion of expertise in

deep machine learning, artificial intelligence, advanced visualization, and large-scale data processing and analytics."

The discussion that follows demonstrates INL's commitment to this strategy and highlights successes and impacts.

Collaborative Computing Center

Recognizing the limitations of INL's legacy facilities and the importance of a gathering place for people involved in Scientific Computing, INL undertook a bold initiative to construct a new facility focused on computing. The Collaborative Computing Center (C3) was designed to meet the current and future scientific computing needs of INL. The State of Idaho became a key enabling partner by providing the funding for the new leased facility. Construction began in April 2018 and was completed in August 2019.

The C3 facility provides office space for 196 people arranged in a manner that encourages collaboration, communication, and innovation between people – INL staff, university collaborators, and industry. The fifteen 'pods' allow small workgroups to have a gathering place, while the flexible shared common areas encourage ad-hoc and impromptu work, such as team programming, user help, and mentoring. Multiple conference rooms of varying sizes provide ample opportunities for collaboration, scientific data visualization, and meetings. The C3 facility is designed with multiple physical security zones to allow public training meetings and public access as required.

A foundational enabling component of Scientific Computing is a capable data center with adequate space, power, and cooling for power-hungry HPC systems. The C3 facility includes data center space for up to 197 computer equipment racks. Racks are arranged in eleven rows, with

the first eight rows configured for HPC hardware – up to 1MW of electrical power per row. The remaining three rows are designed for networking, hard disk storage, and other utility systems with power up to 150KW per row. The data center under floor infrastructure is designed for water-cooled systems and includes the latest data center energy efficiency innovations. Current power and cooling are provisioned up to a max limit of 4 MW with the ability to add an additional 4 MW of capacity when required.

New HPC Systems

INL's Falcon supercomputer has been consistently oversubscribed since installation in 2014. Several updates increased its computational performance by a factor of two, yet the system was still not keeping up with demand.

In early FY18, INL decided to add some institutionally funded compute capacity as a 'bridge' to support INL HPC requirements until the C3 facility was complete and the new Sawtooth machine could be commissioned. Accordingly, in early FY19, a 20,160 core, 1.0 Petaflop Dell system, Lemhi, was installed. This machine was key in supporting Consortium for Advanced Simulation of Light Water Reactors (CASL). This system is also utilized by DOE-NE programs such as: VERA user group training, MAMBA calibration, and several CASL milestones. Lemhi's queueing policies were configured to support large compute jobs with shorter runtimes.

Planning for Sawtooth started in 2014 after the installation of Falcon. This planning work included: numerous vendor meetings, nondisclosure briefings, C3 facility design meetings, and other reviews. The conclusion of this work was a Request for Proposal (RFP) that was released on April 22, 2019. The RFP evaluation and award process included extensive internal reviews, an external review by staff at the National Renewable Energy Laboratory, and several RFP addendums to answer vendor questions. On August 19, 2019, a contract award was made to Hewlett Packard Enterprise (HPE) for a $19.2M four-year lease-to-own system. This new computer has a performance rating of 5.6 Petaflops with 99,792 compute cores. In addition, GPU capabilities add an additional 0.56 Petaflops of compute capability. The system was installed in December 2019 and moved to full production in March 2020. This new system will have a positive impact on DOE-NE's ability to deliver science results at a much larger scale than ever before.

Institutions

The following table lists the HPC user count and institution name for users who utilized INL HPC systems in FY19.

10/01/2018 – 9/30/2019	
Institution	**User Count**
Analysis and Measurement Services Corporation	1
Analytical Mechanics Associates	1
Argonne National Laboratory	2
Bechtel Marine Propulsion Corporation	2
Blue Wave A.I. Labs LLC	1
Boise State University	19
Brigham Young University Idaho	1
Charmworks Inc	2
Clemson University	4
Colorado School of Mines	1
Department of Energy	3
Electric Power Research Institute	4
Electricite de France	1
Exelon Nuclear	6
Framatome	2
General Atomics	1
GSE Systems	1
Idaho National Laboratory (INL)	201
Idaho State University	8
James Madison University	1
Jozef Stefan Institute	1
Kairos Power	2
Kansas City National Security Campus	1
Kansas State University	1
Knolls Atomic Power Laboratory	1
Korea Nuclear International Cooperation Foundation	2
Los Alamos National Laboratory	2
Massachusetts Institute of Technology	9
MPR Associates	7
North Carolina State University	10
Nuclear Regulatory Commission	4
NuScale Power, LLC	1
Oak Ridge National Laboratory	15
Oregon State University	5
Pacific Northwest National Laboratory	4
Pennsylvania State University	3
Politecnico di Milano	2
Purdue University	2

10/01/2018 – 9/30/2019	
Institution	**User Count**
Rolls-Royce	1
Sandia National Laboratory	1
Sapienza University of Rome	2
SCANA	1
Seoul National University	1
Southern Nuclear	3
Southwestern Scientific Ltd. Co.	1
Statehouse, LLC	1
Structural Integrity Associates	1
Texas A&M University	7
Universities Space Research Association	4
University of Colorado Boulder	1
University of Idaho	16
University of Illinois at Urbana-Champaign	5
University of Kentucky	1
University of Massachusetts Lowell	1
University of Michigan	3
University of Nevada, Reno	1
University of New Hampshire	1
University of New Mexico	3
University of South Carolina	1
University of Tennessee	2
University of Tennessee Knoxville	2
University of Texas at Arlington	1
University of Utah	4
University of Wisconsin	1
University of Wyoming	2
Utah State University	1
Virginia Tech	5
Walsh Engineering Services	1
Washington State University	1
Westinghouse Electric Company	14
Yellowstone Energy	1
Grand Total	**425**

Utilization

The Falcon and Lemhi systems combined delivered more than 326 million core-hours of compute time in FY19. This is an increase of 75 million core-hours over FY18, largely due to the deployment of the new Lemhi system. Our operational goal of 80% utilization equates to a target of 315 million core-hours based on the mid-year deployment of Lemhi. The actual compute time delivered exceeded our operational goal.

The average queue size, in terms of oversubscription factor, is another important measure of demand for computational resources. In FY19, the average oversubscription of Falcon was 2.3× (meaning the average wait queue for the year was 79,654 processor cores). The average oversubscription of Lemhi was 1.7× (meaning the average wait queue was 33,352 processor cores).

HPC job scheduling policies give priority to DOE-NE programs such as NSUF, CASL, NEAMS, GAIN, NEUP, FCT, and LWRS. Idaho university students and faculty have a lower priority; their jobs will run when the system has unused compute capacity available – essentially backfilling the system to maintain high utilization while helping build computational science expertise in the state.

The following pages highlight some user-contributed summaries of the modeling and simulation work that made use of INL's supercomputers Falcon and Lemhi in FY 2019.

Ab initio Molecular Dynamics Simulations of Metallic Fuel

REPORT PARTICIPANTS:

Benjamin Beeler[1], David Andersson[2], Chao Jiang[3], Yongfeng Zhang[4]
1 North Carolina State University
2 Los Alamos National Laboratory
3 Idaho National Laboratory
4 University of Wisconsin-Madison

SCIENTIFIC ACHIEVEMENT:

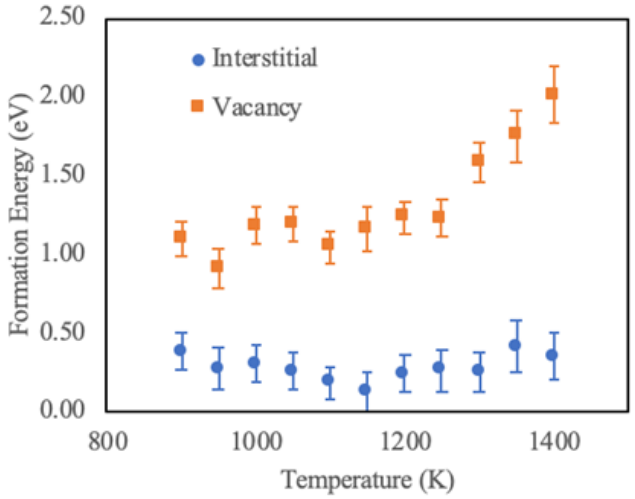


Fig. 1 The point defect formation energy for bcc U from 900 K to 1400 K. Error bars represent plus/minus one standard error of the data set.

Uranium (U) is often alloyed with molybdenum (Mo) or zirconium (Zr) in order to stabilize the high-temperature body-centered cubic (bcc) phase of uranium when used for fuel in nuclear reactors. Relatively few experimental or computational investigations have centered on bcc U, largely due to the mechanical instability of this phase at room temperature. This is particularly true for density functional theory calculations that typically investigate 0 K properties. However, *ab initio* molecular dynamics (AIMD) allows for quantum mechanical-based calculations to be performed at non-zero temperatures. AIMD can account for the inherent anharmonicity responsible for making the bcc phase stable at high temperature, and as such allows for direct investigation of the bcc phase without any other required assumptions or restrictions. While AIMD has been utilized to study a variety of systems, there have been no AIMD investigations into the defect formation energies in bcc U at high temperatures nor have there been any studies into the bcc U-Zr phase. This work performed the first AIMD simulations of the point defect properties of bcc U and subsequently calculated surface energies of several surface orientations in bcc U and bcc U-Zr.

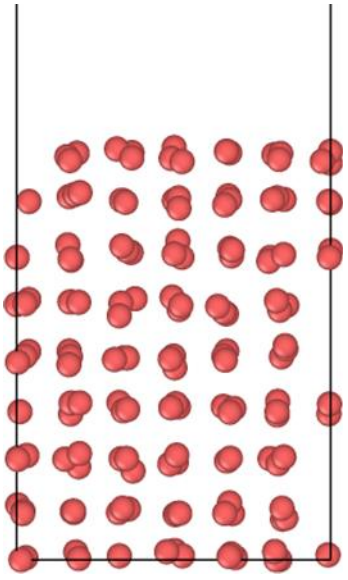


Fig. 2. Surface termination of bcc U along the (110) plane, taken from AIMD simulations at 1100 K.

SIGNIFICANCE:

It has been previously suggested that bcc U exhibits anomalously low interstitial formation energies, however, these calculations relied upon density functional theory that artificially induced a stabilized bcc structure and, as such, introduced a large amount of unquantifiable

uncertainty. This work has shown that bcc U does indeed have extraordinarily low interstitial formation energy for a metal (0.25 eV, compared to typical values of 2-5eV for most metals), and additionally that the vacancy formation energy is substantially larger than the interstitial formation energy. This in turn provides evidence to the suggestion that self-diffusion in bcc U occurs via an interstitial mechanism, as opposed to a vacancy mediated mechanism, as is typical in metals.

In addition, surface energy calculations via AIMD simulations were utilized to inform fuel performance models that incorporated fission gas bubble swelling in metallic fuels. The existing fuel performance models utilized a value that was based upon neither experimental nor computational evidence and as such was yielding incorrect bubble physics. The utilization of AIMD provided a rigorous determination of the fuel surface energy that was incorporated into BISON to construct higher fidelity fission gas swelling simulations.

KEY PUBLICATIONS:

- To be submitted

Computational Modeling of Fission Product Behavior in SiC Layer of TRISO fuels

REPORT PARTICIPANTS:

Chao Jiang[1], Isabella J. Van Rooyen[1], Subhashish Meher[1]
1 Idaho National Laboratory

SCIENTIFIC ACHIEVEMENT:

Understanding phase stability in the palladium-silicon-carbon (Pd-Si-C) ternary system is important for predicting the high-temperature behavior of tristructural isotropic (TRISO) nuclear fuels for high-temperature gas-cooled reactors. In this project, we have performed *ab initio* evolutionary searches and *ab initio* molecular dynamics simulations to predict the atomic structures and energetics of solid and liquid phases in Pd-Si-C and its binary sub-systems, Pd-Si, Si-C and Pd-C. With the incorporation of the present theoretical results, an *ab initio* informed thermodynamic description of the Pd-Si-C ternary system has been successfully obtained.

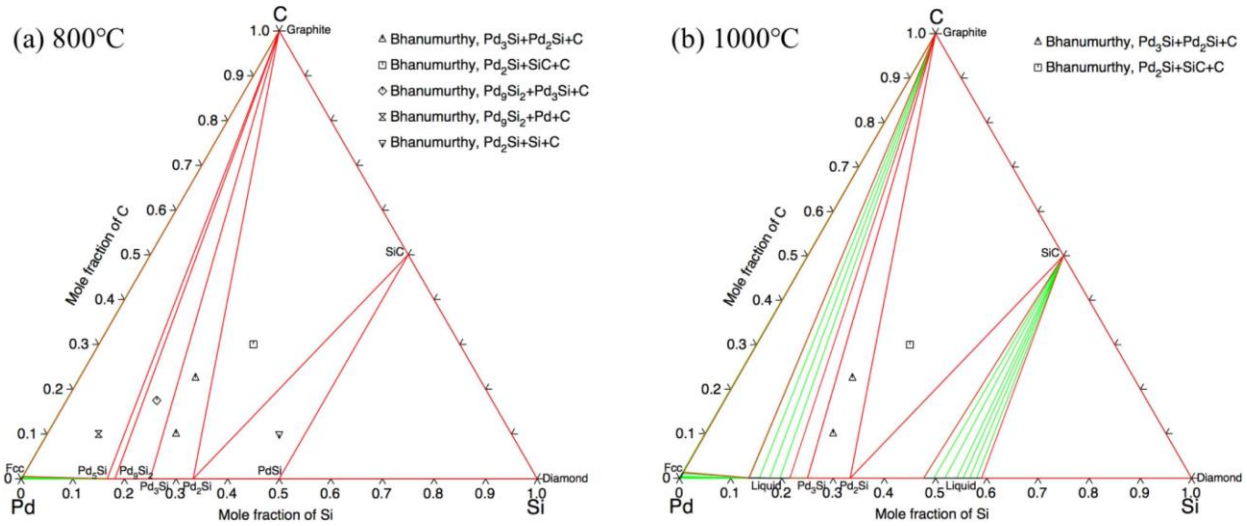


Fig. 1: Model-predicted Pd-Si-C isothermal sections at (a) 800 and (b) 100°C, in comparison with experimental measurements. The symbols indicate the experimentally explored compositions. The green lines are tie-lines, and red triangles indicate three-phase equilibrium.

SIGNIFICANCE:

Silicon carbide currently finds application as one of the layers in tristructural isotropic nuclear fuels for high-temperature gas-cooled reactors by providing high-temperature mechanical strength and a diffusion barrier for fission-product containment. Palladium, a major fission product of uranium and plutonium, has been observed in the TRISO fuel SiC layers, both inter- and intra-granularly, with movement along grain boundaries alongside various other fission or transmutation products to form palladium silicides and other complex multi-element compounds. The only identified SiC layer failure mechanism in fuel from the U.S. Department of Energy Advanced Gas Reactor program is one where the formation of a crack in the TRISO particle inner pyrolytic carbon layer allowed fission products (primarily Pd) to concentrate at and interact with the SiC layer. As these fission products are examined in post-irradiation examination to gain

knowledge on the location, compound compositions, and/or phases, it is unclear what compounds will be present during the high-temperature irradiation cycle to eliminate the effects of segregation during cooling after irradiation. Therefore, knowledge of the phase equilibria in the Pd-Si-C ternary system, as provided by the present research, is invaluable for understanding the safety and performance of the TRISO fuels for advanced nuclear reactors, particularly at the elevated temperatures (≳1600°C) characteristic of accidents.

KEY PUBLICATIONS:

- C. Jiang, I. J. van Rooyen, S. Meher. 2020. "*Ab initio* Study and Thermodynamic Modeling of the Pd-Si-C System." Computational Materials Science 171, 109238.
- S. Meher, I. J. van Rooyen, C. Jiang. 2019. "Understanding of Fission Products Transport in SiC Layer of TRISO Fuels by Nanoscale Characterization and Modeling." Journal of Nuclear Materials 527, 151793.

LOCA Toolkit for US Light-water Reactors (LOTUS)

REPORT PARTICIPANTS:

Cole Blakely[1]
1 Idaho National Laboratory

SCIENTIFIC ACHIEVEMENT:

The LOCA Toolkit for US light-water reactors (LOTUS) is a multiphysics best estimate plus uncertainty (MP-BEPU) environment. Essentially, LOTUS combines both legacy and modern codes into a single plug and play environment. LOTUS allows for massively parallel Monte Carlo based SA/UQ analysis for any resulting integrations. LOTUS employs codes from the disciplines of fuel performance, systems analysis, and core design automation. To date, LOTUS has successfully incorporated seven codes, namely PHISICS and VERA-CS from core design automation, RELAP5-3D from systems analysis, as well as FRAPCON, FRAPTRAN, and BISON from fuel performance. LOTUS stores all data from these codes in a compact and flexible HDF5 database. This year has focused on implementing a novel code execution strategy which results in 100% convergence for RELAP5-3D and FRAPCON cases.

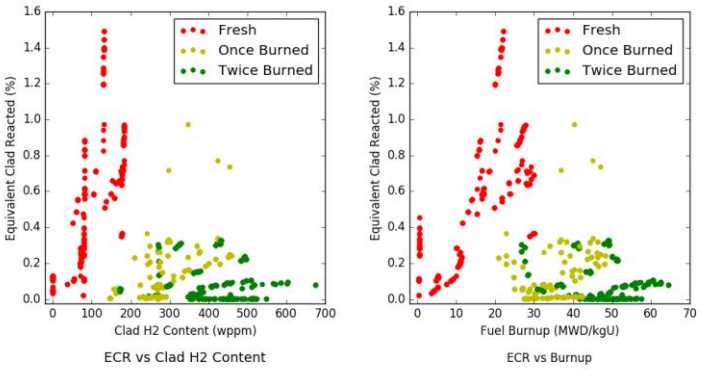


Fig. 1: The ECRR is the ratio between the equivalent cladding reacted, a systems analysis FOM, and an ECR limit based off cladding hydrogen pickup, a FOM unique to fuel performance

SIGNIFICANCE:

The multiphysics nature of LOTUS has allowed it to evaluate figures of merit (FOM) which are impossible to study in isolation, specifically the Equivalent Cladding Reacted Ratio (ECRR) and the Peak Clad Temperature Ratio (PCTR). The ECRR (see Figure 1) is the ratio between the equivalent cladding reacted, a systems analysis FOM, and an ECR limit based off cladding hydrogen pickup, a FOM unique to fuel performance.

Similarly, the PCTR (see Figure 2) is a ratio of the peak clad temperature to a limit also dependent on hydrogen pickup. To the best of our knowledge, the BEPU evaluation of PCTR and ECRR for a full-scale core is only possible within the LOTUS environment.

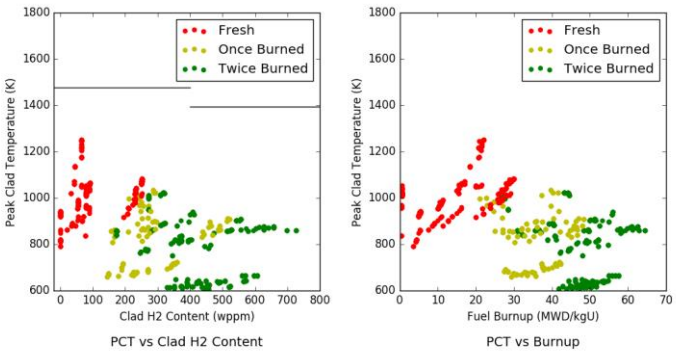


Fig. 2: The PCTR is a ratio of the peak clad temperature to a limit also dependent on hydrogen pickup

KEY PUBLICATIONS:

- Blakely, C., Zhang, H., Szilard, R., Epiney, A., Vaghetto, R., and Ban, H. 2018. "Demonstration of LOTUS Multiphysics BEPU Analysis Framework for LB-LOCA Simulations." *Annals of Nuclear Energy* 122: pp. 8-22.

Point Defect Energetics in Random FeNiCr Austenitic Stainless Steel

REPORT PARTICIPANTS:

Anus Manzoor[1], Yongfeng Zhang[2], Dilpuneet S. Aidhy[1]
1 Department of Mechanical Engineering, University of Wyoming
2 Department of Engineering Physics, University of Wisconsin

SCIENTIFIC ACHIEVEMENT:

The goal of the study is to understand the role of various parameters, such as first- and second-nearest neighbor chemistry, structural arrangements of nearest neighbors, and anti-ferromagnetism, on the vacancy formation energy in random FeNiCr austenitic stainless steel. The work is aimed at developing a generic understanding of defect energetics in concentrated alloys, including high entropy alloys. Density functional theory (DFT) calculations are performed on two different special quasi-random (SQS) structures of FeNiCr to explain large variation of vacancy formation energy observed in different atomic environments in an alloy of a given composition.

SIGNIFICANCE:

This work isolates the individual contribution of various parameters that can lead to a large variation of vacancy formation in an alloy. We find that the vacancy formation energy could vary by more than 0.6 eV in any given alloy. Surprisingly, the large variation is primarily due to the arrangement of first-nearest neighbors so despite the same number of Ni, Fe, and Cr atoms surrounding a vacancy, the different arrangements of the elements could lead to significantly different formation energies.

KEY PUBLICATIONS:

- N/A

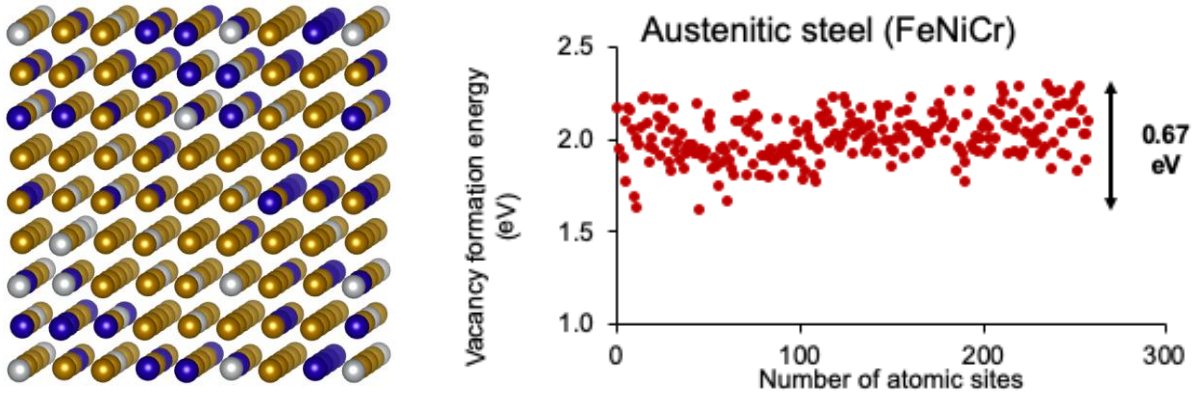


Fig. 1: (a) A 256-atom special quasi-random structure (SQS) of austenitic steel used to perform DFT calculations. (b) Vacancy formation energies of each atomic site showing a variation of 0.67 eV in the supercell.

Computational Fluid Dynamics Modeling to Improve Bubbling and Cavity Formation Processes

REPORT PARTICIPANTS:

Donna Guillen[1], Alexander Abboud [1]
1 Idaho National Laboratory

SCIENTIFIC ACHIEVEMENT:

This project used computational fluid dynamics (CFD) modeling to improve understanding of bubbling and cavity formation processes in laboratory and pilot-scale melters at different scales.

SIGNIFICANCE:

This study supports operations at the Waste Treatment and Immobilization Plant, a $16.8 billion facility being constructed to process legacy nuclear waste into a stable form for disposal. Computational modeling is a powerful complement to laboratory experiments and testing of systems at various scales. When properly applied and validated, CFD can provide information not readily obtainable by physical testing, especially in cases where the operating environment does not permit visual observation or the insertion of typical data acquisition instrumentation, as in the case of waste glass vitrification. A series of CFD and heat transfer models over a range of scales are being developed to support melter operations at the Hanford Waste Treatment and Immobilization Plant. The study provides a description of the models and the resulting information they provide that can be used to improve melter throughput, as well as aid in evaluating and resolving operating plant issues or upsets. Increases in the rate of glass production and avoiding idling can significantly decrease the duration and cost of the vitrification campaign, potentially saving billions of dollars.

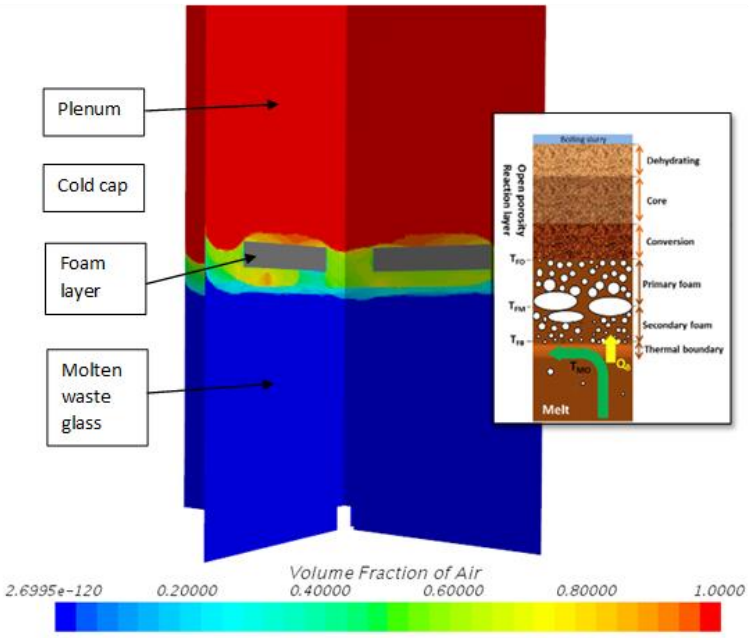


Fig. 1 Cutaway image of regions modelled by physicochemical processes in the CFD model

KEY PUBLICATIONS:

- Guillen, D. P. and Abboud, A. W. 2019. “Sensitivity Study of Forced Convection Bubbling in a Transparent Viscous Fluid as a Proxy for Molten Borosilicate Glass.” Annals of Nuclear Energy 125, pp. 38-49.
- Guillen, D. P., Abboud, A. W., and Fox, K. 2019. “Particle Settling in a Simulated Melter Discharge Riser.” Materials Letters 236, pp. 38-41.

- Abboud, A. W., Guillen, D. P., and Pokorny, R. “Effect of Glass Viscosity on Foaming Behavior and Heat Transfer in a Laboratory-Scale Waste Glass Melter.” American Nuclear Society 2019 Advances in Thermal Hydraulics (ATH19), Orlando FL, Nov. 11-15, 2018.
- Guillen, D. P., Abboud, A. W. and Pokorny, R. “Computational Experiments to Characterize Bubble Formation and Movement in Waste Glass Foam Layer.” American Nuclear Society Nuclear Reactor Thermal Hydraulics Meeting (NURETH-18), Portland, OR, August 18-23, 2019.
- Guillen, D. P., Abboud, A. W., Dixon, D., Eaton, W. C., Fox, K., Pokorny, R., Kruger, A. A. “Melter Modeling over a Range of Scales to Support Vitrification of the WTP.” WM2019 Conference, Phoenix, AZ, March 3-7, 2019. Earned Superior Paper recognition.
- Guillen, D. P., Abboud, A. W., and Pokorny, R. “Latin Hypercube Design of Experiments for Multiphase Flow Simulations of Foam Behavior in a Waste Glass Melter.” ASME Verification and Validation Symposium, Las Vegas, NV, May 15-17, 2019.
- Guillen, D. P. Abboud, A. W., Pokorny, R., Eaton, W. C., Schweiger, M. J., and Kruger, A. A. “Comparison of DOE Melter Model and Commercial Glass Furnace Model to Data from Pilot-scale Melter Test.” The 25th International Congress on Glass, Boston, MA, June 9-14, 2019.
- “Effect of Cold Cap Coverage and Emissivity on the Plenum Temperature in a Pilot-Scale Waste Vitrification Melter.” Office of River Protection Glass Science Workshop, June 2019, Richland, WA.
- “Study of Vitrification Tests in a Laboratory-Scale Melter.” Office of River Protection Glass Science Workshop, June 2019, Richland, WA.

Reactor Excursion and Leak Analysis Program (RELAP5)

REPORT PARTICIPANTS:

Donna Guillen[1], Nolan Anderson [1], Cameron Krome [1], Roger Boza [1], Mike Griffel [1], Jadallah Zouabe [1], Ahmad Al-Rashdan [1]
1 Idaho National Laboratory

SCIENTIFIC ACHIEVEMENT:

This research is the first application of the Reactor Excursion and Leak Analysis Program (RELAP5) with machine learning for the analysis of equipment failures at an operating nuclear power plant. A physics-informed machine learning model was created to analyze the failures of two drywell cooling fan coil units (FCUs) at a boiling water reactor nuclear power plant. A RELAP5 thermal hydraulic model was created to simulate the steady-state normal operation of the fans. RELAP5 was used with a recurrent neural network model to prototype a physics-based anomaly detection model for the drywell FCUs in a boiling water reactor.

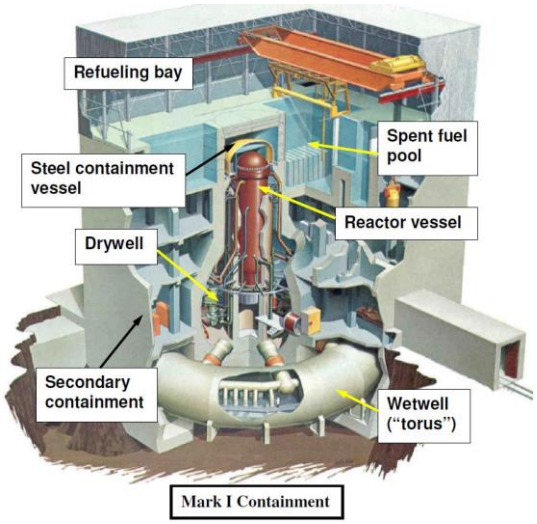
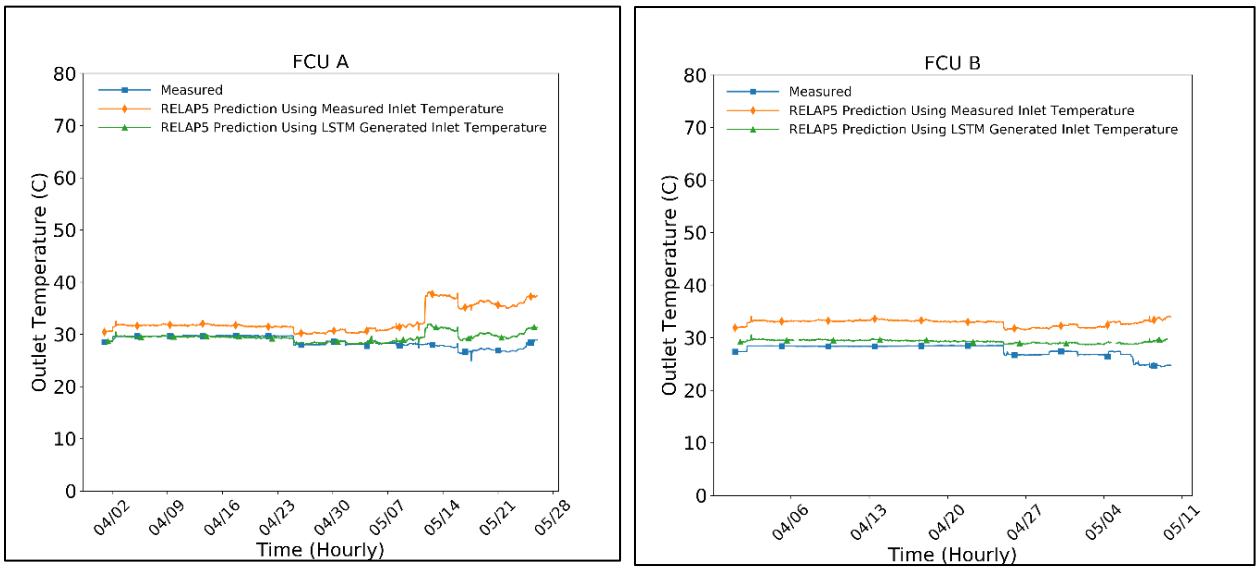


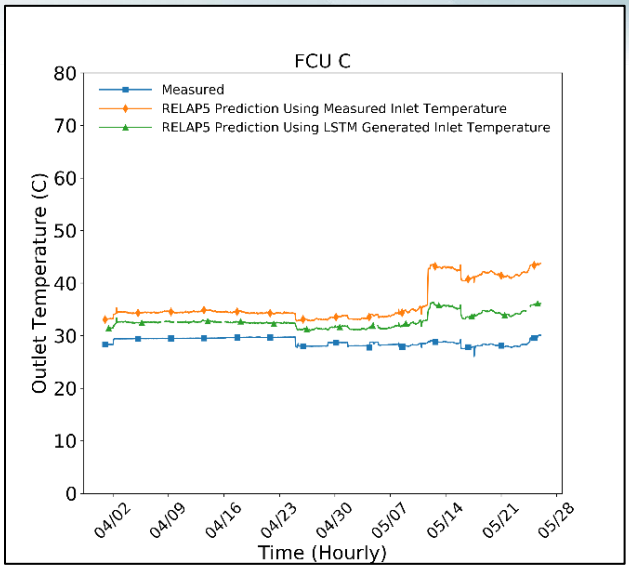
Fig. 1: Boiling water reactor containment structure (Lochbaum, 2014)

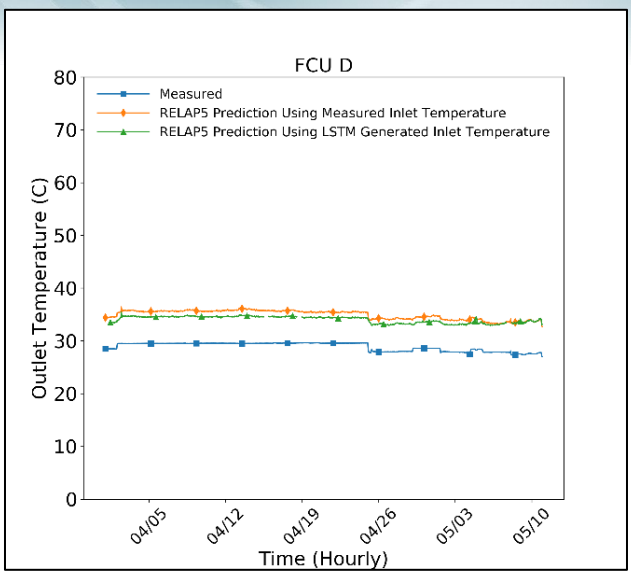
SIGNIFICANCE:

This hybrid approach can be useful for anomaly detection using data from existing plant sensors. The goal is to enable nuclear power plants to detect anomalies that are hidden in the process data, foresee catastrophic failures, and prepare for or mitigate them. Such an approach will enable operators to proactively detect deviations from expected system behaviors that could indicate an impending failure. Solutions such as this can play a key role in the sustainability of light -water reactors.

Fig. 2: Predicted and measured nitrogen outlet temperature for each of the four FCUs.







KEY PUBLICATIONS:

- D. P. Guillen, M. Griffel, R. Boza, A. Al-Rashdan, J. Zouabe, N., Anderson. “A Physics-Informed Machine Learning Model for the Analysis of Drywell Cooling Fan Failure.” Submitted for publication in a special issue of Progress in Nuclear Energy.
- D. P. Guillen, N. Anderson, C. Krome, R. Boza, M. Griffel, J. Zouabe, A. Al-Rashdan. “The Application of Physics-Informed Machine Learning to Predict Drywell Cooling Fan Failure.” Big Data for Nuclear Power Plants workshop at Ohio State University on December 10-11, 2019.
- A. Al Rashdan, L. M. Griffel, R. Boza, and D. Guillen. “Subtle Process-Anomalies Detection Using Machine Learning Methods.” Big Data for Nuclear Power Plants workshop at Ohio State University on December 10-11, 2019.

Scalable Neutron Transport Simulation

REPORT PARTICIPANTS:

Fande Kong[1]
1 Idaho National Laboratory

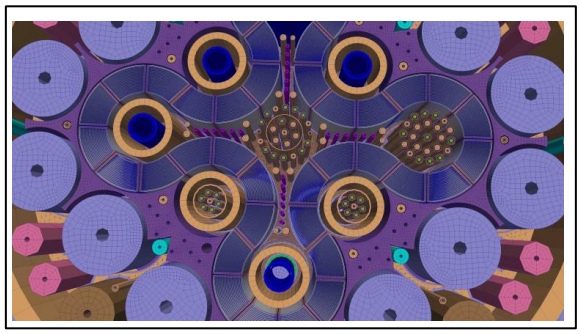


Fig. 1: ATR 3D Mesh

SCIENTIFIC ACHIEVEMENT:

Multigroup neutron transport equations are widely employed in nuclear reactor analysis for studying the motion and interaction of neutrons with materials. Numerical simulation of the multigroup neutron transport equations is computationally challenging because the equations are defined on a high-dimensional phase space (2D in angle and 3D in spatial space), the computational spatial domain is complex, and the materials are heterogeneous. A scalable parallel solver is required to address such a challenge. Utilizing HPC resources, a highly parallel Newton-Krylov-Schwarz method was developed. We have demonstrated that the proposed algorithm is scalable with more than 10,000 processors for a realistic application on 3D unstructured meshes with a few billion degrees of freedom. Neutron transport calculations for ATR (Advanced Test Reactor) using the improved Newton-Krylov-Schwarz algorithm are twice as fast as those based on the unmodified Newton-Krylov-Schwarz solver when over 8,000 processors are employed.

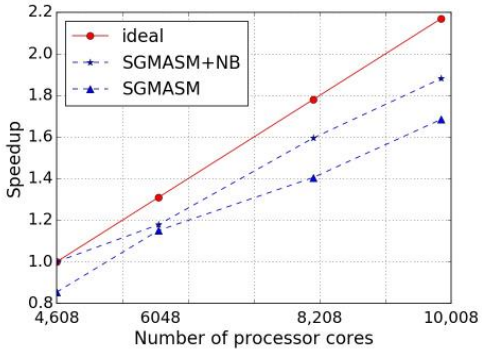


Fig. 2: Strong Scaling

SIGNIFICANCE:

Due to material heterogeneity, spatial domain complexity, and phase space dimensionality, neutron transport calculations are among the most memory and computationally intensive in all computational sciences. A scalable parallel solution strategy that leverages modern supercomputers is critical. The fundamental quantity of interest is the statistically averaged neutron distribution, referred to as “neutron flux”, in a high-dimensional phase space (1D energy, 2D angle, 3D spatial phase space). The neutron flux is a scalar quantity, physically representing the total length traveled by all free neutrons per unit time and volume. In neutron transport simulations, fundamental nuclear data (referred to as “cross sections”) describing the likelihood per unit path length of neutrons interacting with the background materials is required. The cross sections depend on the energy of the neutrons and the temperature of the background materials. The neutron transport equations behave as hyperbolic or elliptic systems depending on changes in cross sections (material properties).

KEY PUBLICATIONS:

- Fande Kong, Yaqi Wang, Derek R. Gaston, Cody J. Permann, Andrew E. Slaughter, Alexander D. Lindsay, and Richard C. Martineau. "A highly parallel multilevel Newton-Krylov-Schwarz method with subspace-based coarsening and partition-based balancing for the multigroup neutron transport equations on 3D unstructured meshes." arXiv preprint arXiv:1903.03659 (2019).
- Fande Kong. 2020. "Neutron Transport Criticality Calculations Using a Parallel Monolithic Multilevel Schwarz Preconditioner Together with a Nonlinear Diffusion Acceleration Method." Annals of Nuclear Energy 141: 107342.

High Temperature Gas-cooled Reactors (HTGRs)

REPORT PARTICIPANTS:

Gerhard Strydon[1]
1 Idaho National Laboratory

SCIENTIFIC ACHIEVEMENT:

This study is the first demonstration of a statistical Uncertainty and Sensitivity Assessment (U/SA) methodology applied to the coupled neutronic and thermal fluid (multiphysics) analysis of a prismatic HTGR design. The approach utilizes the SCALE and RELAP5-3D codes and the latest capabilities build into the INL-developed RAVEN code.

The U/SA of the 350 MW Modular High Temperature Gas-cooled Reactor (MHTGR) was performed in the context of the International Atomic Energy Agency (IAEA) Coordinated Research Project (CRP) on HTGR uncertainties in modeling (UAM).

SIGNIFICANCE:

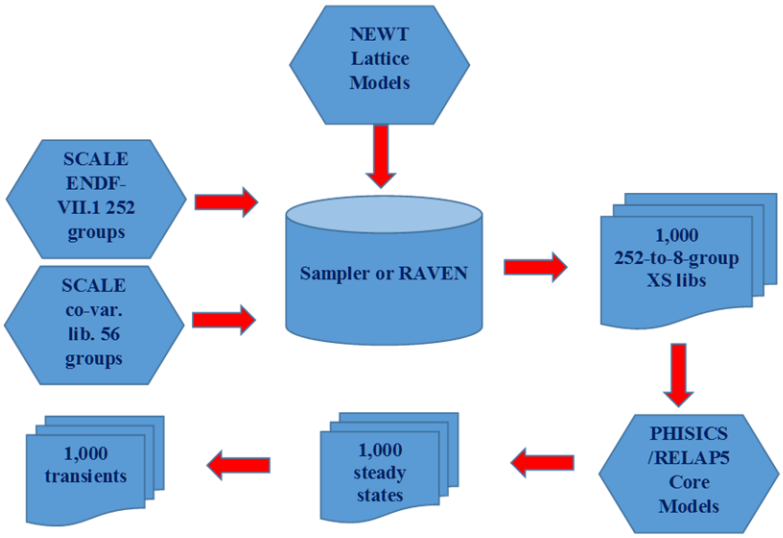


Fig. 1: MHTGR-350 U/SA calculation flow scheme.

The SAMPLER module of SCALE 6.2 was applied to the MHTGR-350 lattice models to obtain several sets of 1,000 perturbed 8- and 26-group AMPX libraries for use in the INL transport core solver PHISICS. The U/SA was performed for the stand-alone neutronics, thermal fluids, and coupled PHISICS/RELAP5-3D core models. Several thousand steady states were subsequently used as the basis for the U/SA of the control rod withdrawal and depressurized loss of forced cooling transients, as shown in Figure 1.

Sensitivity indexes for the major figures of merits were calculated using RAVEN, and the main contributors to the overall uncertainty in these parameters are identified. An example of the MHTGR-350 fuel temperatures obtained for a Loss of Forced Cooling (LOFC) transient for the first 200 perturbed PHISICS/RELAP5-3D models is shown in Figure 2.

Due to the statistical nature of the U/SA approach, a very large number of lattice (SCALE), core steady-state (PHISICS) and coupled transient (PHISICS/RELAP5-3D) had to be performed. It is estimated that more than 200,000 SCALE/NEWT calculations were submitted to Falcon, at least 100,000 PHISICS/RELAP5-3D steady-state calculations, and at least 50,000 LOFC and Control Rod Withdrawal transients, respectively (in FY-19). The resources available at INL to the ART program were crucial to the success of this IAEA CRP on HTR UAM over the last 6 years; it would have been impossible to achieve the results without support.

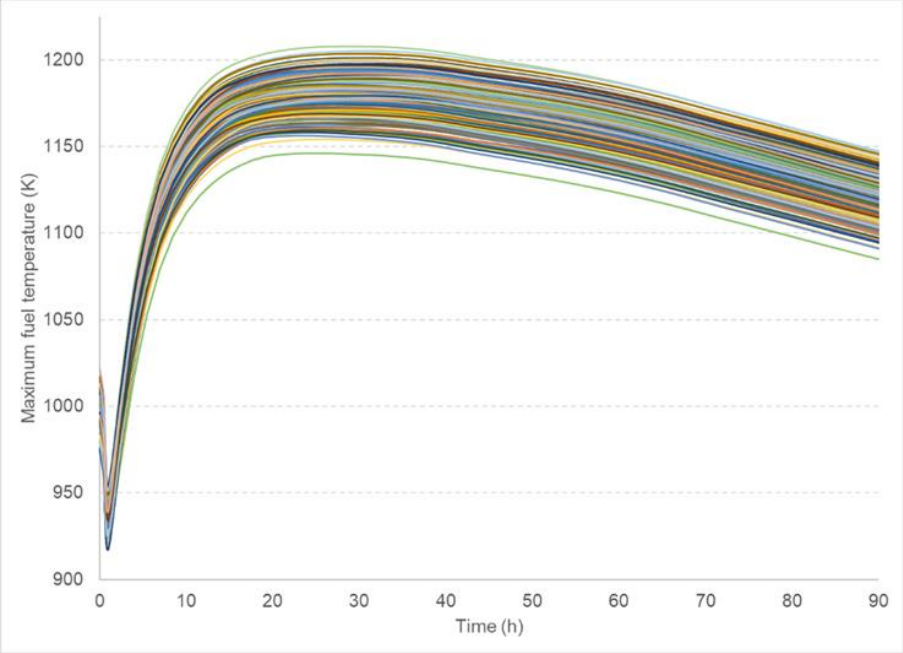


Fig. 2: MHTGR-350 maximum fuel temperature (K) values for 200 perturbed samples of the 0% bypass flow PHISICS/RELAP5-3D model.

KEY PUBLICATIONS:

- Strydom, G. 2019. “IAEA Coordinated Research Project on HTGR Physics, Thermal Hydraulics, and Depletion Uncertainty Analysis: PHISICS/RELAP5-3D Results for the Phase III Coupled Core Exercises.” INL/EXT-19-55546, Idaho National Laboratory.
- Rouxelin, P. N. 2019. “Reactor Physics Uncertainty and Sensitivity Analysis of Prismatic HTGRs.” Ph.D. Thesis, North Carolina State University.
- Strydom, G. 2020. “Consistent Multi-Scale Uncertainty Quantification Methodology for Multi Physics Modeling of Prismatic HTGRs.” Ph.D. Thesis, North-West University, South Africa.
- Strydom, G., Rouxelin, P. N. 2020. “Multi-Physics Uncertainty and Sensitivity Assessment of the MHTGR-350 design with SCALE, PHISICS/RELAP5-3D AND RAVEN.” Submitted to BEPU 2020 conference, Sicily, May 2020.

Molecular Dynamics Simulations of Anisotropic Grain Boundary Mobility in Uranium Dioxide

REPORT PARTICIPANTS:

Jarin French[1], Xian-Ming Bai[1]
1 Department of Materials Science and Engineering, Virginia Tech

SCIENTIFIC ACHIEVEMENT:

Modern reactor designs require an intimate knowledge of material properties throughout reactor use. While the reactor is in use, the fuels undergo complex microstructural changes that impact the fuel performance properties (such as thermal conductivity, fission gas release rate, etc.). One significant microstructural feature is the grain boundary (GB). GBs have five degrees of freedom, making it difficult to generalize individual GB properties from the experiment. GB properties such as mobility and energy are important parameters for mesoscale simulations (such as phase field). Typical mesoscale simulations assume isotropic GB properties or a specific form of anisotropy that may not accurately reflect the topography within the GB five-space. Recent efforts have been made to incorporate anisotropic GB properties directly from atomistic simulation into mesoscale simulations. To aid these efforts, molecular dynamics simulations were performed using LAMMPS to calculate GB mobility for six cylindrical GBs in uranium dioxide: three low-index rotation axes of <100>, <110>, and <111>, with two misorientation angles of 20° and 45° each.

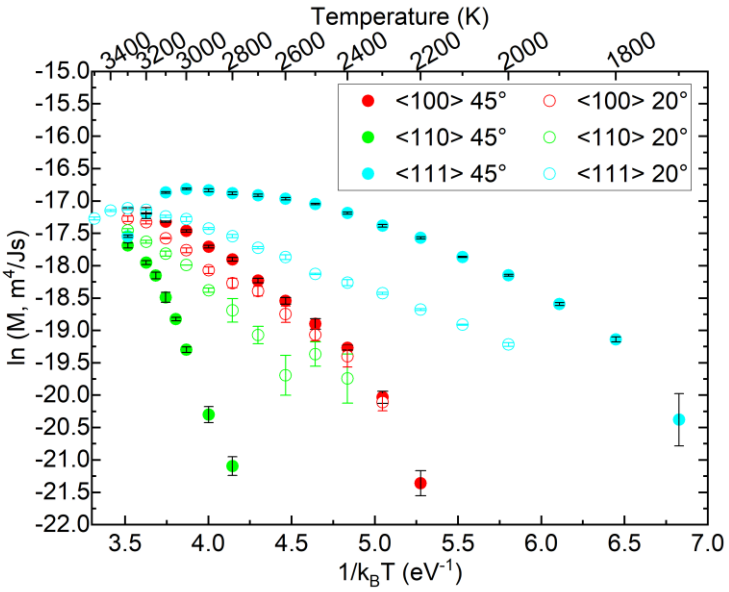


Fig. 1: MHTGR-350 U/SA calculation flow scheme.

SIGNIFICANCE:

The results indicate that anisotropy in GB mobility cannot be ignored, with mobilities varying over three orders of magnitude. GB mobility appears to be highest for the <111> rotation axis, followed by the <100> and <110> for the same misorientation angles. These mobility values can be implemented within a database to use in mesoscale simulations.

KEY PUBLICATIONS:

- N/A

Optical Analysis of 3d and 4d Transition Metals in LiCl-KCl Eutectic Composition

REPORT PARTICIPANTS:

John Fuller[1], Qi An[1]
1 University of Nevada, Reno

SCIENTIFIC ACHIEVEMENT:

Molten salt reactors are a promising design prototype for the Generation IV nuclear reactors that employ a self-contained cycle with high efficiency and stability utilizing molten salts as both the fuel -delivery mechanism and coolant for the system. These reactors, in addition to their safe and environmentally friendly design, offer substantial improvements in recyclability for spent fuel and allow for significant improvement in reactor miniaturization due to the relative simplicity of their design. To better understand the spent fuel reprocessing operation in molten salt reactions, the chemical and structural properties of the salts must be tested and clearly understood through both computational and experimental methods. These properties are of particular interest in pyroprocessing operations (the high-temperature process of recycling reactor waste through extraction and purification of spent fuel) which involve the transport of metal cations inside the salt melt. The exact configuration of these metal complexes in the molten salts can help predict the chemical and structural properties of the melt, leading to a more efficient treatment of the salts in pyroprocessing and better reactor design.

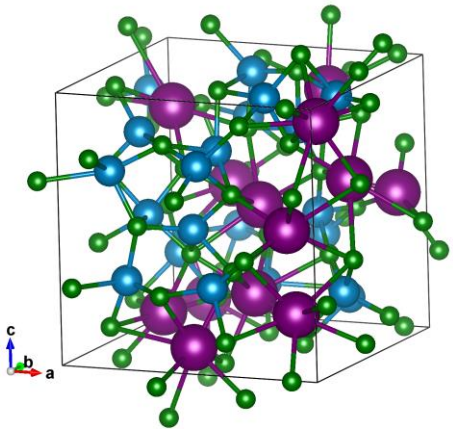


Fig. 1: LiCl-KCl binary eutectic at T=400 C; purple spheres represent K atoms, while blue spheres represent Li atoms and green spheres represent Cl atoms

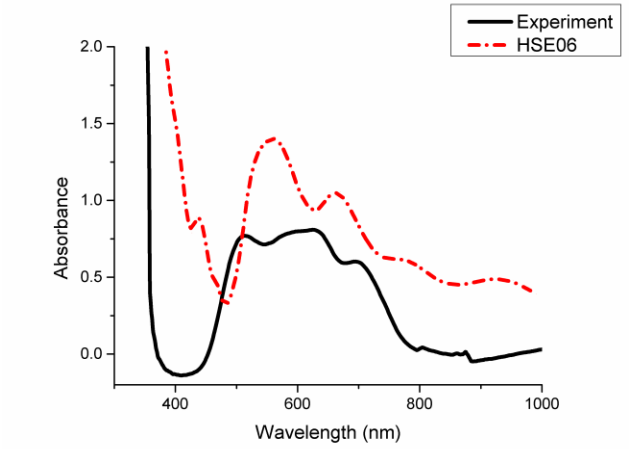


Fig. 2: Absorption intensity by wavelength is shown for both experimentally obtained data and DFT simulation results for NiCl2-LiCl-KCl using the

SIGNIFICANCE:

Our work investigated the configurations of transition metal cations (such as Ni^{2+}, Co^{2+}, Mo^{5+}, and others) in the eutectic composition of the binary molten salt LiCl-KCl using Density Functional Theory (DFT) methods to compare with experimental. We focused on obtaining absorption spectra using quantum molecular dynamics to prepare a simulated molten salt system and a hybrid functional approach (specifically HSE06) to acquire the optical data with reasonable agreement to experimental absorption spectra for the transition metals in the binary eutectic melt. By acquiring these absorption spectra, the configuration (tetrahedral, octahedral, etc.) can be predicted. Investigating these optical property

analysis techniques computationally for transition metals allows a framework of knowledge to be built for treating other elements with the same approach, such as lanthanides and other heavier elements with more complex behavior. Knowing the configurational behavior at the atomic level of the metal cation inside the melt will allow future work to predict physical and chemical properties important to the transport and pyroprocessing mechanisms computationally, saving significant experimental research effort and costs. This work was supported by a graduate student.

KEY PUBLICATIONS:

- N/A

Ab initio Study of the Mechanism for the Initiation of Localized Corrosion on Stainless Steel

REPORT PARTICIPANTS:

Kofi Oware Sarfo[1], Pratik Vinod Murkute[1], Larry Aagesen Jr.[2], Yongfeng Zhang[3], O. Burkan Isgor[1], Julie D. Tucker[1], Líney Árnadóttir[1]
1 Oregon State University
2 Idaho National Laboratory
3 University of Wisconsin - Madison

SCIENTIFIC ACHIEVEMENT:

Stainless steels are widely used as primary piping material in PWR's because of their high corrosion resistance, largely due to the formation of a passive film of metal oxides, such as chromium (e.g., Cr_2O_3). However, upon exposure to aggressive ions like chlorides (Cl^-), stainless steel becomes susceptible to localized corrosion, due to the breakdown of the passive film. It is therefore essential to gain fundamental insights into the mechanism of the passive film breakdown (depassivation) to develop a tailored design to minimize localized corrosion. This project investigates the initial stages of the depassivation of the Cr passive film using density functional theory (DFT), a quantum-based computational method. The mechanism of Cl^- induced depassivation has long been debated, but the two most popular models are the ion-exchange (IE) model and the point-defect (PD) model, illustrated in Figure 1. Pit initiation in chloride containing solutions involves Cl^- adsorption on the surface, insertion by ion exchange with subsurface anion and migration of Cl^- through the oxide film (according to the IE model, A) or Cl^- induced cation vacancy formation on the surface followed by vacancy migration to the metal/film interface (according to the PD model, B).

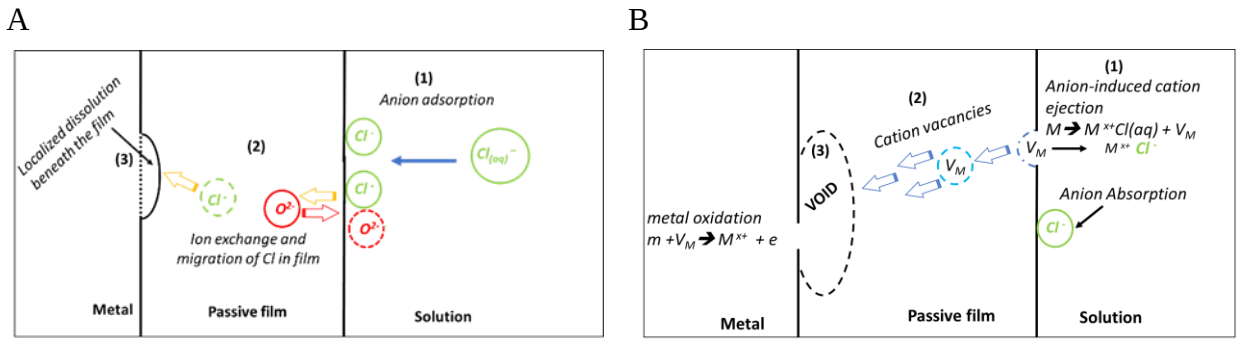


Fig. 1: Schematic of the ion exchange (A) and the point defect models (B) describing chloride induced depassivation mechanism of metals and alloys in three stages, labelled (1)-(3). Both models start with anion adsorption but in the ion exchange model (A) the adsorption (1) is followed by Cl- insertion by ion

Using density functional theory calculations, we have compared the thermodynamic feasibility of certain critical steps of the two depassivation models. We found that the overall mechanism is a concentration dependent interplay between the two models. At low chlorine coverages substitution with weakly adsorbed surface species, such as H_2O or OH^-, is favorable but becomes less favorable at higher Cl coverages. Cl insertion into the film is unfavorable at low coverages but becomes more favorable at higher coverages, which is supported by the IE model. High Cl coverages and subsurface Cl also enhance cation vacancy formation, which is supported by the PD model. This

suggests that, at high Cl coverages, both Cl insertion, described by the IE model, and cation vacancy formation, described by the PD model, are thermodynamically favorable unlike for the chloride enhanced depassivation of iron, where only the PD model was found to be feasible. The initial stages of Cl^- induced breakdown of the chromium oxide passive film differs significantly from iron, a major component of stainless steels, and can be described as an interplay of the two mechanisms, which is concentration dependent, in good agreement with experimental observations.

SIGNIFICANCE:

This work makes a significant contribution to the knowledge about the role of Cl in the depassivation of the chromium-oxide passive layer of stainless steel. It is a part of an NEUP/NEAMS project, which provides kinetic information at the atomistic level to understand and predict the localized corrosion on stainless steel. The overall project combines modeling and experiments to predict corrosion and embrittlement in dual-phase stainless steels within the MARMOT framework.

KEY PUBLICATIONS:

- K. O. Sarfo, P. V. Murkute, Y. Zhang, O. B. Isgor, J. D. Tucker, L. Árnadóttir. “First Principles Study of the Initial Stages of Chloride Enhanced Depassivation of Chromium Oxide Film.” To be submitted to Corrosion Science.

ATR LEU Conversion

REPORT PARTICIPANTS:

Matthew Johnson[1]
1 Idaho National Laboratory

SCIENTIFIC ACHIEVEMENT:

The NNSA Office of Conversion is working with the INL to develop and qualify new fuels and technologies to support low-enriched uranium (LEU) conversion efforts of the remaining U.S. High Performance Research Reactors (USHPRR). Fuel qualification of U-10Mo will be accomplished through the execution of a comprehensive series of irradiations and post-irradiation examinations using the fuel produced by a commercially-viable fabrication process. The LEU qualification for the USHPRR Project will be conducted in stages with multiple irradiation tests. It will be accompanied by fuel design/safety analysis efforts, and the efforts to demonstrate and mature fabrication methods. The irradiation tests are being designed to gather sufficient (i.e., statistically significant) high-quality data under an approved NQA-1 program to demonstrate that the requirements for fuel qualification are met. A series of tests in this strategy are designated as the experiment tests (ET) 1, 2, and 3. For these tests, the newly designed LEU fuel element, called the LOWE element, will be irradiated in a driver position in the Advanced Test Reactor (ATR). A Safety Analysis Report (SAR) addendum needs to be written and approved before the ET can be inserted into the core. Monte Carlo neutron transport simulations are being run to generate fuel-plate power density and cumulative fission density profiles (Fig. 1) as well as other reactor physics metrics that are inputs to nuclear safety analysis, which supports the ATR ET-1 SAR addendum. The simulation results are also being used to inform ET-1 test planning.

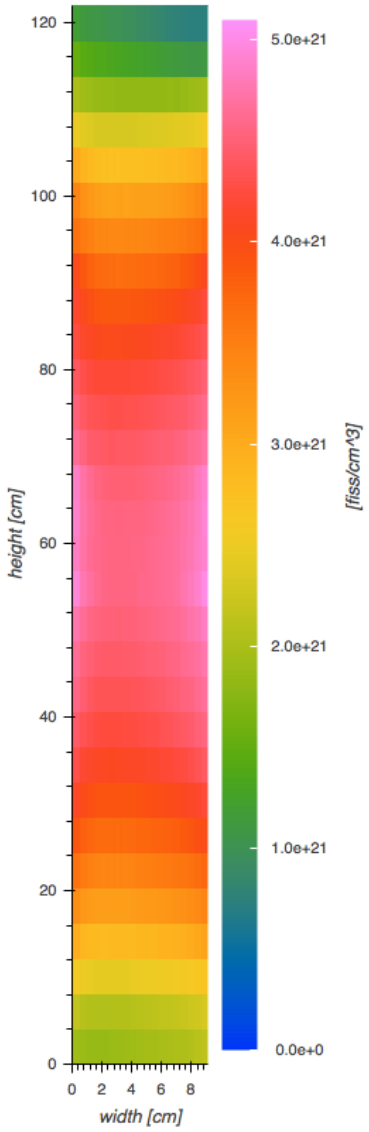


Fig. 1: Cumulative fission density profile at terminal burnup in plate 19 of the LOWE element

SIGNIFICANCE:

Monte Carlo neutron transport simulations are being run on the INL HPC to generate fuel-plate power density and cumulative fission density profiles as well as other reactor physics metrics that are inputs to nuclear safety analysis, which supports the ATR ET-1 SAR addendum. The simulation results are also being used to inform ET-1 test planning.

KEY PUBLICATIONS:

- 2019. “ET-1 Plate Power Density and Cumulative Fission Density Profiles,” ECAR 4460, Rev. 0, Idaho National Laboratory.

Advanced Electrode and Solid Electrolyte Materials for Elevated Temperature Water Electrolysis

REPORT PARTICIPANTS:

Meng Li[1], Dong Ding[1]
1 Idaho National Laboratory

SCIENTIFIC ACHIEVEMENT:

Perovskite is a class of metal oxides that has been widely used in water electrolysis. The compositional and structural disorder of perovskite materials, which determine their catalytic activity and conductivity, are not able to be evaluated directly using experimental methods. We studied the lattice evolution and surface relaxation in proton conducting perovskite using a VASP simulation to reveal the changes in mechanism underpinning performance differences.

- The bulk structures and surfaces for perovskites with different compositions were created
- The compositional and structural disorder of perovskite materials were studied
- The lattice evolution and surface relaxation under reaction conditions were studied
- The water electrolysis reaction barriers were calculated to understand the mechanism in performance differences.

We obtained a better understanding of how the composition and structure disorder of perovskite materials determine their activity for water splitting was obtained, which will provide guidance for the rational design of highly active materials in subsequent research.

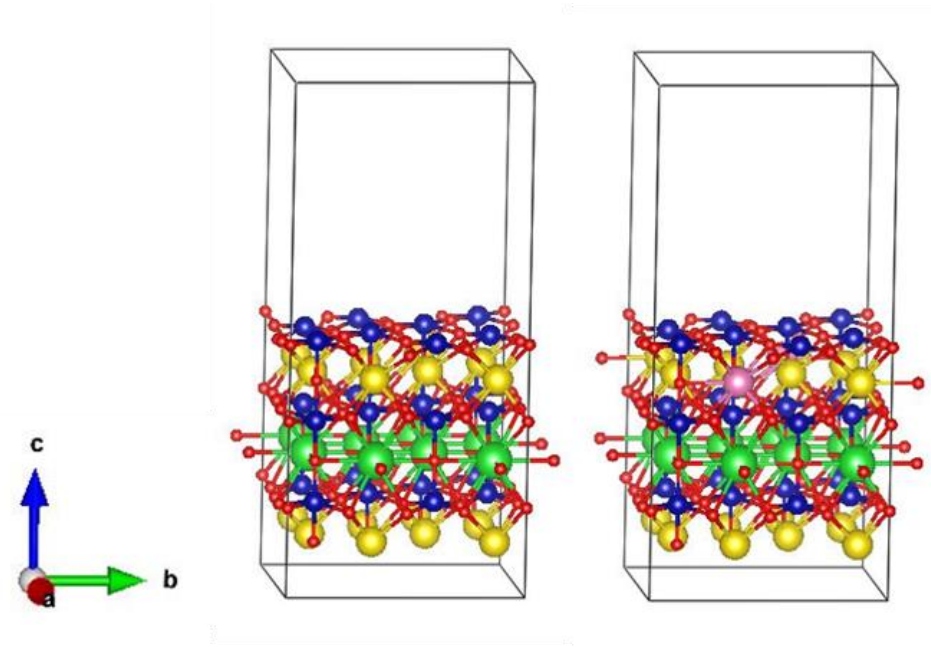


Fig. 1: Doped $PrBaCo_2O_{5+x}$ perovskite surfaces as electrode active sites for water electrolysis.

SIGNIFICANCE:

Elevated-temperature water electrolysis is one of the most efficient technologies for energy storage and conversion. Electrode and solid electrolyte materials are vital to the performance of hydrogen production. The compositional and structural disorder of solid oxide materials, which determine their catalytic activity and conductivity, are not able to be evaluated directly using experimental methods.

While computational study of solid oxides is highly useful in assisting the development of elevated-temperature electrochemical systems, there exist several computational challenges that must be overcome. These computational difficulties mostly originate from the intrinsic compositional disorder within both the cation and anion sublattices in these complex oxide materials, leading to a large number of distinct local environments a proton will encounter. We used a combination of high-throughput density functional theory calculations of proton energetics and of migration barrier cluster expansion techniques to address these challenges. The simulation work on HPC greatly benefits our project by providing a guidance for advanced materials design.

KEY PUBLICATIONS:

- N/A

Radiation Induced Defects in Nuclear Fuel Oxides

REPORT PARTICIPANTS:

Miaomiao Jin[1]
1 Idaho National Laboratory

SCIENTIFIC ACHIEVEMENT:

Primary radiation damage, featuring rapid atomic collisions and thermal spikes, constitutes the foundation of a high-fidelity description of radiation-assisted microstructure evolution. To systematically describe the primary damage in the mixed - fuel oxide systems $Th_{1-x}U_xO_2$, we consider the effect of temperature, composition, and primary-knock atom energy on defect generation. A holistic empirical expression is developed to quantify the number of defects and an exponential truncated power-law is shown to describe the defect size distribution. Furthermore, the defect (cluster) structures are elaborated, where notably vacancy clusters approach being charge balanced, and interstitial clusters can embrace a high symmetry with a cuboctahedral structure. These results present both a high-level description and a detailed atomic understanding towards radiation-induced defects in fuel oxides, which provides the required input for meso-scale simulations of microstructure evolution.

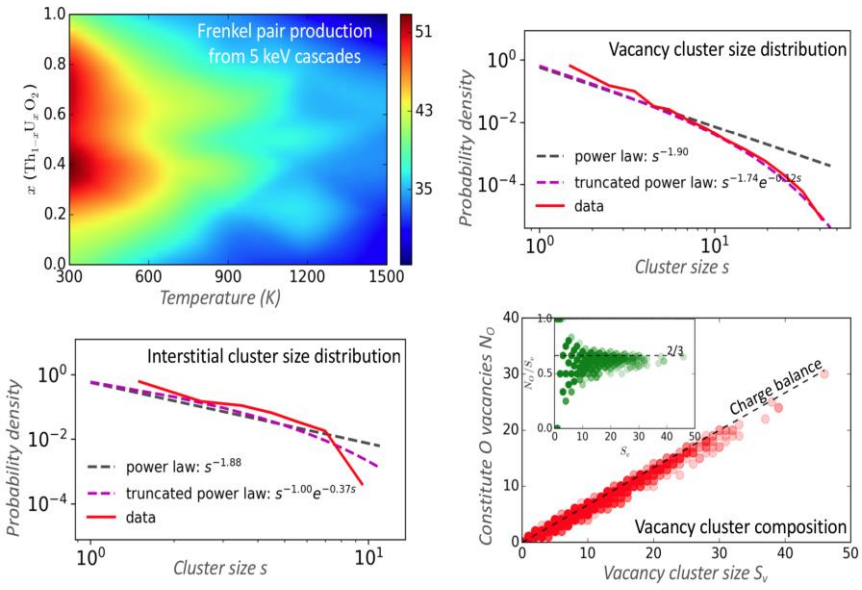


Fig. 1: Defect production from primary damage in $Th_{1-x}U_xO_2$

SIGNIFICANCE:

Understanding of defects behavior is the cornerstone of explaining the impact of additional phonon-defect scattering caused by radiation damage on the thermal transport in nuclear fuels. The detailed behavior can be described to the atomic resolution utilizing molecular dynamics simulations.

KEY PUBLICATIONS:

- Miaomiao Jin, Chao Jiang, Jian Gan, David Hurley. 2019. “Systematic Analysis on the Primary Radiation Damage in Th1−xUxO2 Fluorite Systems.” Submitted to the Journal of Nuclear Materials.

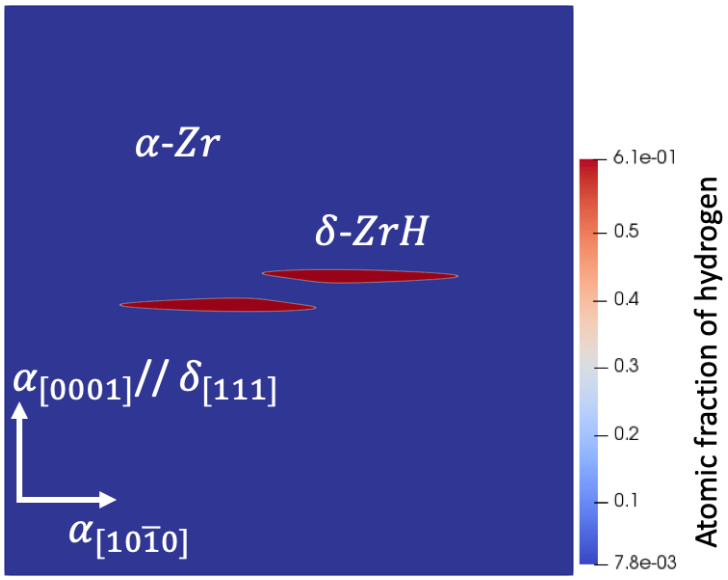
Phase Field Modeling of Zirconium Hydride Morphology

REPORT PARTICIPANTS:

Pierre-Clément A. Simon[1], Michael R. Tonks[2], Arthur T. Motta[1],
1 Penn State University
2 University of Florida

SCIENTIFIC ACHIEVEMENT:

A quantitative-phase field model is being developed for the zirconium hydride system to study nanoscale hydride morphology and nanoscale hydride stacking into mesoscale hydrides in zirconium. The phase field model includes a quantitative description of the chemistry of the two phases and a detailed description of the elastic contribution from volume change during phase transformation, thermal expansion, and hydrogen in solid solution.



SIGNIFICANCE:

In Light Water Reactors, zirconium is commonly used as cladding material. During normal operations, waterside corrosion produces hydrogen, which is in part picked-up by the cladding. Once the concentration of hydrogen in solid solution in the cladding reaches the solid solubility limit, it precipitates into brittle nanoscale hydrides, which aggregate into mesoscale hydride clusters. Depending on their morphology, these brittle mesoscale hydride clusters can affect cladding integrity. Due to the zirconium texture, mesoscale hydrides are usually oriented circumferentially in the cladding. However, under sufficient applied stress, the nanoscale hydrides can stack radially to form radial mesoscale hydrides, which can ease crack propagation through the cladding thickness. To assess cladding integrity, it is thus crucial to understand the physics and mechanisms responsible for hydride morphology under different stress states. This project is part of a larger research project on the ‘Development of a Mechanistic Hydride Behavior Model for Spent Fuel Cladding Storage and Transportation’ from an Integrated Research Project funded by the Department of Energy. The modeling of the hydride microstructure under different thermomechanical treatments informs a larger scale model in BISON focusing on predicting hydrogen and hydride distribution in the cladding during normal operation and preparation for dry storage.

KEY PUBLICATIONS:

- Pierre-Clément A. Simon, Michael R. Tonks, Arthur T. Motta. “Study of the Effect of Zirconium Grain Boundaries on Hydride Precipitation Using Phase Field Model.” Materials in Nuclear Energy Systems (MiNES) by ANS and TMS, Baltimore, MD, October 9, 2019.
- Pierre-Clément A. Simon, Evrard Lacroix, Michael R. Tonks, Arthur T. Motta. “Development of an Experimental Method to Define the Kinetic Parameters of a Phase Field Model – Application to Zirconium Hydride Precipitation.” Materials Research Society (MRS) Spring 2019 - Interfacial Science and Engineering - Mechanics, Thermodynamics, Kinetics and Chemistry, Phoenix, AZ, April 24, 2019.

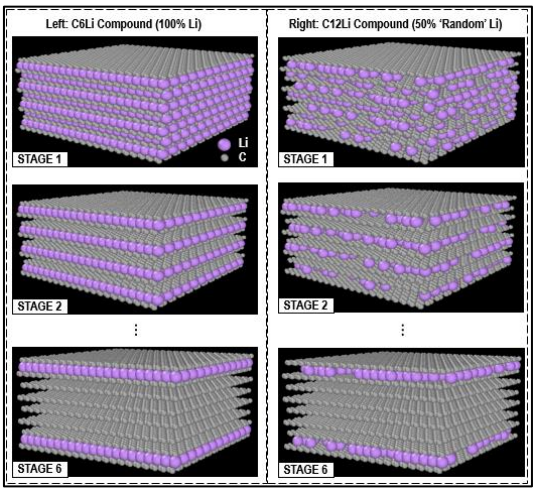
Molecular Modeling of Lithium Self-Diffusion in the Graphite Anode in Lithium Ion Batteries

REPORT PARTICIPANTS:

Rajni Chahal[1,2], Gorakh Pawar[2]
1 Idaho National Laboratory
2 University of Texas at Arlington

SCIENTIFIC ACHIEVEMENT:

The graphite electrode in lithium (Li) ion batteries is known to have high energy/power density, due to its high surface area. Also, due to high chemical stability and rich natural resources of graphite, it is becoming a popular material to fulfill future energy needs. In order to determine the battery performance (charging/discharging), it is important to understand the lithium diffusion into the graphite anode.



This research problem has been tackled by various researchers following experimental or *ab initio* calculations. Whereas the inherent limitations, such as nanoscale measurements and sample preparation, cost inhibit the experimental techniques, *ab initio* methods are limited by the small size of the system under study. Therefore, a molecular dynamics method is used that allows the modelling of a representative graphite anode in order to study the effect of state of charge on Li diffusion and on the mechanical properties of the system.

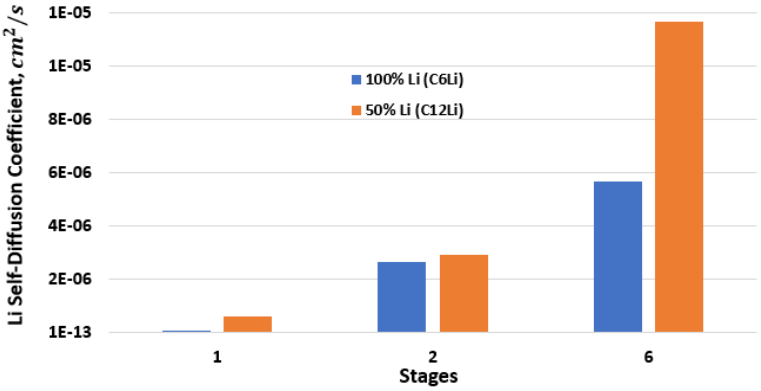


Fig. 1: Effect of state of charge and Li concentration on Lithium Diffusion.

SIGNIFICANCE:

The molecular dynamics study to evaluate the Li self-diffusion coefficient helps understand that both state of charge (staging) and concentration of Li play a significant role in determining the self-diffusion coefficient of Li in lithium ion batteries. Knowledge of mobility or diffusion of Li inside the graphite anode is critical in determining the performance of the batteries. The study performed to characterize the mechanical behavior of the graphite anode at different Li concentration is important in predicting the reliability of Li ion batteries. As the Li concentration at the anode increases (charging) the anode material becomes more ductile and its strength decreases. The results drawn

from these simulations contribute towards predicting the performance and reliability of lithium ion batteries.

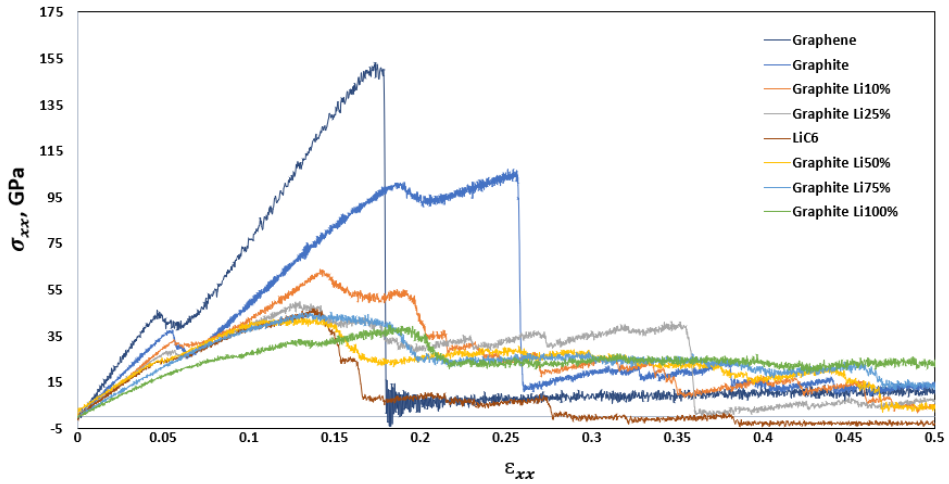


Fig. 2: Mechanical behavior of graphite anode at different Li concentration

KEY PUBLICATIONS:

- N/A

Molecular Simulations to Predict Mechanical Properties of Silica Nanofibers

REPORT PARTICIPANTS:

Rajni Chahal[1,2], Gorakh Pawar[2]
1 Idaho National Laboratory
2 University of Texas at Arlington

SCIENTIFIC ACHIEVEMENT:

Silica dioxide grows naturally on silicon in the presence of oxygen at room temperature or under thermally controlled conditions. Silica possess excellent mechanical, thermal, and optical properties and hence is routinely used in a wide variety of technological applications. It is a popular material used in manufacturing micro- and nano-electronic devices, optical fibers for telecommunications, and glass fibers to form fiber-reinforced polymer composites. A fundamental understanding of the mechanical properties of silica nanowires will help increase their reliability when integrated into functional nanodevices.

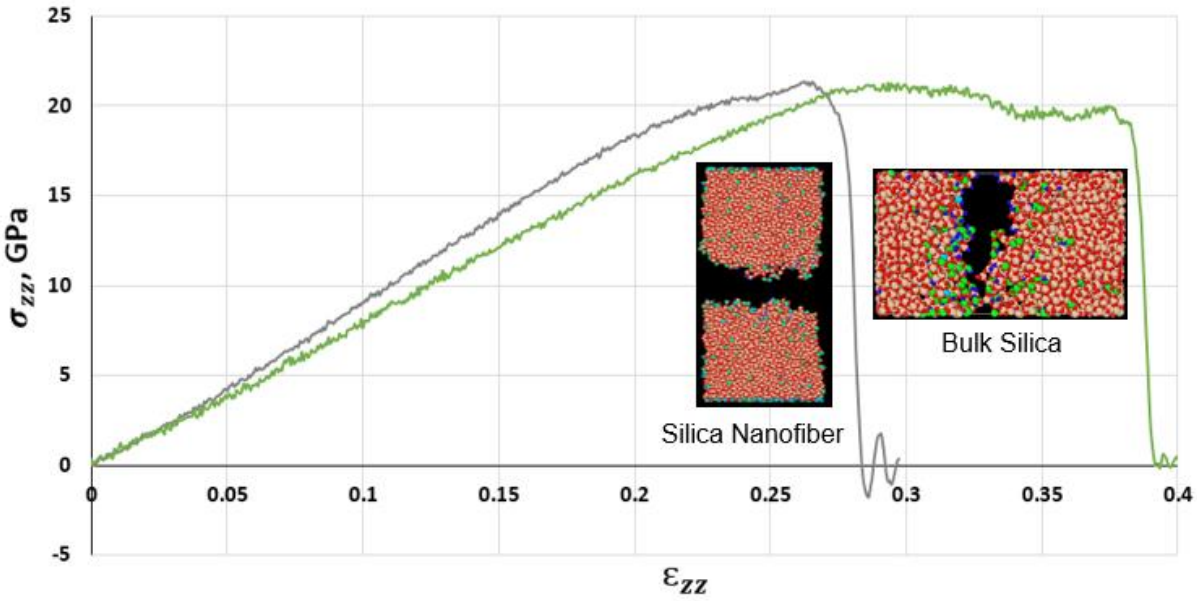


Fig. 1: Stress-strain behavior of bulk silica vs silica nanofiber (diameter = 63 A, length = 100 A)

Recent findings about the size-dependent mechanical properties of individual silica nanofibers have encouraged the molecular modelling of silica nanofibers to understand the fracture process. At INL, a workflow is being developed to evaluate the overall mechanical properties of electrospun silica nanofiber matts with different fiber arrangements and sizes.

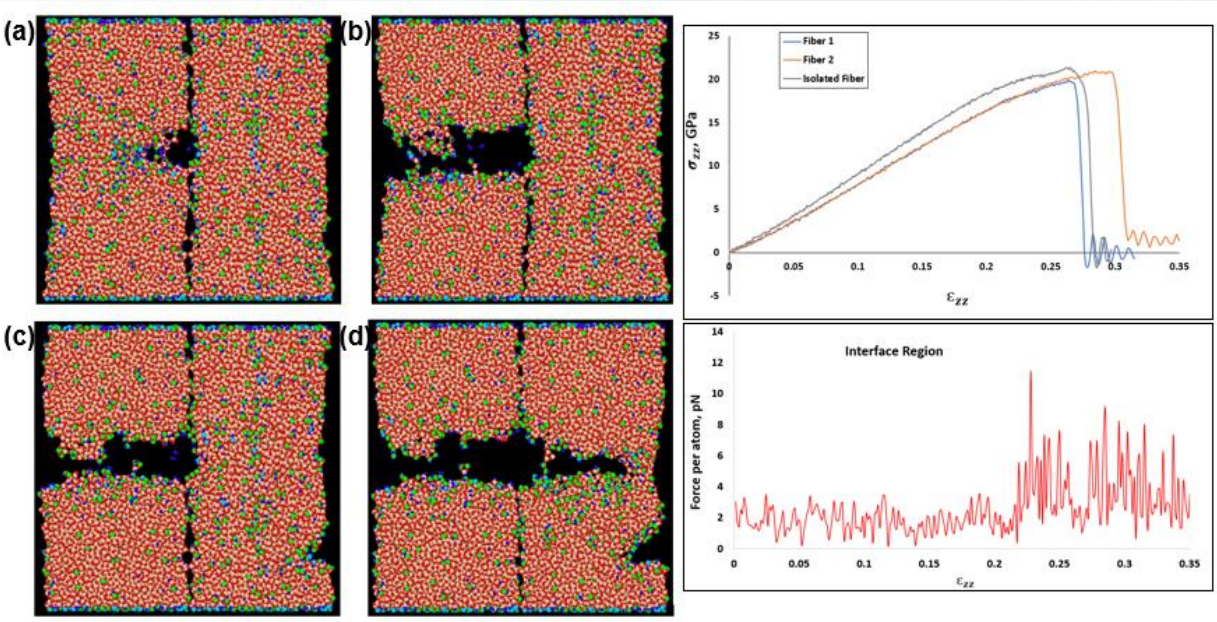


Fig. 2: (a) Atomic configuration at strain of 27.23% (Crack Initiating from nanofiber 1 surface) (b) Fractured nanowire 1 (c) Atomic configuration at strain of 30.10% (Crack Initiating from nanofiber surface) (d) Fracture nanowire 2 (Color: O-red, Si-yellow, Under-coordinated O-Blue, Under-coordinated Si-Green)

SIGNIFICANCE:

Molecular dynamics simulations assisted in elucidating the fracture behavior of silica nanofiber. The obtained results can be applied to telecommunications and integrated electronics. The ongoing work to formulate a multiscale stochastic model of different sizes and arrangement will help to predict the macroscale mechanical properties driven by nanoscale failure criteria.

KEY PUBLICATIONS:

- N/A

Pressurized Water Reactor Optimization

REPORT PARTICIPANTS:

Hongbin Zhang[1], Cole Blakely[1], Ryan Stewart[1]
1 Idaho National Laboratory

SCIENTIFIC ACHIEVEMENT:

Most pressurized water reactors (PWRs) in the U.S. typically operate on an 18-month cycle before shutting down to refuel approximately a third of their core. Increasing the cycle length to 24 months would provide a myriad of benefits for the current PWR fleet. Over a ten-year period, a plant operating on a 24 month cycle can provide an additional two months of power compared to a typical 18-month cycle length. This excess power production can help alleviate some of the financial pressures that nuclear power plants currently face. To achieve a longer cycle length, two major hurdles must be addressed.

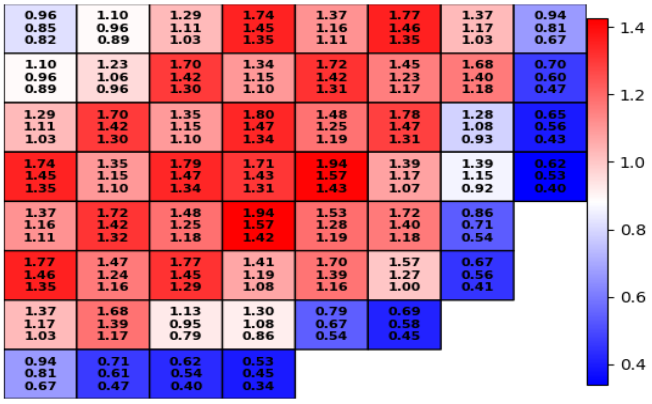


Fig. 1: Peaking Factors for Core Design 2 at Cycle 11

The first hurdle includes increasing the current regulatory limits for the fuel- discharge burnup limit. Currently, the limit on fuel exposure is set at 62 GWD/MTU (rod averaged). Increasing this limit to 75 GWD/MTU allows a higher fuel utilization, meaning more power is being extracted from a given amount of fuel. Along with this, increasing the burnup limit has the potential to reduce the amount of refueling (i.e. increase the cycle length) which causes an increase in the capacity factor. Increasing the fuel burnup has been shown to increase the economic competitiveness of current nuclear plants, even under the restriction of a 5 w/o fuel.

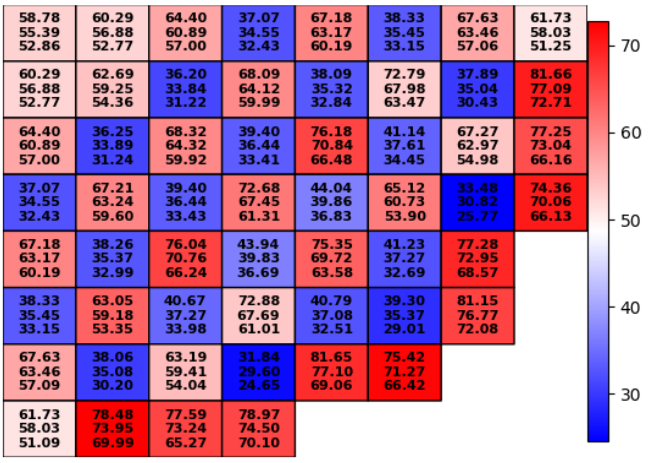


Fig. 2: Burnup Distribution for Core Design 2 at EOC

The second major hurdle is the current regulatory limit on enrichment for light water reactors. The limit for ^{235}U enrichment in nuclear fuels is currently set at 5 w/o. Increasing this level from 5 to 6-7 w/o could significantly help increase the cycle length. Similar to increasing the limit on burnup, previous work has shown that increasing the limit on enrichment can help decrease overall fuel costs while simultaneously increase the burnup of an assembly before it is discharged.

The core redesign process involved configuring a PWR core, which has the capability to operate for a minimum of 24-months, while retaining adequate operating and safety constraints. For this, the average burnup for a fuel assembly was increased to 75

GWD/MTU, and an enrichment of 6 w/o was allowed. These constraints are currently not allowed by NRC regulations. The calculations provide evidence that if the constraints were relaxed, there would be a potential for increased fuel utilization, lower fuel costs, and more limited reactor outages.

SIGNIFICANCE:

The design process provides evidence that a 24-month cycle is possible with the proposed increased burnup and enrichment limits. Multiple designs tradeoffs allow for the decrease in reactor batch fraction and increase in fuel utilization, while retaining a majority of stringent safety constraints. This approach allows researchers to determine which safety constraints are the most challenging when it comes to increasing burnup and enrichment limits. Furthermore, it allows researchers to determine which safety constraints should be reexamined to further increase the ability of reactors to operate for longer cycles.

KEY PUBLICATIONS:

- N/A

Multiphase CFD Modeling and Simulation for Boiling Water Reactor Applications

REPORT PARTICIPANTS:

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1 Idaho National Laboratory
2 Massachusetts Institute of Technology – Nuclear Science and Engineering Department

SCIENTIFIC ACHIEVEMENT:

This project aimed at developing the advanced multi-phase flow and boiling models for the boiling water reactor (BWR) application. While extensive effort is being devoted to evaluate and improve the closure validity and predictive capabilities, as part of the Consortium for Advanced Simulation of Light Water Reactors (CASL) program, the heat and mass transfer characteristics in two-phase flow boiling still remain challenging, especially for BWRs. For instance, the extension of existing boiling closures to the high-void fraction conditions of Boiling Water Reactors (BWR) is still an open issue. The scales that need to be resolved vary widely, from the millimeter scale of the multiphase structures to the meters scale of the core geometry. This multi-scale problem requires extremely high computational effort in order to avoid geometric simplifications that would introduce large uncertainty in the computational result. This project provides a baseline closure model for the BWR application that has been developed by leveraging the closure model developed for the pressurized water reactor (PWR) and research experiences from the Numerical Nuclear Reactor project. The predictive capability of the closure model has been assessed against the international benchmark, OECD/NRC BWR Full-size Fine-mesh Bundle Test (BFBT) data. The limitation of baseline model has been addressed by the computational fluid dynamics (CFD) benchmark of the Westinghouse FRIGG experiment, and the advanced modeling approach using the Large Scale Interface (LSI) model was proposed and evaluated for a further model development.

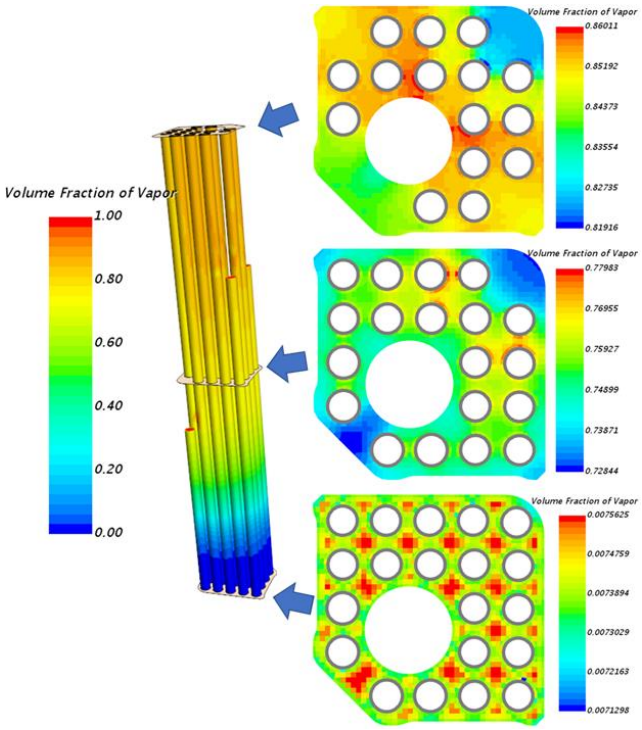


Fig. 1: FRIGG Benchmark-Void Distribution in the Fuel Assembly

SIGNIFICANCE:

The objectives of this project were to develop and evaluate a multi-phase CFD capability for BWR applications, address the limitation of the current modeling approach, and provide a direction for the further model development. Although improved void drift prediction is obtained, inaccuracies are still observed, which are attributed to the deficiency of the two-phase turbulence model and the rough representation of the interaction area density at a high void fraction regime. A further study is needed to investigate the fundamental mechanism of two-phase flow mixing and the effect of interphase momentum transfer closures in order to improve the CFD prediction.

KEY PUBLICATIONS:

- SuJong Yoon. 2016. “High Fidelity BWR Fuel Simulation.” INL/EXT-16-39678, CASL-THM-CFD-P13-03.
- SuJong Yoon, Emilio Baglietto, and Giulia Agostinelli. 2017. “BWR Full Fuel Assembly Testing and Validation.” INL/EXT-17-42714, CASL-THM-CLS-P15-10.
- SuJong Yoon and Emilio Baglietto. 2018. “Gen-0 BWR Modeling Application and Validation.” INL/EXT-18-51009, CASL-THM-P18-01.
- SuJong Yoon, Jinyong Feng, and Emilio Baglietto. 2019. “BWR Application Validation using Advanced CFD-BWR Model.” INL/EXT-19-55758, CASL-THM-BWR-P19-03.
- SuJong Yoon, Giulia Agostinelli, and Emilio Baglietto. 2017. “Evaluating the Practicability of Multiphase CFD for BWR Fuel Assembly Analysis.” M&C 2017, Jeju, Korea, April 16-20.
- SuJong Yoon, Giulia Agostinelli, and Emilio Baglietto. 2017. “Assessment of Multiphase CFD with Zero Closure Model for Boiling Water Reactor Fuel Assemblies.” NURETH-17, Xi’an, Shaanxi, China, Sept. 3-8.
- SuJong Yoon, Emilio Baglietto, and Jinyong Feng. 2020. “Multi-phase Computational Fluid Dynamics Modeling and Simulation for Boiling Water Reactor Applications,” CASL Symposium, Oak Ridge National Laboratory, April 7-9.

CFD Modeling and Simulation of Wire Wrapped Fuel Assembly

REPORT PARTICIPANTS:

SuJong Yoon[1], Samuel Bays[1], Aballa Abou-Jaoude[1], Dillon Shaver[2], Florent Heidet[2],
1 Idaho National Laboratory
2 Argonne National Laboratory

SCIENTIFIC ACHIEVEMENT:

The objectives of this work are to develop the computational fluid dynamics (CFD) model of a wire wrapped fuel assembly and to evaluate the Reynolds Averaged Navier-Stokes (RANS) based turbulence models of a CFD code in prediction of turbulent flow mixing and pressure loss. A special mesh treatment technique to reduce the computational cell was adopted to model the complex geometry of wire-wrapped fuel. CFD analyses of 217 pin wire wrapped fuel assemblies were developed with 92 million computational cells and were carried out to evaluate the temperature and pressure distribution. Various sensitivity tests of mesh structure and turbulence models were also performed. The pressure drop of fuel assembly was evaluated against the existing empirical correlations showing a CFD model with a high wall y+ value and wall treatment provides a better prediction of the pressure drop. Swirling flow through the edge subchannel modeled by the CFD would be complicated and not one-directional as assumed for the empirical correlations.

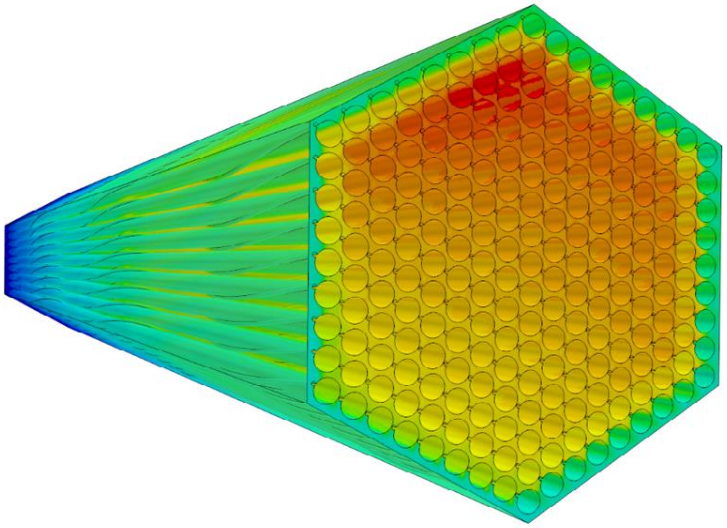


Fig. 1: CFD model of 217-pin wire-wrapped fuel assembly

SIGNIFICANCE:

This work aims at evaluating the performance of the wire wrapped fuel assembly that is supported by the Versatile Test Reactor (VTR) program. The turbulent flow mixing, mainly induced by the wire wrap spacers in the fuel assembly, is a key phenomenon in predicting the temperature distribution and peak cladding temperature. In general, empirical correlations have been used in the system thermal-hydraulic and subchannel codes to model the effect of turbulent flow mixing. CFD can provide high resolution and high fidelity data to improve the flow mixing model in the system and/or subchannel codes, but there are some technical challenges in CFD modeling of a wire-wrapped fuel assembly to be resolved. Due to the complex geometry of the helically coiled wire-wraps, the CFD analysis would take a lot of effort on geometry modeling, preprocessing

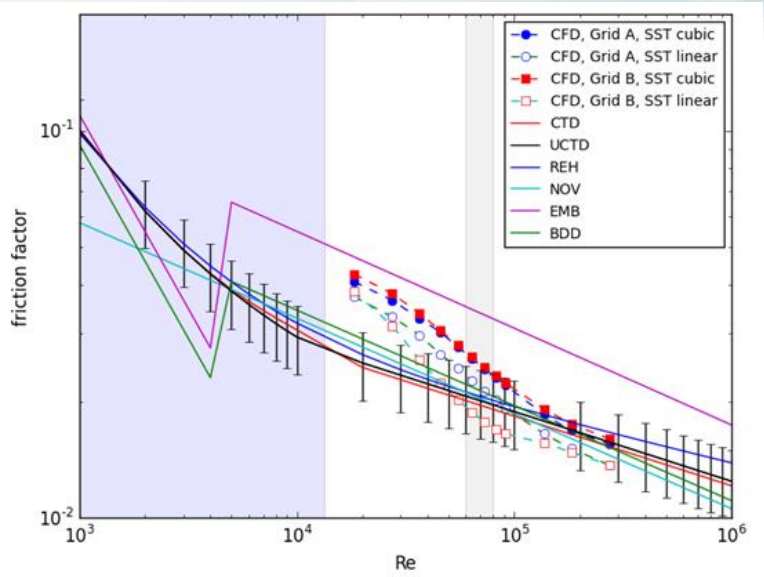


Fig. 2: CFD pressure drop evaluation with existing correlations

of computational domain, and running the simulation. In addition, liquid metal coolants have different thermo-physical properties from water and gases. For instance, a typical liquid -metal coolant, sodium, is a low Prandtl number fluid of the order of 10^{-3} that has a high thermal conductivity and low dynamic viscosity. It is known that typical RANS based turbulence models predict the thermal behavior of liquid metal systems inaccurately as they are developed based on the Reynolds analogy that assumes a Prandtl number of one. This work developed a CFD model of a 217 pin wire wrapped fuel assembly and addressed the scientific and technical challenges of modeling the thermal-hydraulic behavior of wire wrapped fuel assembly.

KEY PUBLICATIONS:

- SuJong Yoon and Florent Heidet. 2020. “Evaluation of Pressure Drop Correlations for the Wire-wrapped Rod Bundles.” Submitted to the 2020 ANS Annual Meeting, Phoenix, AZ, June 7-11.
- Abdalla Abou-Jaoude, SuJong Yoon, and Samuel E. Bays. 2019. “MCNP and CFD Modeling of a Sodium Fast Reactor Subassembly Channel to Capture Localized Power Peaking.” M&C 2019, Portland, Oregon, August 25-29.

DEM Simulation of Biomass Particle Flow for Bioenergy Conversion Process

REPORT PARTICIPANTS:

Yuan Guo[1], Feiyang Chen[1], Zakia Tasnim[1], Qiushi Chen[1]
1 Clemson University - Glenn Department of Civil Engineering

SCIENTIFIC ACHIEVEMENT:

The work focuses on developing the Discrete Element Method (DEM) model to better improve the current understanding of biomass particle flow properties in the bioenergy conversion process, so as to provide recommendations to describe biomass flow in the system scale. Biomass particles, (e.g., wood chips and switchgrass particles), feature unique particle morphology and particle size distribution with a high particle deformability, which contribute to a unique mechanical property that may lead to processing failures in the biomass preprocessing stage. Using DEM as a numerical tool, we are trying to simulate the mechanical and flow behavior of various biomass particles in different scenarios, including a biomass compression test, a biomass ring shear test, and biomass transport in screw conveyors, hoppers, and drag chain conveyors.

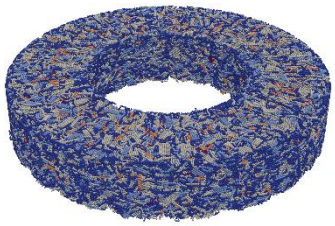


Fig. 1: Ring shear test model

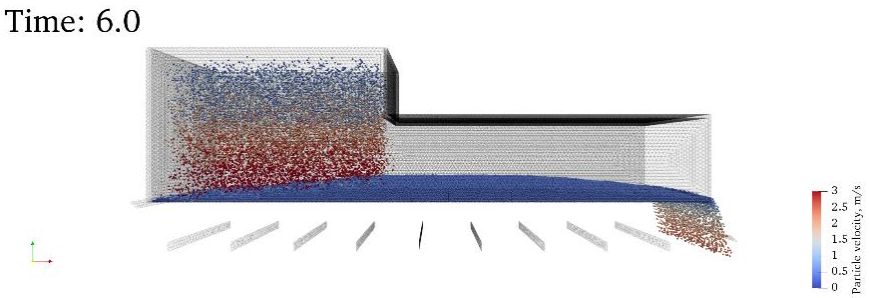


Fig. 2: Switchgrass transport in a drag chain conveyor

SIGNIFICANCE:

DEM simulation contribute to a more accurate estimation of particle flow in process demonstration unit (PDU) systems. The simulations incur a high computational cost, especially for industrial-scale models. Our model is able to consider fibrous biomass particles with a high particle deformability and moisture content. It is shown that the DEM model replicates the physical and mechanical behavior with a high fidelity. It is also able to describe various biomass unique properties, e.g., moisture-dependent flow behavior, arching and clogging in certain conditions.

KEY PUBLICATIONS:

- N/A

Computational Study of CO Adsorption and Disproportionation on Mo_2C Supported Pt Nanoparticles

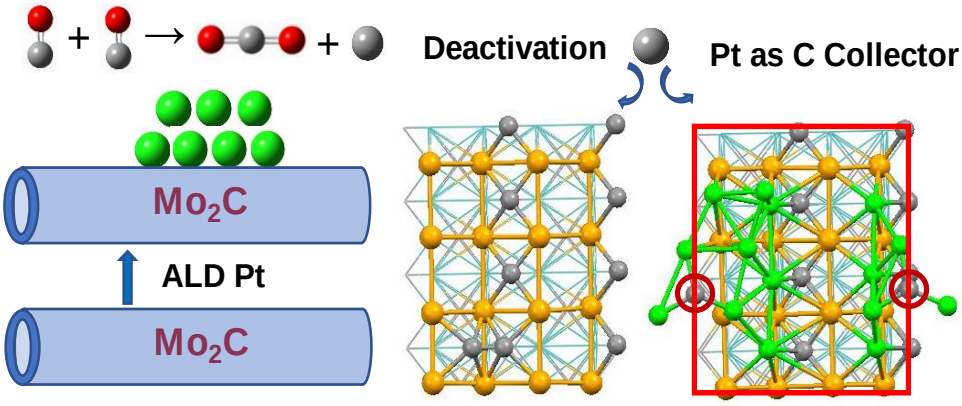
REPORT PARTICIPANTS:

Zongtang Fang[1], Ember Sikorski[2,3], Lan (Samantha) Li[2,3], Rebecca Fushimi[1]

1 Idaho National Laboratory
2 Boise State University
3 Center for Advanced Energy Studies (CAES)

SCIENTIFIC ACHIEVEMENT:

CO reactions on Mo_2C nanotube-supported Pt nanoparticles (NPs) under TAP conditions shows the formation of CO_2 via the process of CO disproportionation. Detailed plane-wave density functional-theory calculations of the CO adsorption and disproportion reactions on Mo_2C-supported Pt nanoparticles (NPs) were performed. The Mo_2C was represented by the β-Mo_2C (100) surface, and the Pt/Mo_2C interface was modeled by the addition of 12 Pt atoms to the Mo_2C (100) surface (12Pt@Mo_2C). The potential energy surfaces of the Boudouard reaction were calculated on pure Mo_2C, 12Pt@Mo_2C, as well as Pt (111) surfaces. CO dissociation readily occurs on the Mo_2C (100) surface, but not on the Pt (111) surface, with the former being exothermic and the latter being endothermic. At the Pt/Mo_2C interface, CO dissociation is still exothermic, but with a larger energy barrier. The Boudouard reaction takes place on the Mo_2C region, where CO_2 is formed from a surface O atom dissociated from one CO molecule



in reaction with another CO molecule, leaving one C atom on the surface. C adsorption is preferential on the Pt site in comparison to the Mo site. The supported Pt domains can collect the remaining C atoms, facilitating further CO_2 formation on the active Mo sites. A Bader charge analysis shows that the surface metal-carbon bond is a mixture of covalent and ionic bonds, whereas the surface metal-oxygen bond is ionic. Electron localization function and partial charge density calculations agree well with the Bader charge analysis. These computational results are consistent with experimental observations of the interaction of CO with Mo_2C nanotube-supported Pt domains in the transient regime under far from equilibrium conditions. The Boudouard reaction is an important side reaction, and the unexpected role found for Pt as a carbon collector, with Mo serving as a disproportionation site, provides a unique vantage point for understanding carbon and coke formation on catalytic materials.

SIGNIFICANCE:

The role of Pt nanoparticles as a carbon collector may be helpful for the design of new catalytical materials. Carbon and coke formation resulting in deactivation of catalysts is generally unavoidable in various industrial processes such as CO methanation and steam reforming. The Boudouard reaction is also an important side reaction in many catalytic processes. For such processes, the doping of a small amount of Pt on the catalytic active species could be potentially useful to mitigate the deactivation, if C atoms prefer to adsorb on the Pt domain rather than the catalytic active sites.

KEY PUBLICATIONS:

- Fang, Z., Wang, L., Wang, Y., Sikorski, E., Tan, S., Li-Oakey, K. D., Li, L., Yablonsky, G., Dixon, D. A., Fushimi, R. 2020. “Pt-Assisted Carbon Remediation of Mo2C Materials for CO Disproportionation.” ACS Catal., 10(3), 1894-1911.

Long Timescale Molecular Dynamics Annealing of Radiation Damage in Metals

REPORT PARTICIPANTS:

Charles Hirst[1], Penghui Cao[2], Scott Middlemas[3], Michael Short[1]
1 Massachusetts Institute of Technology
2 University of California, Irvine
3 Idaho National Laboratory

SCIENTIFIC ACHIEVEMENT:

Bridging the timescale gap between simulations and experiments remains one of the key limitations for computer modelling using atomistic techniques. The objective of this research, coupled with the latest advances in Fast Scanning Chip Calorimetry (FDSC), is to decelerate simulations and accelerate experiments to the point of a functional overlap, when one technique can reliably inform the other (at the same timescale). This project has successfully simulated the annealing of electron irradiation damage in pure metals across timescales up to 2 μs. In doing so, we have visualized the defect migration and annihilation mechanisms and have determined the evolution of stored energy in the system as a function of temperature. This release of energy with increasing temperature has been used to predict and interpret the equivalent, experimentally observed, FDSC signal. Further work is being conducted, with increasingly complex defect systems, to explore the recovery of neutron irradiation damage.

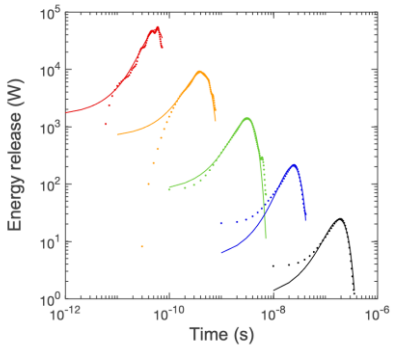


Fig. 1: Stored energy release from defect annihilation with increasing temperature (and time)

SIGNIFICANCE:

Experimental validation of radiation damage simulations has long been sought. Due to diffraction and transmission limitations, electron microscopy can only partially authenticate models of radiation damage evolution in materials. The investigation of defect annealing, through calorimetric methods, has the potential to further verify atomistic simulations, particularly for sub-nanometer scale features. In addition, this technique has the capability to *directly measure* radiation damage. This is a key advantage over the current estimate of damage (the average number of displacements per atom) and is a fundamental requirement when evaluating structure-property relationships for radiation materials science. Coupling computer modelling to experimental measurement of defect reactions also provides significant mechanistic input into the analysis of radiation damage evolution. This synergy is a promising

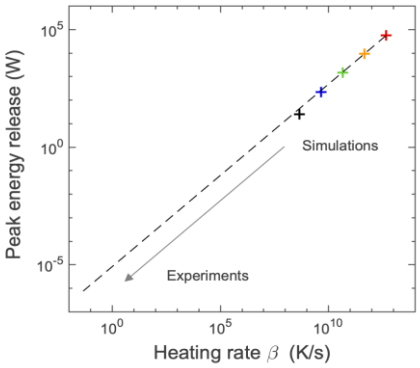


Fig 2.: Extrapolation of peak energy release from atomistic to experimental timescales

advance towards the development of accelerated materials testing methods for nuclear materials characterization.

KEY PUBLICATIONS:

- N/A

Feasibility Assessment of a Molten Salt Loop inside the Advanced Test Reactor

REPORT PARTICIPANTS:
Abdalla Abou Jaoude[1]
[1]Idaho National Laboratory

SCIENTIFIC ACHIEVEMENT:
This project is assessing the feasibility of deploying a molten salt loop experiment inside the Advanced Test Reactor (ATR). Multiple private entities are pursuing novel molten salt reactor (MSR) concepts. These advanced reactors promise to upend the nuclear industry and improve reactor safety/economics/resource utilization. It is anticipated that many of the fueled salts proposed will need to be irradiated within a test reactor before they are commercialized. High-Performance Computing (HPC) capabilities were leveraged to scope neutronic behavior of the proposed loops within different ATR testing positions. The study recommended the I-position for further analysis. The HPC was also utilized to conduct system code analysis to evaluate the potential for natural circulation within the loop. The results were benchmarked to more complex computational fluid dynamics (CFD) models and showed good agreement. This provided the basis for the preliminary design of the salt loop.

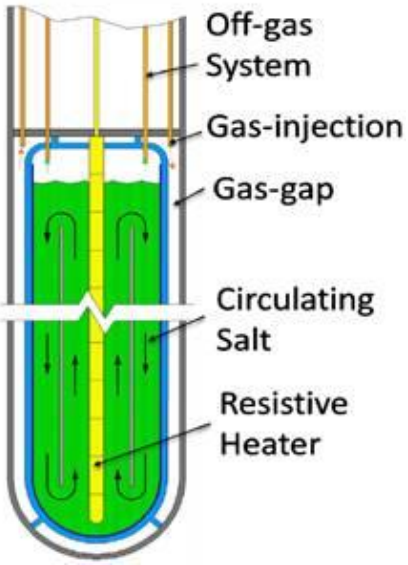


Fig. 1: Illustration of the proposed natural circulation irradiation salt loop.

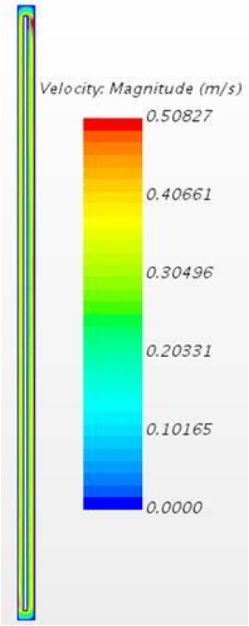


Fig. 2: Computational Fluid Dynamics (CFD) simulation of a 2-D representation of the proposed salt loop, highlighting the velocity field throughout the experiment.

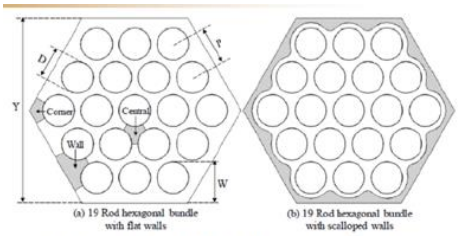
SIGNIFICANCE:
This project provides a key stepping stone in the commercialization of MSR concepts. The feasibility study concluded that the ATR is a suitable venue to conduct salt irradiation testing. Preliminary designs were also developed and are expected to be further refined in the near future. If deployed, the proposed salt irradiation loop would provide critical data to support the licensing and commercialization of new reactor concepts.

KEY PUBLICATIONS:

- Abou-Jaoude, J., Sterbentz, J., Palmer, P., Calderoni. 2019. “Evaluation of a Versatile Experimental Salt Irradiation Loop (VESIL) inside the Advanced Test Reactor.” INL/EXT-19-52917-Rev001, Idaho National Laboratory.
- Abou-Jaoude, J., Sterbentz, J., Palmer, P., Calderoni., 2019. “A Versatile Experimental Salt Irradiation Loop (VESIL) in the Advanced Test Reactor,” ANS Annual 2019, Minneapolis, (June) 2019.

CFD Analyses and Friction Factor Correlation in Hexagonal Bundles with Flat and Scalloped Walls

REPORT PARTICIPANTS:
Mohamed El-Genk[1,2,3,4], Luis Palomino[1,2], and Timothy Schriener[1,2]
[1]Institute for Space and Nuclear Power Studies, University of New Mexico
[2]Nuclear Engineering Department, University of New Mexico
[3]Mechanical Engineering Department, University of New Mexico
[4]Chemical and Biological Engineering Department, University of New Mexico



Section views of bundles of bare rods with (a) flat and (b) scalloped walls

SCIENTIFIC ACHIEVEMENT:
The flat-walled hexagonal rod bundles that have previously been used in liquid-metal-cooled reactors result in non-uniform radial flow and coolant temperature distributions. This non-uniformity is a result of a large fraction of the flow passing through the space adjacent to the shroud wall, bypassing the rods in the center of the bundle. The non-uniform flow distribution also causes non-uniformity of the friction factor, f, which is used for estimating the bundle pressure losses. The University of New Mexico's Institute for Space and Nuclear Power Studies (ISNPS) has recently developed a small modular reactor concept, the Scalable Liquid Metal cooled small Modular (SLIMM) reactor and a very small modular reactor concept, the Very-Small Long-LIfe Modular (VSLLIM) reactor, which instead employ hexagonal rod bundles with scalloped walls. Scalloping the bundle wall effectively enhances the uniformity of the flow, and hence the friction factor, as well as the coolant and fuel temperatures within the fuel rod bundle.

To quantify the effects of scalloping the shroud walls, this research project investigates the pressure loss and friction factor in hexagonal bundles of bare rods or tubes with either flat or scalloped bundle walls. It develops a continuous correlation of the friction factor for hexagonal bundles of bare tubes with flat walls, covering the range of inlet Reynolds number, Re_{in}, from 10^2 to 4 x 10^5, pitch-to-diameter ratios (P/D) up to 3.0, and for bundle sizes between 7 and 331 rods or tubes. The bundle average friction factor, f_b, correlation has the following form:

$$f_b = (f_l^2 + f_t^2)^{1/2}$$

where the laminar and turbulent flow friction factors being $f_l = A/Re_{in}$ and $f_t = B/Re_{in}^{0.198}$. The coefficients A and B are correlated in terms of P/D and number of rods, N, as:

$$A = (87.2 + 22.4/N^{0.22}) + (70.8 - 106.4/N^{0.32})\,[P/D - 1] - [((87.2 + 22.4/N^{0.22}) - 25)/(P/D)^{15.6-(10.6/N\text{^}0.123)}]$$

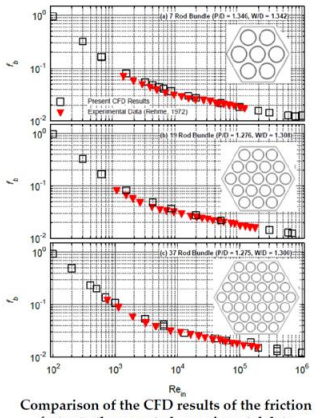
$$B = 0.186 + 0.00047[(P/D) - 1] - [0.06/(p/D)^{18.2}].$$

This correlation is based in part on the reported experimental data of Rehme (1972), complemented by data generated using computational fluid dynamics (CFD) analyses.

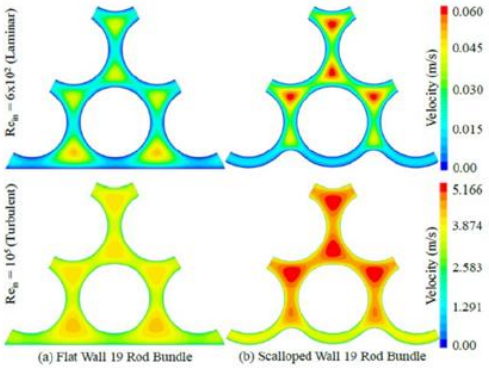
The CFD analyses is are used to generate additional bundle friction factor data within the laminar, transition, and turbulent flow regimes to extend the applicable range of the present correlation beyond that possible using the reported experimental data alone. This continuous correlation agrees with the compiled database of 1049 experimental and 375 CFD data points to within 5-10%. The developed friction factor correlation is then used to help quantify the effects of using scalloped walls on the friction factor by comparing against results of CFD analyses for the friction factor of hexagonal bundles of 19 and 37 bare tubes, but with scalloped walls. The results show that the developed correlation of the friction factor is applicable to bundles of bare tubes with scalloped walls, agreeing to within 5-8% of the CFD data.

SIGNIFICANCE:

The present friction factor correlation for hexagonal rod bundles with either flat or scalloped walls is a useful tool for engineering design and calculation of pressure losses in hexagonal bundles of bare tubes. It is applicable with either flat or scalloped walls. It provides a continuous correlation applicable for flows throughout the laminar, transition, and turbulent flow regimes, and it incorporates the effects of the bundle P/D as well as the number of rods or tubes within the bundle. The developed correlation has applications to the design and modeling of liquid- metal- cooled small modular reactors, space nuclear reactors, and tube and shell heat exchangers.



Comparison of the CFD results of the friction factor to the reported experimental data



Flow distribution for bundle with (a) flat and (b) scalloped walls

In addition to calculating the effects on the pressure losses, the CFD analyses demonstrate the scalloped bundle wall reduces bypass flow along the periphery of the bundle while increasing the flow through the middle of the bundle. This results in more uniform flow, reduces the peak fuel and cladding temperatures, and produces a more even coolant exit temperature. The uniform flow distribution enhances the thermal hydraulics of the fuel bundles, with the lower maximum fuel temperature enabling an increase in the power density in the fuel rods compared to that possible using bundles with flat walls.

KEY PUBLICATIONS:

- Palomino, L.M., El-Genk, M.S. 2019. “Friction factor correlation for hexagonal bundles of bare tubes / rods and with flat and scalloped walls,” J. Nuclear Engineering and Design.

Thermo-mechanical Performance of SiC-SiC Cladding and Channel Box

REPORT PARTICIPANTS:

Gyanender Singh[1]
[1]University of Tennessee

SCIENTIFIC ACHIEVEMENT:

Silicon carbide composites are candidate materials for accident tolerant fuel cladding and channel boxes. Currently, these materials are under evaluation for applications in light-water reactors (LWRs). The computing work performed using HPC resources at INL provided detailed information about the thermo-mechanical performance of SiC-SiC cladding and the channel box. This information includes the pellet cladding mechanical interaction, stresses, temperature and gap closure behavior for cladding, and details of the lateral bending phenomenon for the channel box, see Figure 1. The computing work performed using HPC resources generated important information about whether these materials can deliver the required performance under normal reactor operating conditions and off-normal conditions. This information will be highly significant as it will inform critical decisions regarding the development and deployment of these materials in LWRs, thus enhancing the efficiency and safety of nuclear reactors and meeting the energy demands of the world.

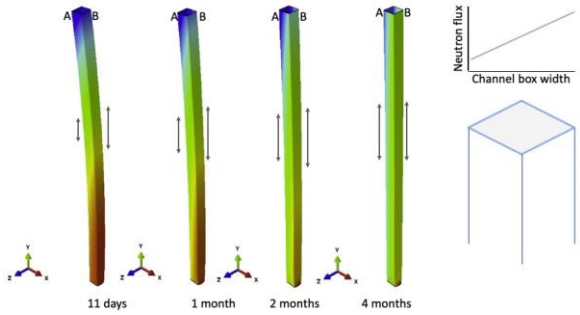


Fig 1: SiC-SiC channel box undergoes lateral displacement during the initial operating phase of a BWR, and gradually straightens during the course of time. Channel bowing is caused by the differential swelling of SiC-SiC under the influence of non-uniform neutron irradiation across the width of the channel box.

SIGNIFICANCE:

The is study generated important information about whether SiC-SiC materials can deliver the required performance under normal reactor operating conditions and off-normal conditions. This information will be highly significant as it will inform critical decisions regarding the development and deployment of the materials in LWRs, thus enhancing the efficiency and safety of nuclear reactors and meeting the energy demands of the world. The computing work performed using HPC resources at INL provided detailed information about the thermo-mechanical performance of SiC-SiC cladding and the channel box. This information includes the pellet-cladding mechanical interaction, stresses, temperature and gap closure behavior for cladding, and details of the lateral bending phenomenon for the channel box. This novel scientific investigation directly helps the nuclear community (government, academia, and industry) to determine the next steps for the development of SiC-SiC core components for light-water reactor applications.

KEY PUBLICATIONS:

- Singh, G., Sweet, R., Schappel, D., Nelson, A., Harp, J., Wirth, B.D., Katoh, Y. 2019. “Preliminary Analysis of PCMI Behavior of SiC-SiC Cladding with U_3Si_2 and UO_2 Fuel Systems,” ORNL/SPR-2019/1247.
- Singh, G., Gorton, J., Schappel, D., Brown, N.R., Katoh, Y., Wirth, B., Terrani, K. 2019. “Deformation Analysis of SiC-SiC Channel Box for BWR Applications,” Journal of Nuclear Materials, Vol. 513, pp. 71-85.
- Singh, G., Sweet, R., Brown, N., Wirth, B., Katoh, Y., Terrani, K. 2018. “Parametric Evaluation of SiC/SiC Composite Cladding with UO_2 Fuel for LWR Applications: Fuel Rod Interactions and Impact of Nonuniform Power Profile in Fuel Rod,” Journal of Nuclear Materials, Vol. 499, pp. 155-167.

AFC Project SiC/SiC Composite Clad Bowing and Stresses

REPORT PARTICIPANTS:

Danny Schappel[1]
[1]University of Tennessee

SCIENTIFIC ACHIEVEMENT:

This work is focuses on the SiC/SiC composite cladding simulation capability research efforts. BISON was selected for this work due to its adaptability to most fuel performance related activities. In the past year, we have added and improved boundary conditions to allow for the simulation of SiC/SiC composite clad bowing as a result of neutron flux and temperature profiles.

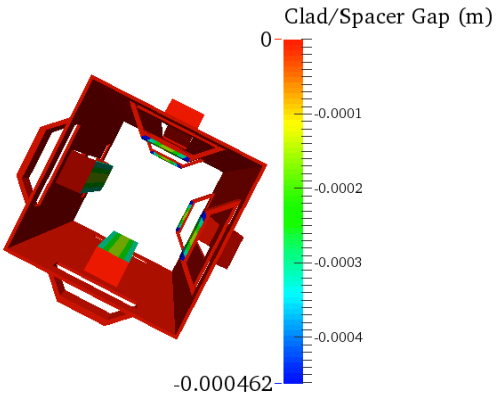


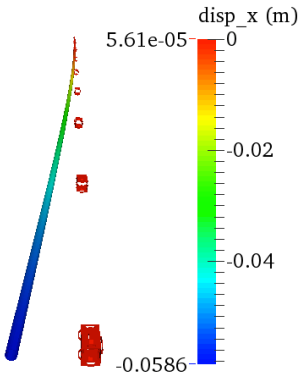
Fig 1: Sample spacer grid

SIGNIFICANCE:

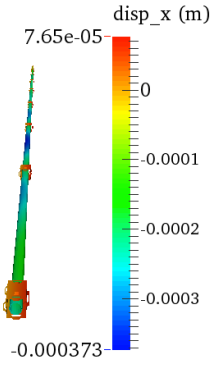
Using explicit thermal and mechanical contact models, a bowing displacement predictor, adaptable penalty Dirichlet boundary conditions, and improved auxkernels, it is possible to estimate the displacements and stresses in a SiC-SiC cladding tube under asymmetric operating conditions. Figure 1 shows the simulated spacer grid channel geometry, which was based on a 17x17 PWR spacer grid. Methods were also developed to allow for mechanical contact between the grid springs and dimples, and the cladding tube, without resulting in an excessively expensive simulation.

KEY PUBLICATIONS:

- In progress



Rod bowing displacement without grid/cladding contact.



Bowing with grid/cladding contact.

Fig. 2: Shows an example of clad bowing with and without active spacer grid/cladding contact. Maximum clad/grid contact overlap was about 0.2 µm, which surpassed expectations. Additionally, the monolythic fuel rod was stabilized so that oscillatory hot spots did not form in the cladding tube throughout its large displacement. This shows that BISON can simulate relevant fuel conditions for SiC/SiC cladding, where most other codes have difficulty.

Aluminum-clad Spent Nuclear Fuel

REPORT PARTICIPANTS:

Alexander Abboud[1]
[1]Idaho National Laboratory

SCIENTIFIC ACHIEVEMENT:

This project used Computational Fluid Dynamics (CFD) coupled with radiolytic chemical reactions to model potential buildup of hydrogen and nitric acid within ATR storage canisters over extended interim storage scenarios.

SIGNIFICANCE:It examines a preliminary three-dimensional (3D) multi-physics CFD model of the unsealed canisters containing aluminum-clad spent nuclear fuel from INL's ATR in the irradiated fuel storage facility. This 3D CFD model considers fully resolved fuel plates in an unsealed canister. There is small mass exchange with surrounding air as time evolves in the simulation and contains a network of chemical reactions to consider due to several of the side reactions occurring in the presence of water vapor, nitrogen, oxygen, and carbon dioxide rather than in helium-backfilled DOE standard canisters. Prior to the CFD modeling, the full set of chemical reactions under these conditions was analyzed, reduced, and refit to a more manageable number of equations for the computational efficiency of the 3D CFD simulation. To deal with the long timescale of interest for tracking the possible buildup of trace species such as nitric acid, NOx, and hydrogen, a segregated time stepping algorithm is used, wherein the velocity field is only updated periodically, and assumed to be in a pseudo- steady state.

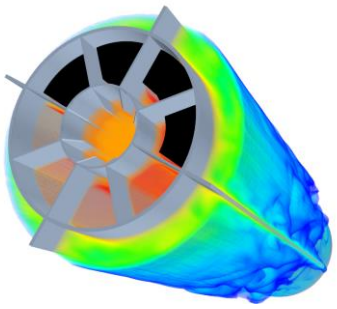


Fig 1.: Temperature field in an IFSF bucket loaded with ATR fuel.

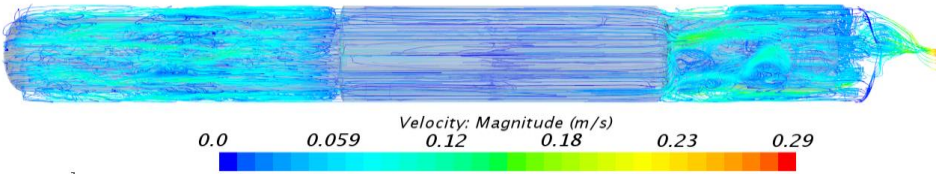


Fig. 2: Velocity streamlines within a loaded IFSF canister (canister bottom is right side of image).

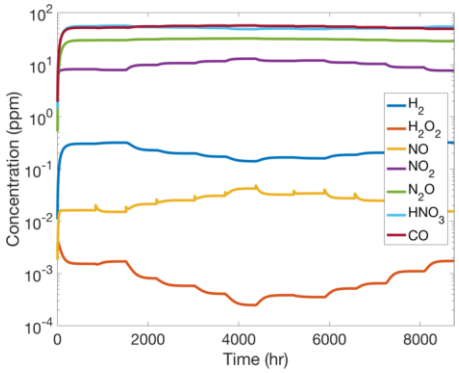


Fig. 3: Evolution of average chemical concentrations over 1-year, when model is coupled with seasonal-changing ambient temperature and humidity.

SIGNIFICANCE:

This study first examines the theory of the model, workflow to establish radiolysis reaction network, and initial simulations of the evolutions of thermal fields, hydrogen gas and nitric acid concentrations within unsealed canisters in conditions relevant to the INL INTEC CPP-603 facility over a long period of time.

KEY PUBLICATIONS:

- Abboud A.W., Huang, H. 2019. “Reactive CFD of Dry Storage of Unsealed Canisters of Aluminum Clad SNF,” Waste Management Symposium, Phoenix, AZ (March 3-7).
- Abboud A.W., Huang, H. 2019. Full-scale Model of Dry Storage of Aluminum Clad Spent Nuclear Fuel, Idaho National Laboratory, INL/EXT-19-5518.

Dynamic Line Ratings

REPORT PARTICIPANTS:

Alexander Abboud[1]
[1]Idaho National Laboratory

SCIENTIFIC ACHIEVEMENT:

The WindSim computational fluid dynamics (CFD) software was used to calculate wind fields over large regions of terrain around transmission lines of interest. The local wind fields were used in calculating the convective cooling rates along transmission lines, providing an increase in the current carrying capacity above typical conservative static ratings. These wind fields were coupled to local weather observation data to calculate the benefit of dynamic line ratings over a year-long period. In addition, the cases were also tested using mesoscopic forecasted data from the High-resolution Rapid Refresh model. This project used Computational Fluid Dynamics (CFD) to calculate cooling rates along overhead transmission lines to show possible improvements for current carrying capacity.

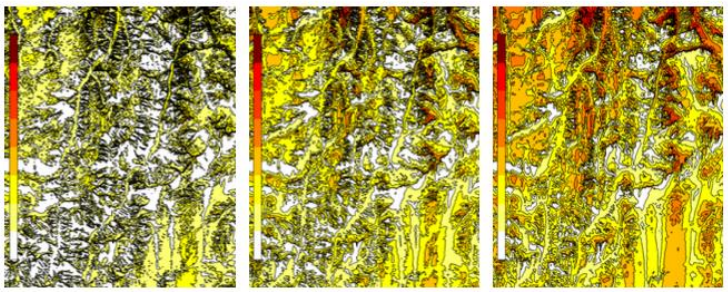


Fig. 1: Wind speeds in Hells Canyon at 10, 50, and 100m above ground elevation.

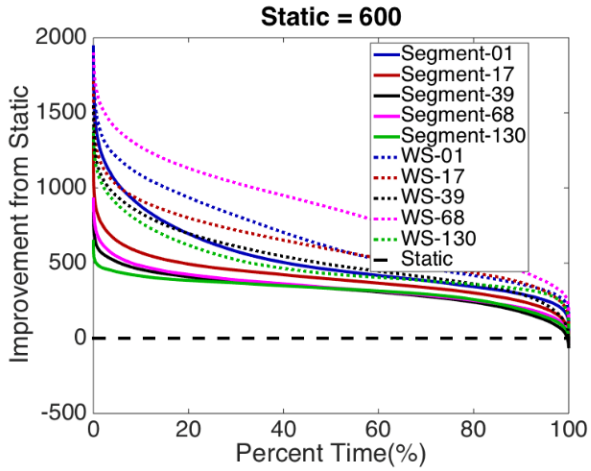


Fig. 2: Improvement of current carrying capacity above static ratings due to convective cooling.

SIGNIFICANCE:

This project used CFD to calculate cooling rates along overhead transmission lines to show possible improvements for current carrying capacity.The WindSim CFD software was used to calculate wind fields over large regions of terrain around transmission lines of interest. The local wind fields were used in calculating the convective cooling rates along transmission lines, providing an increase in the current carrying capacity above typical conservative static ratings. These wind fields were coupled to local weather observation data to calculate the benefit of dynamic line ratings over a year-long period. In addition, the cases were also tested using mesoscopic forecasted data from the High-resolution Rapid Refresh model.

KEY PUBLICATIONS:

- Abboud, A.W., Gentle, J.P., McJunkin, T.R., Lehmer, J.P. 2019. “Using Computational Fluid Dynamics of Wind Simulations Coupled with Weather Data

to Calculate Dynamic Line Ratings," IEEE Transactions on Power Delivery, Accepted June 2019.

- Abboud, A.W., Fenton K.F., Ferhinger, B.A., Gentle, J.P., McJunkin, T.R., Lehmer, J.P., LeBlanc K.L., Petty, M.A., Wandishin, M.S. 2019. "Coupling Computational Fluid Dynamics with the High-Resolution Rapid Refresh Model for Forecasting Dynamic Line Ratings." Electric Power Systems Research, Vol. 170, pp. 326-327.

Computational Design of Alloy Chemistry to Mitigate Fuel - Cladding Chemical Interactions in Uranium-based Metallic Fuels

REPORT PARTICIPANTS:
Samrat Choudhury[1] and Rabi Khanal[1]
[1]University of Idaho

SCIENTIFIC ACHIEVEMENT:
In U-based metallic fuels, lanthanide fission products react with the cladding materials leading to fuel-cladding-chemical interactions (FCCI). The FCCI results in reduced cladding integrity and potential rupture of the cladding. The addition of dopant(s) to hold lanthanides within the fuel matrix by forming intermetallic compounds has generated considerable attention due to its effectiveness. However, there is no generic rule of thumb to choose an appropriate dopant that can be effective in arresting lanthanides. Here, we present *ab initio* based thermodynamic alloy design principles that can be effective in identifying dopant(s) that can bind a lanthanide inside the fuel matrix. It was shown that, solely based on readily available intrinsic features of dopants such as electronegativity, atomic size, and electronic configuration, it is possible to predict the tendency of a given dopant to form intermetallic within the metallic matrix. Our approach correctly identifies both known dopants like Pd and new dopants such as As and Se that can be effective in binding lanthanides within U-matrix.

SIGNIFICANCE:
This research provides a significant leap in alloy design beyond typically used empirical approaches, such as Hume-Rothery rules or the Darken-Gurry map. Our approach correctly identifies both known dopants like Pd and new dopants such as As and Se that can be effective in binding lanthanides within U-matrix. It was shown that, solely based on readily available intrinsic features of dopants such as electronegativity, atomic size, and electronic configuration, it is possible to predict the tendency of a given dopant to form intermetallic within the metallic matrix. Further, desired alloy chemistry can be predicted without creating complicated binary/ternary phase diagrams, as are currently needed.

KEY PUBLICATIONS:
- Khanal, R., Jerred, N., Charit, I., Benson, M., Mariani, R., Choudhury, S. 2019. "Guiding Principles of the Dopants Selection to Immobilize Lanthanide Fission Products in Uranium-based Metallic Fuels," *TMS Annual Meeting*, San Antonio, TX.
- Khanal, R., Jerred, N., Charit, I., Benson, M., Mariani, R., Choudhury, S. 2018. "A Novel Approach of Dopant Selection to Immobilize Lanthanides in Uranium-Based Metallic Fuels,", *MRS Fall Meeting & Exhibit*, Boston, MA (Nov.)
- Khanal, R., Jerred, N., Benson, M., Mariani, R., Charit, I., Choudhury, S. 2018. “Effect of Dopants on Uranium-based Metallic Fuels to Mitigate Fuel-Cladding Chemical Interactions,” *TMS Annual Meeting & Exhibition*, Phoenix, AZ.

Battery500

REPORT PARTICIPANTS:
Alexander Abboud[1]
[1]Idaho National Laboratory

SCIENTIFIC ACHIEVEMENT:
This project utilized microscale modeling of a lithium battery cell to understand non-uniform current density fields during charging with different sized cathode particles. Lithium plating and dendrite growth are challenging issues for Li metal electrode (LME) performance in high-energy rechargeable Li battery (RLB) development. The morphology of Li plating is affected by local current density variations on LME.

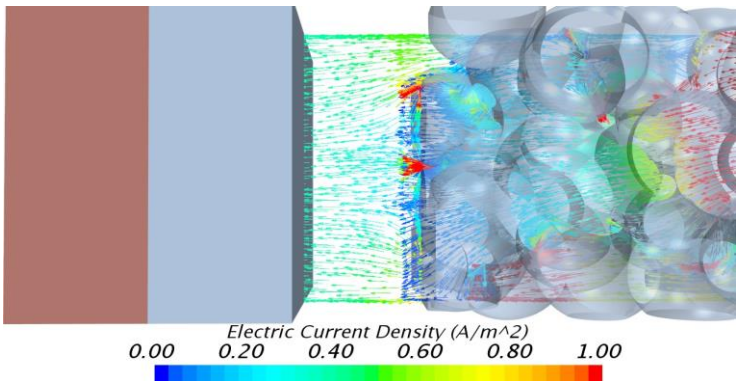


Fig. 1: Electric Current Density

The Star-CCM+ software was used to model microscopic electrochemical fields for rechargeable lithium metal batteries. A three-dimensional RLB cell model is used to investigate current density variations induced by cathode particle size. It was shown that decreasing particle size leads to more uniform electrical current density across the battery. Smaller cathode particles show lower variances in the current density distribution throughout the separator. The results suggest particle size could affect uniformity of Li plating, propensity for dendrite formation, and, ultimately, cycle life of RLB.

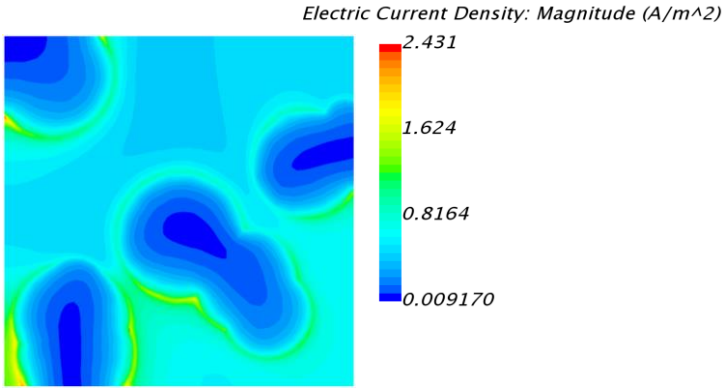


Fig. 2: Current density distribution across cell and at cathode-separator interface.

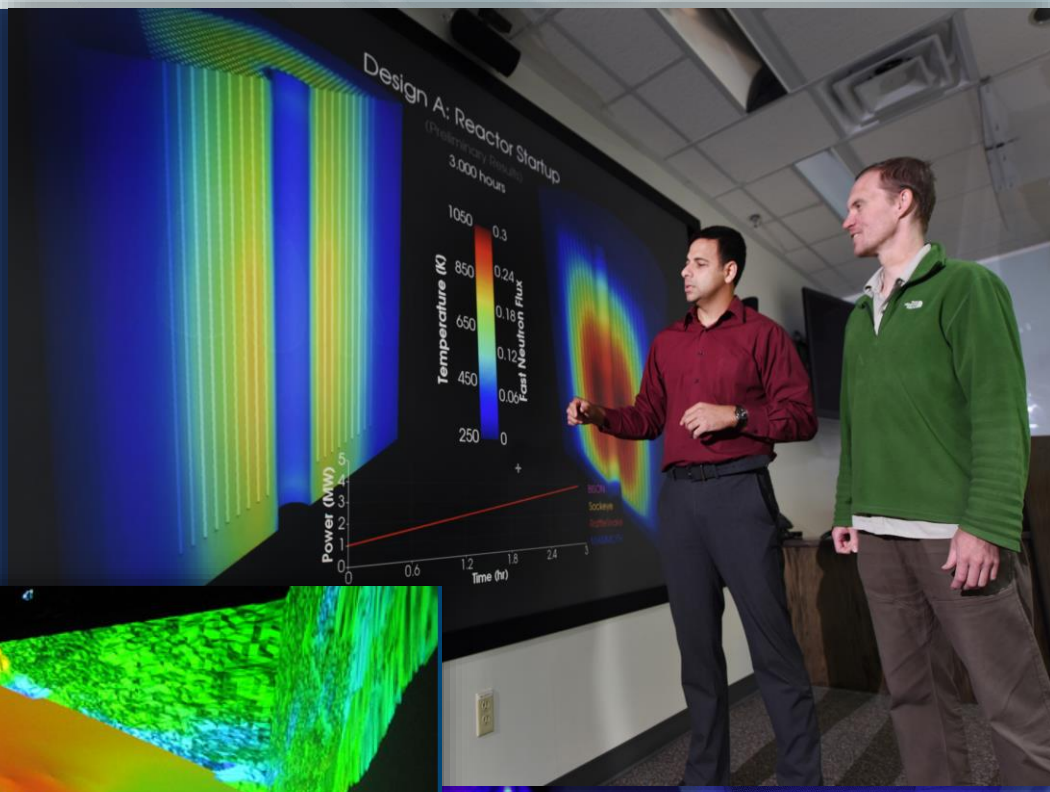
SIGNIFICANCE:
Consistent performance of a Li metal electrode (LME) relies on a well-distributed current across the electrode surface. A more uniform electrical current density should lead to more uniform electrodeposition rather than dendritic growth on the anode. This result may indicate a possibility for increasing cycle life expectancy for lithium metal batteries.

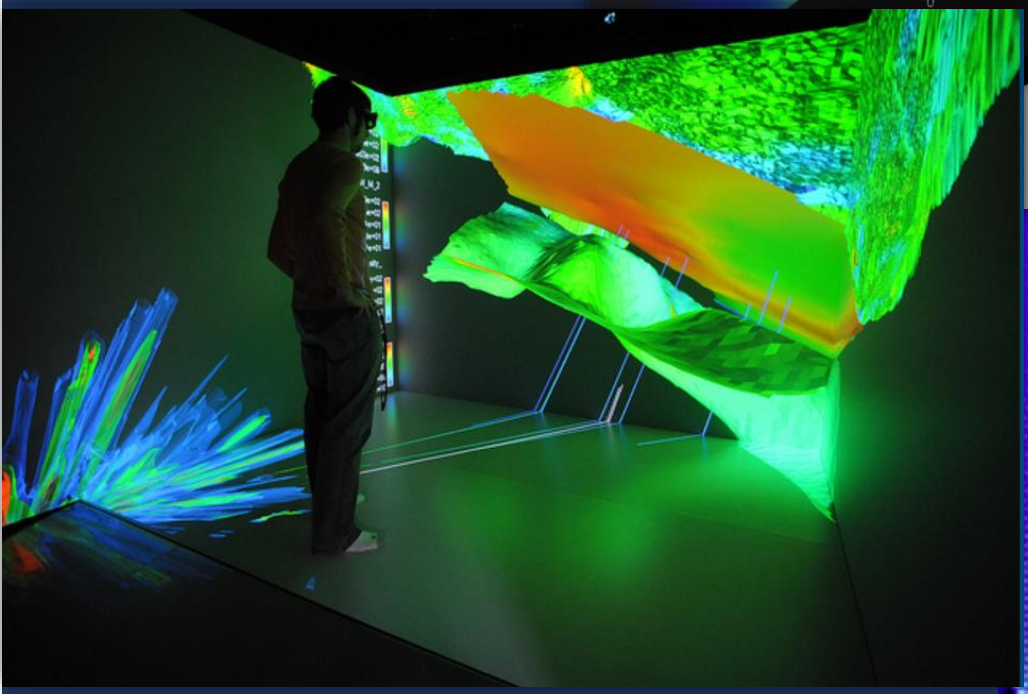
KEY PUBLICATIONS:

- Abboud, A.W., Dufek, E.J., Liaw, B. 2019. “Implications of Local Current Density Variations on Lithium Plating Affected by Cathode Particle Size.” *Journal of the Electrochemical Society*, Vol. 166, No. 4, A667-A669.

https://inl.gov/

http://hpcweb.hpc.inl.gov





Prepared by Idaho National Laboratory, Idaho Falls, Idaho 83415.