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Nuclear Science User Facilities High Performance Computing

FY 2020 Annual Report

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Nuclear Science User Facilities High Performance Computing

FY 2020 Annual Report

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Idaho National Laboratory
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Idaho Falls, Idaho 83415

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EXECUTIVE SUMMARY

Idaho National Laboratory (INL), supported by the Department of Energy Office of Nuclear Energy (DOE-NE) through the Nuclear Science User Facilities (NSUF), provides access to supercomputer systems and data storage along with support staff for system management, software installation, cybersecurity and user support to the broader DOE-NE user community. Users include individuals at universities, industry, and government laboratories, enabling a wide range of research and development and mission-supporting activities. The availability of high-performance computing (HPC) capabilities is a key foundation of collaboration and innovation in nuclear energy systems research. HPC resources and INL staff directly support the mission and objectives of DOE-NE.

In FY20, INL enhanced its HPC capabilities with full occupancy of the Collaborative Computing Center (C3), which includes data center space for up to 197 computer equipment racks. The Advanced Scientific Computing (ASC) division expanded in FY20 to include a new Artificial Intelligence (AI), Data and Visualization department. In addition, the Nuclear Computational Resource Center (NCRC) was established in FY20 to provide easy access to computational tools, HPC resources, and training.

In March 2020, a new $19.2 million supercomputer named Sawtooth was made available to users. With a performance rating of 5.6 petaFLOPS coming from 99,792 compute cores and an additional 0.56 petaFLOPS of compute capability coming from GPUs, Sawtooth is the largest INL supercomputer installed to date. Sawtooth, along with the supercomputers Falcon and Lemhi, delivered a total of 630 million core hours of compute time to researchers. In December 2020, a new deep learning system named Hoodoo was also made available to users, with a performance rating of 429 teraFLOPS double precision or 858 teraFLOPS single precision.

During FY20, INL HPC capabilities were utilized by a diverse set of computing and applied researchers. The majority (522) came from National Laboratories (309) with university researchers (as a group), making up the second largest group of users (155), while industry partners also accounted for a substantial number of users (58). In addition, INL also supported users from nuclear regulatory agencies, demonstrating our commitment to foster relationships between research and regulatory personnel.

INL HPC capabilities were utilized for a wide range of research and engineering activities in FY20, with summaries of a number of these activities presented as project reports (see Appendices A through J). A large portion of HPC use was geared towards nuclear energy, with numerous computational studies on important topics relevant in nuclear energy and well as and other energy systems. The subset of projects presented in this report give a clear indication of the high value and strong utilization of the INL HPC capabilities supported by 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 usage.

CONTENTS

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ACRONYMS

AI	Artificial Intelligence
ARPA-E	Advanced Research Projects Agency - Energy
AIMD	ab initio molecular dynamics
AKMC	Atomic Kinetic Monte Carlo
ALD	Atomic Layer Disposition
ANL	Argonne National Laboratory
ASC	Advanced Scientific Computing
ATF	Accident-tolerant Fuel
ATR	Advanced Test Reactor
bcc	body-centered-cubic
BWR	Boiling-Water Reactor
C3	Collaborative Computing Center
CASL	Consortium for Advanced Simulation of Light Water Reactors
CFD	Computational Fluid Dynamics
CNN	Convolutional Neural Network
CSAP	Core Safety Assurance Package
DEM	Discrete Element Modeling
DFT	Density Functional Theory
DNB	Departure from Nucleate Boiling
DOE-NE	Department of Energy Office of Nuclear Energy
EBSD	Electron Backscatter Diffraction
EERE	Office of Energy Efficiency and Renewable Energy
EM	Office of Environmental Management
EXAFS	Extended X-ray Absorption Fine Structure
FCCI	Fuel-cladding Chemical Interface
FCU	Fan Coil Unit
FGR	Fission Gas Release
GAIN	Gateway for Accelerated Innovation in Nuclear
HFIR	High-Flux Isotope Reactor
HTGR	High-Temperature Gas Reactor
HPC	High Powered Computing
HPGe	High-Purity Germanium
IES	Integrated Energy Systems

INL	Idaho National Laboratory
IUC	Idaho University Consortium
KTH	Kungliga Tekniska högskolan (Royal Institute of Technology)
LaRomance	Los Alamos Reduced Order Models for Advanced Nonlinear Constitutive Equations
LDRD	Laboratory Directed Research and Development
LWR	Light-Water Reactor
LWRS	Light Water Reactor Sustainability
MATHAM	Mars Active Tracer High Resolution Atmospheric Model
MCNP	Monte Carlo N-Particle
MCO	Moisture Carryover
ML	Machine Learning
MOOSE	Multiphysics Object-Oriented Simulation Environment
MPCMIV	multiphysics pellet cladding mechanical interaction validation
NEAMS	Nuclear Energy Advanced Modeling and Simulation
NCRC	Nuclear Computational Resource Center
NE	Nuclear Energy
NEUP	Nuclear Energy University Program
NRC	Nuclear Regulatory Commission
NRIC	National Reactor Innovation Center
NSUF	Nuclear Science User Facilities
NF	nanofiber
NRAD	Neutron Radiography Reactor
NRS	North Radiography Station
OS	Office of Science
PBR	Pebble-Bed Reactor
RCCS	Reactor Cavity Cooling System
RE	Reactor Engineering
RELAP5	Reactor Excursion and Leak Analysis Program
RIS	Radiation-Induced Segregation
RPV	Reactor Pressure Vessel
SQS	Special Quasirandom
TES	Thermal Energy Storage
TREAT	Transient Reactor Test
UIUC	University of Illinois at Urbana-Champaign
VASP	Vienna ab initio Simulation Package

VBMC	Variational Bayesian Monte Carlo
vdW	van der Waals
VERA	Virtual Environment for Reactor Analysis
VTT	Valtion Teknillinen Tutkimuskeskus (Technical Research Centre [of Finland])

1. INTRODUCTION

Idaho National Laboratory (INL), supported by the Department of Energy Office of Nuclear Energy (DOE-NE) through the Nuclear Science User Facilities (NSUF), provides access to supercomputer systems and data storage along with support staff for system management, software installation, cybersecurity and user support to the broader DOE-NE user community. Users include individuals at universities, industry, and government laboratories enabling a wide range of research and development and mission-supporting activities. The availability of high-performance computing (HPC) capabilities is a key foundation of collaboration and innovation in nuclear energy systems research. HPC resources and INL directly support the mission and objectives of DOE-NE.

Due to continuous and rapid transformation developments in the field of scientific computing, the INL continues to look for new and innovative ways to expand our computational research capabilities through:

- Investments in scientific computing capacity
- Development and validation of innovative modeling tools
- Expansion of expertise in deep machine learning, artificial intelligence, advanced visualization, and large-scale data processing and analytics

Fiscal Year 2020 was one that saw many significant accomplishments associated with HPC at INL. INL's capacity for both HPC hardware and infrastructure expanded significantly. INL completed and took occupancy of the Collaborative Computing Center (C3), which can house up to 196 staff members and 197 computer equipment racks, greatly expanding the HPC capabilities. In additional the Advanced Scientific Computing (ASC) Division was expanded by adding a new department focused on artificial intelligence and data science.

INL HPC systems doubled the core-hour usage time between FY19 and FY20, delivering more than 630 million core-hours of compute time in FY20. This is an increase of 304 million core-hours from the previous year, largely due to the deployment of the new 5.6 petaFLOPS Sawtooth system. A new deep learning system (Hoodoo) was also installed, with a performance rating of 0.43 petaFLOPS (double precision) or 0.86 petaFLOPS (single precision).

A total of 79 user supplied HPC usage summaries are included as appendices to this report. These summaries are submitted as part of a newly implemented process for user account renewals. While the breadth and depth of the user reports vary, they serve to document and demonstrate the types of work being conducted on INL HPC resources. The vast majority support nuclear energy research and development.

The discussion that follows expands on these topics and serve to demonstrate INL's commitment to expanding its HPC capabilities and resources.

2. MAJOR ACCOMPLISHMENTS

INL recognizes the importance of HPC in all areas of science and, as such, is strongly committed to growing its capabilities and enhancing its ability to support DOE-NE's computational science programs. Major accomplishments for INL HPC in FY20 are listed below and discussed in the following subsections.

- Expansion of the Advanced Scientific Computing (ASC) division
- Full occupancy of the Collaborative Computing Center (C3)
- Installation of the Sawtooth HPC system

- Procurement of the Hoodoo system for Deep Learning
- Modeling COVID in Rural Areas
- Establishment of the Nuclear Computational Resource Center (NCRC)

2.1. Advanced Scientific Computing Division

The ASC division expanded in FY20 to include a new Artificial Intelligence (AI), Data and Visualization department. The ASC division now houses three departments:

- Computational Frameworks Department
- High Performance Computing Department
- Artificial Intelligence, Data Analytics and Visualization Department.

This organizational realignment will help INL to take advantage of opportunities in the increasingly important field of Artificial Intelligence and Machine Learning (ML).

2.2. Collaborative Computing Center

C3 was designed to meet the current and future scientific computing needs of INL. The state of Idaho became a key partner by providing the funding for the leased facility. Construction began in April 2018 and was completed in August 2019. In early FY20 people and equipment moved into the facility. Figure 2-1 shows the front of the C3 building, looking to the west,

Figure 2-1. Collaborative Computing Center (C3).

The C3 facility provides office space for 196 people arranged in a manner that encourages collaboration, communication, and innovation between INL staff, university collaborators, and industry. Fifteen separate work areas are arranged in a “pod” configuration, allowing for technical discipline focus areas to exist within each pod. Thirteen pods configured as open collaboration space and two pods configured as hard wall offices. Specifically, the pods provide 40 hard-wall offices and 156 open office cubicles. Pods allow small workgroups to have a gathering place, while the flexible shared common areas

encourage ad hoc and impromptu collaboration, such as team programming, user help, and mentoring. Pod technical focuses consist of:

- National & Homeland Security Data Science (one pod)
- Digital Engineering and Advanced Analytics (one pod)
- Materials/Modeling and Simulation (one pod)
- AI, Data Analytics and Visualization (one pod)
- High Performance Computing Operations (two pods)
- Computation Materials (three pods)
- Reactor Physics (one pod)
- Computational Frameworks/MOOSE (two pods)
- Subsurface Science and Seismic Structural (one pod)
- ASC/C3 Leadership (one pod)
- INL Scientific Data Management (planned for future; one pod)

In addition to the pods, there are seventeen conference rooms of varying sizes which provide ample opportunities for collaboration, scientific data visualization, and meetings. The C3 facility is designed with multiple physical security zones to allow public meetings and general access as required. Figures 2-2 and 2-3 provide a few views of the interior of C3, with Figure 2-1 showing the entry way and Figure 2-3 showing an upstairs collaboration space, respectively.

Figure 2-2. C3 entrance.

Figure 2-3. C3 collaboration area.

A foundational enabling component of scientific computing is a capable data center with adequate space, power, and cooling for HPC systems. The C3 facility includes 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 1 MW of electrical power per row. The remaining three rows are designed for networking, hard disk storage, and other utility systems with power up to 150 KW 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 systems have a maximum limit of 4 MW with the ability to add an additional 4 MW of capacity when required.

2.3. Sawtooth

Sawtooth is INL's newest HPE SGI 8600 distributed-memory system consisting of 99,792 cores, 395 TB of total memory, high-speed EDR interconnect network, high-speed storage, and 0.56 petaFLOPS of GPU capabilities. This new computer has a performance rating of 5.6 petaFLOPS.

Planning for Sawtooth started in 2014 after the installation of Falcon cluster. This planning work included numerous vendor meetings, nondisclosure briefings, C3 facility design meetings, and other reviews. The conclusion of the planning was a Request for Proposal that was released on April 22, 2019. On August 19, 2019, a contract award was made to Hewlett Packard Enterprise for a $19.2 million four-year lease-to-own system.

The system was installed in December 2019 and moved to full production in March 2020. This new system has a positive impact on DOE-NE's ability to deliver results at a much larger scale than ever before. Figure 2-4 shows the C3 data center.

Figure 2-4. C3 Data Center.

2.4. HOODOO System for Deep Learning

Hoodoo, with over 400 teraFLOPS of performance, is a Lambda Hyperplane deep learning distributed memory system. It has 44 NVIDIA A100 tensor core GPUs and 7.2 TB of total memory. The system was delivered to HPC INL in late November 2020 and provides a maximum performance of 429 teraFLOPS double precision or 858 teraFLOPS single precision. Hoodoo became available to users the middle of December 2020.

2.5. Modeling Covid-19 in Rural Areas

The CityCovid model is a multi-agent simulation framework developed at Argonne National Laboratory (ANL) aimed at large scale COVID-19 infection simulations of transmission vectors related to public transportation in populations in excess of one million people. This model was a Gordon Bell finalist in the SC-20 conference. The CityCovid model was shared with INL in August 2020 and was modified to support modeling and prediction of COVID-19 spread in rural areas using data provided from the East Idaho Public Health District. Several hundred large scale simulations were executed for populations of less than 200,000 without public transportation, resulting in predicted ICU bed capacity and infection rate based on different public health policy decisions including partial closing of schools, obligatory mask usage, and closing of in-person dining at restaurants. Results of these simulations were shared with public health officials and a subsequent seed LDRD was submitted to continue research efforts.

2.6. Nuclear Computational Resource Center

Modeling and simulation are essential to nuclear energy innovation as well as the continued safe, secure, and efficient operation of existing nuclear systems. In FY20, the NCRC was established at INL to provide easy access to computational tools, HPC resources, and training. The target audience includes users from the private sector, national laboratories, universities, and federal agencies.

Available computational tools include INL's extensive library of software based on the Multiphysics Object-Oriented Simulation Environment (MOOSE) modeling and simulation framework and are relevant to nuclear energy, advanced manufacturing, and environmental science applications. The NCRC also allows for consolidated user management of INL licensed simulation codes, as well as selected codes developed at other national laboratories or research centers.

3. UTILIZATION

The Sawtooth, Falcon, and Lemhi systems combined delivered more than 630 million core-hours of compute time in FY20. This is an increase of 304 million core-hours from FY19, largely due to the deployment of the new Sawtooth system. The compute time observed exceeded our operational goals.

The average queue size, in terms of the oversubscription factor, is an important measure of demand for computational resources. In FY20, the average oversubscription of Sawtooth was 2.81 (meaning the average queue was 280,639 processor cores for the year. The average oversubscription of Lemhi was 2.38 (queue was 48,036 processor cores). The average oversubscription of Falcon was 1.22 (queue was 42,701 processor cores).

The HPC job scheduler utilizes fair-share metrics along with other considerations for prioritizing work. Given a specific need, users may request higher priority. The scheduler maintains very high overall system utilization while assuring that the most critical work runs first. Total utilization has increased by a factor of ten over the past few years. Figure 3-1 shows the increase of HPC usage from 2011 to 2020.

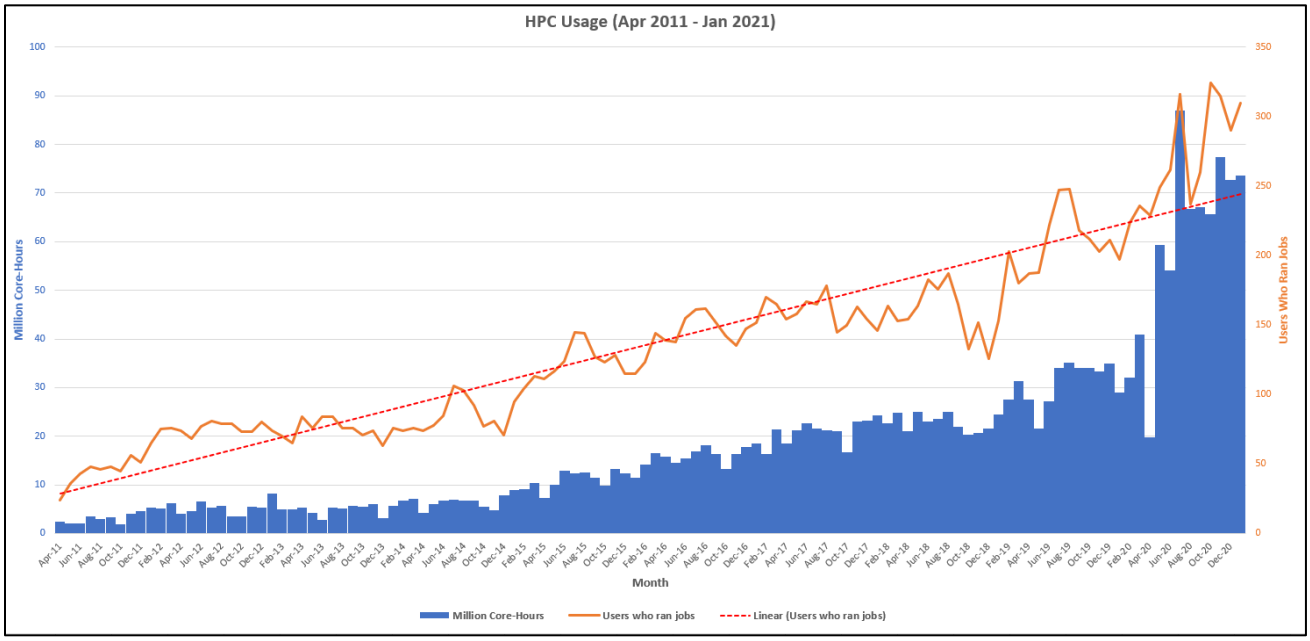


Figure 3-1. HPC utilization for April 2011-2020.

4. USER INSTITUTIONS

The following pages present a summary of institutions utilizing HPC, followed by user-contributed summaries of their modeling and simulation work that made use of INL's HPC resources in FY20. As shown in Figure 4-1, INL HPC capabilities were utilized by 522 researchers during FY20, with the majority coming from National Laboratories (309) using 402.47 million core hours. University researchers/students, as a group, made up the second largest group of users (155) utilizing 180.32 million core hours, while industry partners also accounted for a substantial number of users (58) with 46.03 million more hours.

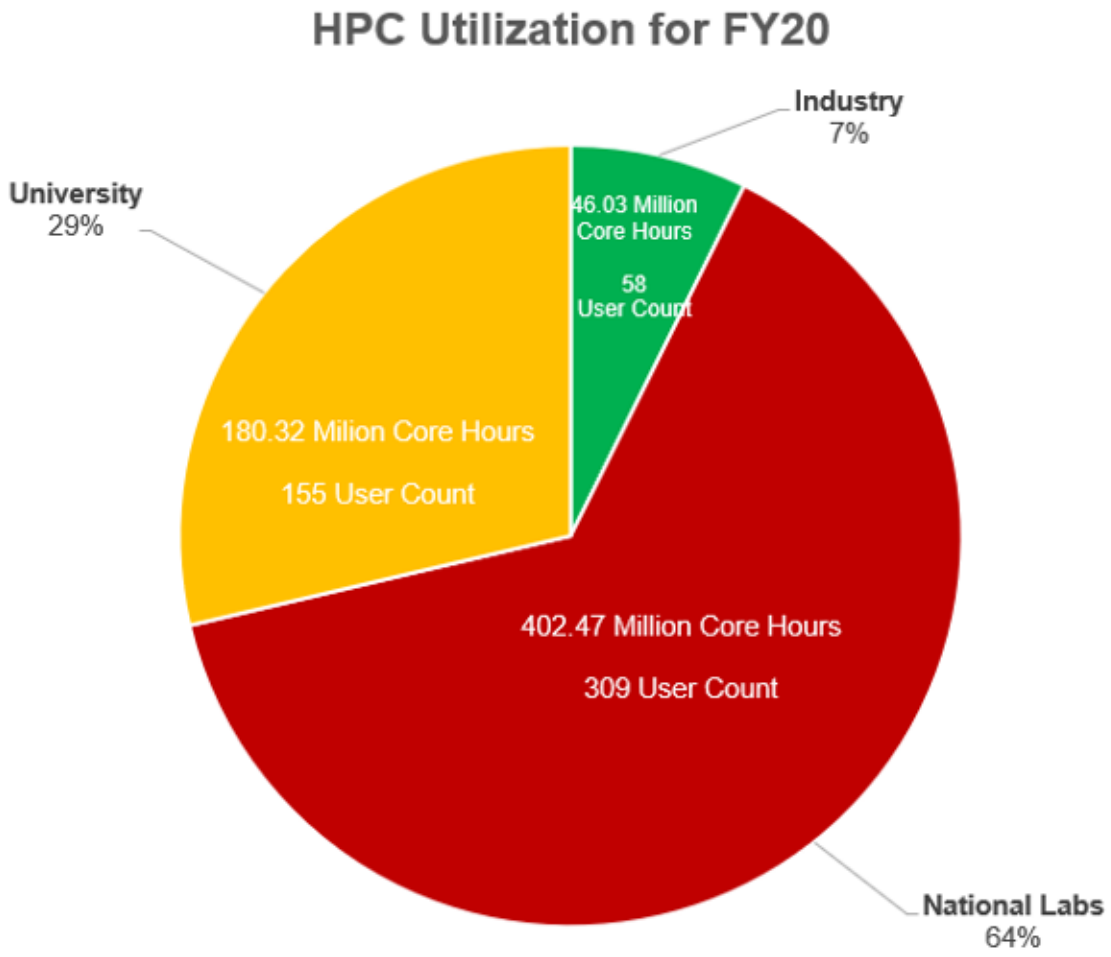


Figure 4-1. HPC utilization for FY20.

Table 1. lists the top thirty organizations with the largest number of active HPC users in FY20. The majority of users coming from the INL (252), followed by the second largest from Naval Nuclear Laboratory (27). The remaining top thirty organizations include a mix of universities (131), industry partners (32) other national laboratories (28), and Nuclear Regulatory Commission (6).

Table 1. Top 30 HPC User Count and Institution Name Utilizing INL HPC Systems

10/01/2019 – 9/30/2020	
Institution	**User Count**
Idaho National Laboratory	252
Naval Nuclear Laboratory	27
University of Idaho	17
Boise State University	16
Idaho State University	16
Oak Ridge National Laboratory	15
North Carolina State University	14
MPR Associates	12
Texas A&M University	11
Argonne National Laboratory	9
Westinghouse Electric Company	9
Massachusetts Institute of Technology	8
University of Michigan	7
Nuclear Regulatory Commission	6
Hewlett Packard Enterprise	5
University of Illinois at Urbana-Champaign	5
Framatome	4
Los Alamos National Laboratory	4
Oregon State University	4
University of New Mexico	4
University of Tennessee	4
Virginia Tech	4
Clemson University	3
Purdue University	3
University of Florida	3
University of South Carolina	3
University of Tennessee Knoxville	3
University of Utah	3
University of Wisconsin	3
Blue Wave A.I. Labs LLC	2

A total of 79 reports were submitted by researchers for this FY20 Annual Report. Reports were grouped in categories based on the primary funding source for the research as shown in Figure 4-2.

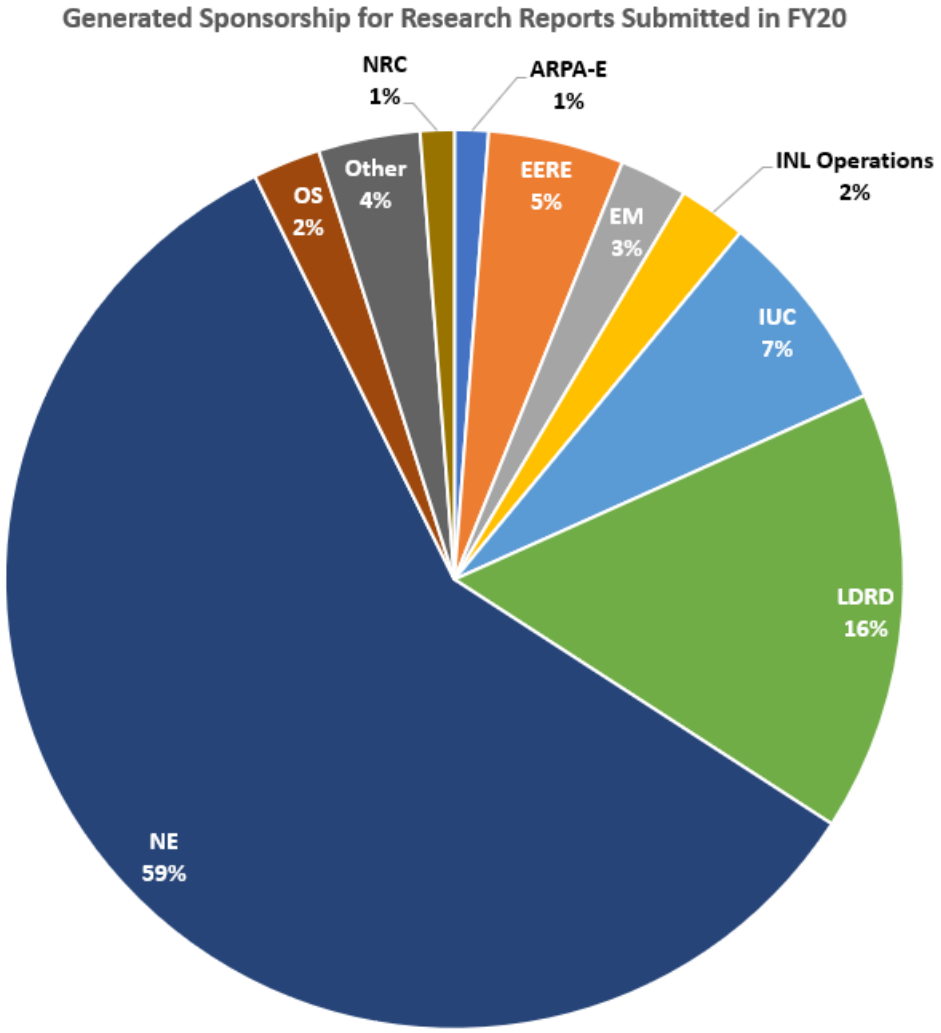


Figure 4-2. Generated sponsorship for research reports submitted in FY20.

The percentages shown on Figure 4-2 have some inconsistencies in the way usage and user data were recorded. In some cases, work was directly supported by a DOE Office (e.g., Office of Nuclear Energy), while other work was supported by other sources such as LDRD or university funding, which taken together make up over 20% of the submitted reports. It is important to note that some of the work conducted using the LDRD or university funding also supported nuclear energy, but our reporting system wasn't configured to differentiate the type of work conducted for these categories. Also note that the user supplied reports only account for a portion of the HPC usage in FY20. Changes are being implemented in FY21 to the reporting system to both capture more information from users and better differentiate HPC usage.

The following appendices highlight a subset of projects that were completed in FY20 by researchers using INL's HPC resources, grouped in categories based on the primary funding source for the research. This research made use of the resources of the HPC INL which is 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.

Appendix A

NUCLEAR ENERGY

Table of Contents

A.1. A Novel Approach for Selecting Dopants in FCCI-Resistant Metallic Fuel Systems

Report Participants

Rabi Khanal[1], Samrat Choudhury[1]

1 University of Idaho

Scientific Achievement

Previous works have proposed the formation of intermetallic compounds of lanthanide fission products within uranium-based metallic fuels with added dopant(s) to arrest fission products within the metallic-matrix, before lanthanides chemically react with cladding materials, leading to the degradation of the cladding. In this project, we proposed ab-initio-based alloy-design principles, which can be useful in identifying dopants that can bind a lanthanide inside the fuel matrix. Based on our principle, we have predicted new dopants, As and Se, that can be effective in binding all lanthanides within the uranium matrix. We have also explored the interactions between various dopants and the lanthanides within the uranium-based metallic fuel for the dopant's effectiveness in binding lanthanide within a uranium-based matrix.

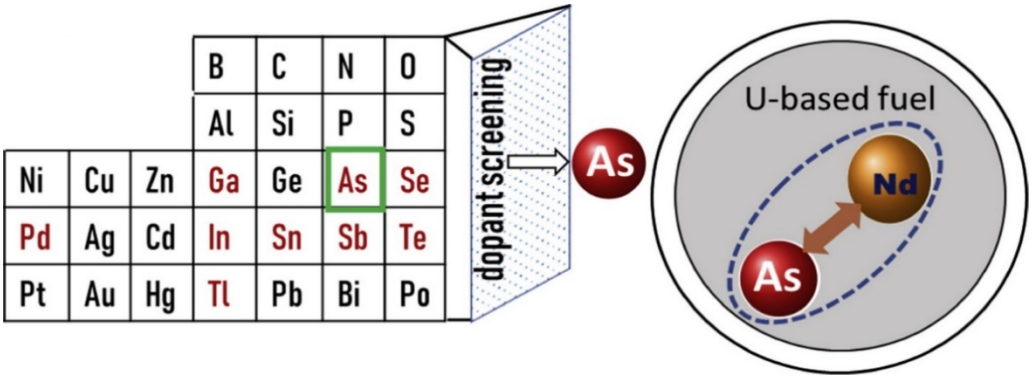


Figure A-1. Schematic diagram showing the screening of a dopant based on the alloy design principle.

Significance

In uranium-based fuels, the production and migration of lanthanide fission products and subsequent chemical interactions with cladding constituents lead to an FCCI, limiting fuel performance. In general, a dopant addition to the fuel matrix to arrest lanthanides within the fuel by forming intermetallics is effective in mitigating FCCI. Previous attempts to choose potential dopants based on lanthanide-dopant binary phase diagrams and macroscopically measured thermodynamic properties (e.g., melting point) had limited success in arresting lanthanides (Ln), plausibly due to the lack of understanding of the chemical and electronic interaction between elements as well as a lack of a comprehensive list of U-Ln-dopant ternary phase diagrams. Alternatively, ab initio calculations can be adapted to predict novel dopants, as they provide a fundamental understanding regarding the electronic structure and chemical interactions between elements, without a particular need for their binary and ternary phase diagrams. In this work, we present a combined ab initio calculation and experimental approach on screening dopants to immobilize Nd, the primary lanthanide fission product. We show that dopants can be screened based on readily available features, such as electronic configuration, electronegativity, and the covalent radius of dopants. Our approach correctly identifies previously known dopants like Pd as well as predicts novel dopants (As and Se), which can bind with the Nd fission product within the U matrix. Overall, this research helps to develop generic alloy-design principles for complex multicomponent systems based on lanthanide and dopant intrinsic characteristics.

Key Publications

- Khanal, R., Jerred, N., Benson, M., Xie, Y., Mariani, R., Charit, I, Choudhury, S., (2020). "Interactions and Immobilization of Lanthanides with Dopants in Uranium-based Metallic Fuels," *J. Nucl. Mater.,* vol. 540, no. 152372. https://doi.org/10.1016/j.jnucmat.2020.152372
- Jerred, N., Khanal, R., Benson, M., Mariani R., Choudhury, S., Charit, I., (2020). "Nd, SbNd and Sb3Nd4 and their interactions with the cladding alloy HT9," *J. Nucl. Mater.,* vol. 541, no. 152387. https://doi.org/10.1016/j.jnucmat.2020.152387
- Khanal, R., Jerred, N., Benson, M., Andersson, D.A., Mariani, R., Charit, I., Choudhury, S. (2020). "A novel approach to selection of dopant to immobilize neodymium in uranium-based metallic fuels," *J. Nucl. Mater.,* vol. 529, no. 151922. https://doi.org/10.1016/j.jnucmat.2019.151922
- Jerred, N., Khanal, R., Benson, M., Perez, E., King, J., Charit, I., Choudhury, S., Mariani R., (2019). "Evaluation of Tellurium as a Fuel Additive in Neodymium-Containing U-Zr Metallic Fuel," *Scientific Reports, vol.* 9, no. 16043. https://doi.org/10.1038/s41598-019-51852-z
- Khanal, R., Ayers, N., Jerred, N., Benson, M., Mariani, R., Charit, I., Choudhury, S., "Role of Zr in Lanthanides-Dopants Interactions within Uranium-Based Metallic Fuels," in progress.

Sponsor/Program

Nuclear Energy University Program

A.2. An Evaluation of the Computational Fluid Dynamics Capabilities in MOOSE

Report Participants

Abdullah Weiss[1], M. Gomaa Abdoelatef[1], Mohammed Ottom[1], Mark Kimber[1], John Peterson[2], Alexander Lindsay[3], Fande Kong[3], Karim Ahmed[1]

1 Texas A&M University

2 Akselos

3 Idaho National Laboratory

Scientific Achievement

The MOOSE framework is a high performance, opensource, C++, finite element toolkit developed by Idaho National Laboratory. OpenFOAM is a free opensource computational fluid dynamics software developed by OpenCFD Ltd. The purpose of this project is to assess the MOOSE capabilities in utilizing the navier stokes equations. Flow over a cylinder CFD problem with laminar flow (Reynolds number of 200) was used. The problem is transient by nature and, thus, requires an extra computational effort. We were able to capture the vortices that happen in the wake of the cylinder using both codes and compared the results. The priminarly results (as long as the sensitivity analysis) shows a good agreement between both codes (MOOSE and OpenFOAM), but further studies need to be taken to examine different Reynolds numbers, geometries, and meshes.

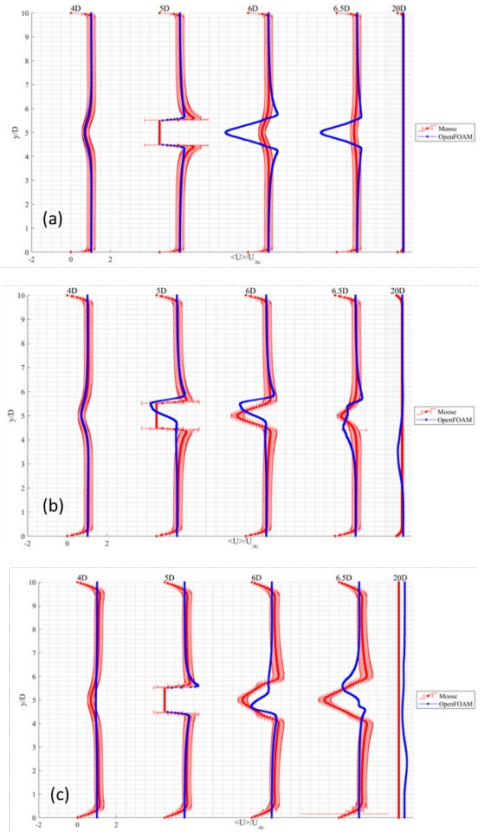


Figure A-2. Comparisons between MOOSE (red) and OpenFOAM (blue) at (a) 0.1 seconds, (b) 1 second, and (c) 5 seconds.

Significance

This project describes one such study to determine the extent to which MOOSE's navier_stokes module can be used for CFD work by running a set of 2D simulations for the CFD problem of flow past a round cylinder. The flow past a cylinder problem is useful in many applications, such as the assessment of flow past a fuel rod in a nuclear reactor or flow past a solid obstacle for aerodynamic foil studies. As such, there are many numerical and experimental solutions available for this problem, making it an ideal problem to benchmark the MOOSE CFD capabilities. In this study, 2D velocity fields as well as pressure and vorticity fields are calculated in the simulation. Additionally, a mesh sensitivity analysis is performed to determine the grid convergence index, and therefore estimate the numerical error in the results. An input sensitivity analysis was also performed with multiple simulation inputs to estimate the input error in the simulation. The errors were analyzed as a function of time and space, showing the evolution of uncertainties in the flow fields and allowing for a visual understanding of the limitations of MOOSE's navier_stokes module. A StarCCM+ simulation has also been run, and its results, alongside some results from literature, are also shown to illustrate how well MOOSE stacks up against results from experiments and other CFD codes.

Key Publications

The proposed manuscript is under preparation for submission and publication.

Sponsor/Program

Nuclear Energy Advanced Modeling and Simulation

A.3. Assessment of Core Performance of Advanced Light-Water Reactor Fuel Concepts in Normal and Accident Conditions

Report Participants

Lap-Yan Cheng[1], Michael Todosow[1], Arantzazu Cuadra[1]

1 Brookhaven National Laboratory

Scientific Achievement

The team performed analyses to assess the characteristics of several accident-tolerant fuel (ATF) concepts for light-water reactors. The study includes neutronics analyses to evaluate the impact on performance parameters (e.g., cycle length/burnup, power distributions), safety-related characteristics (e.g., reactivity and control coefficients/worths, kinetics parameters), and performance in a broad spectrum of transient and accident scenarios (e.g., peak cladding and fuel centerline temperatures).

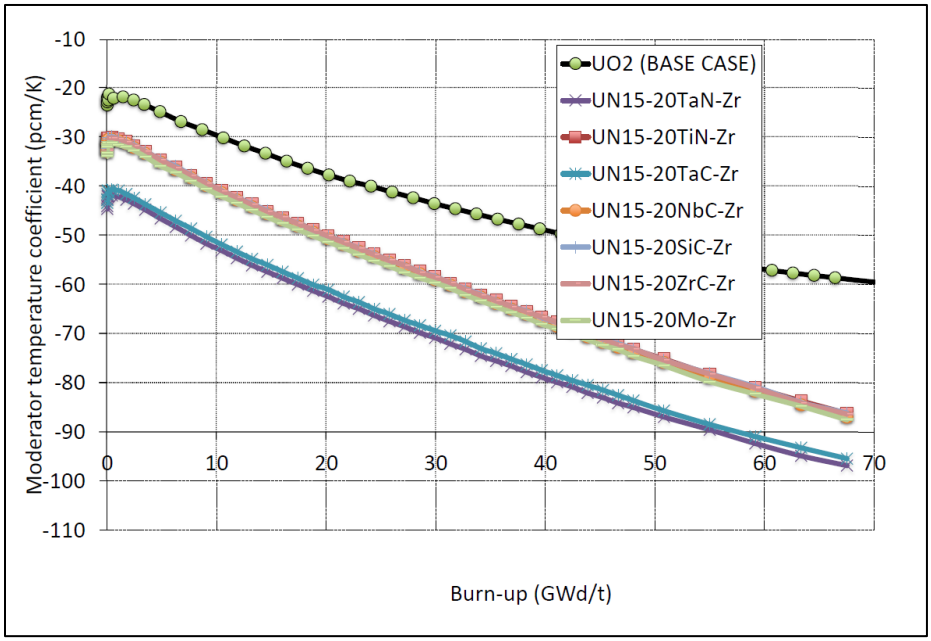


Figure A-3. Moderator temperature coefficient vs. burnup.

Significance

The neutronics and accident analyses are to screen advanced fuel/ATF concepts to ensure that a proposed concept has at least an equivalent performance and safety characteristics relative to current uranium dioxide (UO_2) fuel and zirconium alloy (Zry) cladding as well as offering potential performance or safety benefits. In FY19, the assessment demonstrated the use of an uncertainty analysis (via the TRACE-DAKOTA interface) to inform ATF designers in a systematic and quantitative fashion in how each fuel parameter (thermophysical properties) will impact the figure of merit used in comparing the performance of different design options under accident conditions. In FY20, the assessment evaluated the neutronics impact of coating fuel pellets to mitigate the fuel-coolant interactions for water-reactive high-density UN fuel. Pellet coatings proposed by LANL included TaN, TiN, TaC, NbC, SiC, ZrC, Mo, and Zr.

The assessment of the impacts of advanced fuels on reactor performance and safety characteristics will continue, with a focus on a greater utilization of the multiphysics computational platform provided the Consortium for Advanced Simulation of Light Water Reactors (CASL) suite of codes (e.g., VERA78).

Key Publications

- Todosow, M., Cheng, L-Y., Cuadra, A., "Assessment of Core Performance of Advanced LWR Fuel Concepts in Normal and Accident Conditions–Summary Report on FY19 Activities," BNL-AFC-2019-001, September 27, 2019.
- Todosow, M., Cuadra, A., "Assessment of Core Performance of Advanced LWR Fuel Concepts in Normal and Accident Conditions–Summary Report on FY20 Activities," BNL-AFC-2020-001, September 28, 2020.

Sponsor/Program

Department of Energy Office of Nuclear Energy, Advanced Fuels Campaign

A.4. Assessment of Empirical Interatomic Potential to Predict Thermal Conductivity in ThO_2 and UO_2

Report Participants

Miaomiao Jin[1]

1 Idaho National Laboratory

Scientific Achievement

This study assesses the efficacy of an extensively utilized embedded-atom potential, developed for actinide oxides, to predict phonon mediated thermal transport. This work involves an active interplay between theoretical approaches and experimental results in terms of phonon properties in ThO_2 and UO_2. The accuracy of the potential to represent harmonic and anharmonic interatomic force constants is evaluated by comparing the prediction of phonon dispersion, lifetime, and branch specific thermal conductivity to first-principles calculations and inelastic neutron scattering measurements. The empirical potential can reasonably capture the dispersion of acoustic modes but exhibits significant discrepancies for optical modes, leading to a reduction in the phonon scattering space and the subsequent overestimation of phonon lifetimes and thermal conductivity. This study performs DFT calculations with the VASP package and applys the EP calculation with the LAMMPS package.

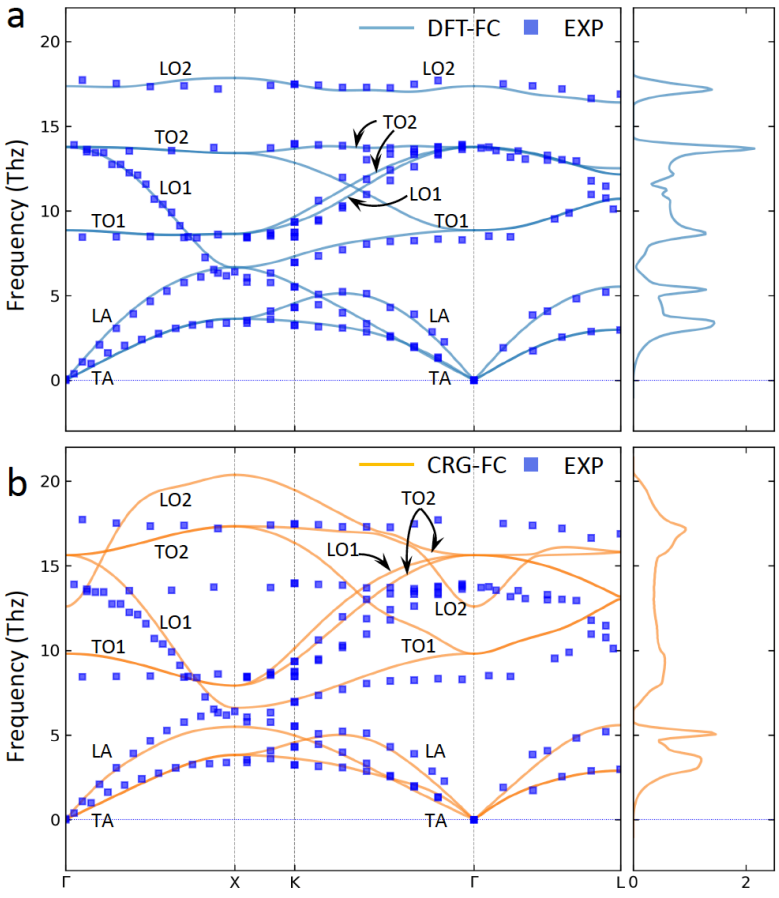


Figure A-4. Comparison of dispersion curve and density of states in ThO_2 from DFT-FC and CRG-FC. The experimental measurements (blue squares) are overlapped for comparison.

Significance

The findings in this work help identify potential shortcomings in previous efforts using this potential to characterize thermal transport. Thses results provide a pathway for the further optimization of potentials to better capture (an)harmonic effects for robust predictions of thermal conductivity in materials with nontrivial defects.

Key Publications

This work has been submitted to the Journal of Physics: condensed matter.

Sponsor/Program

Center for Thermal Energy Transport under Irradiation

Department of Energy, Office of Science, Office of Basic Energy Sciences, Energy Frontier Research Center

A.5. BISON Development and Validation for Priority LWR-ATF Concepts

Report Participants

Kyle A. Gamble[1], Giovanni Pastore [2], Michael Cooper[3]

1 Idaho National Laboratory

2 University of Tennessee Knoxville

3 Los Alamos National Laboratory

Scientific Achievement

This project involved the implementation of lower-length scale-informed models for the fission gas behavior and creep of the accident-tolerant fuel concepts, U_3Si_2 and Cr_2O_3-doped UO_2, into the BISON fuel performance code. The newly developed material models were then used in validation cases from the Halden and Advanced Test Reactors. We completed a sensitivity analysis by coupling BISON to the Dakota software to identify the most influencial fuel performance parameters that affect the output metrics of interest. This study also summarized INL participation in an international benchmark on FeCrAl cladding analysis.

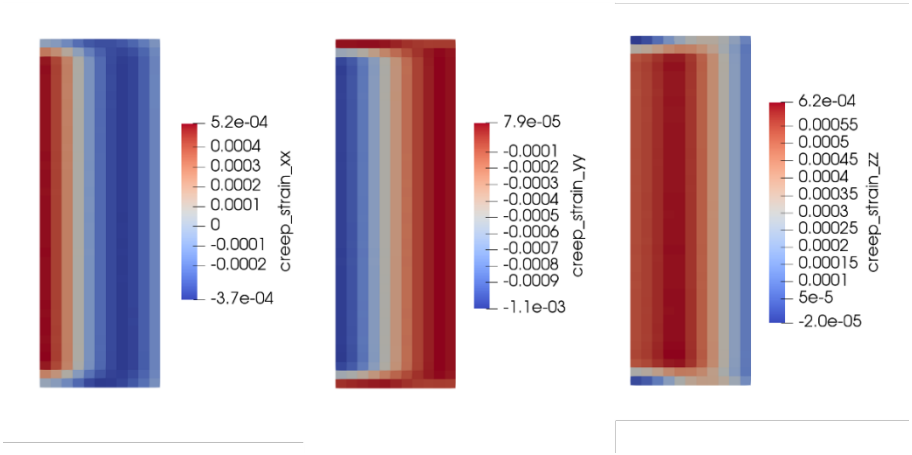


Figure A-5. The creep strain in the (a) radial, (b) axial, and (c) hoop directions within the fuel at the time of cladding failure during a loss-of-cooling accident transient.

Significance

This work helped develop physics-based informed models from first principles in an attempt to describe the physical behaviors of nuclear fuel systems for which limited experimental data exists. These models can than be used to help guide further irradiated experiments and help reduce the uncertainties in modeling predictions. INL authors led the development of the specifications of the international benchmark on FeCrAl cladding performance. The results of this work show a reduction in the uncertainty of fuel concept models that are informed from the lower length scale as well as a good comparison amongst international participants on FeCrAl behavior.

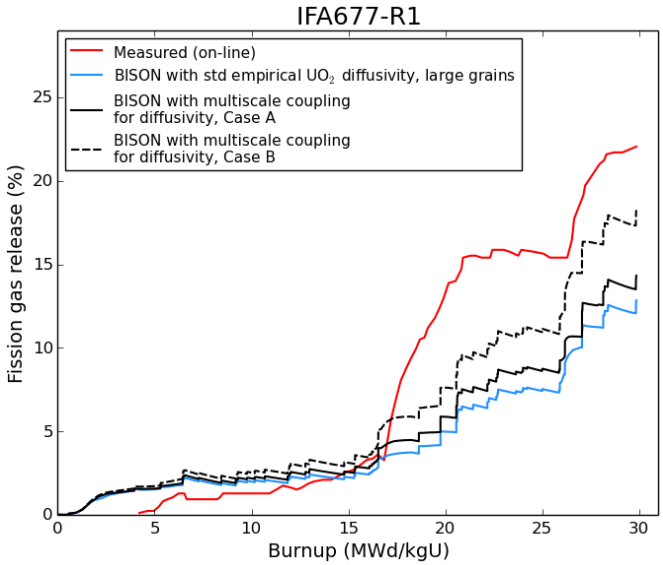


Figure A-6. The measured FGR during the IFA-677 test on doped fuel for IFA-677 Rod 1. BISON results for case A and case B using the multiscale enhanced diffusivity model developed in this work are shown with the black lines. They are compared to results using the standard empirical undoped UO_2 model with large grains (blue lines).

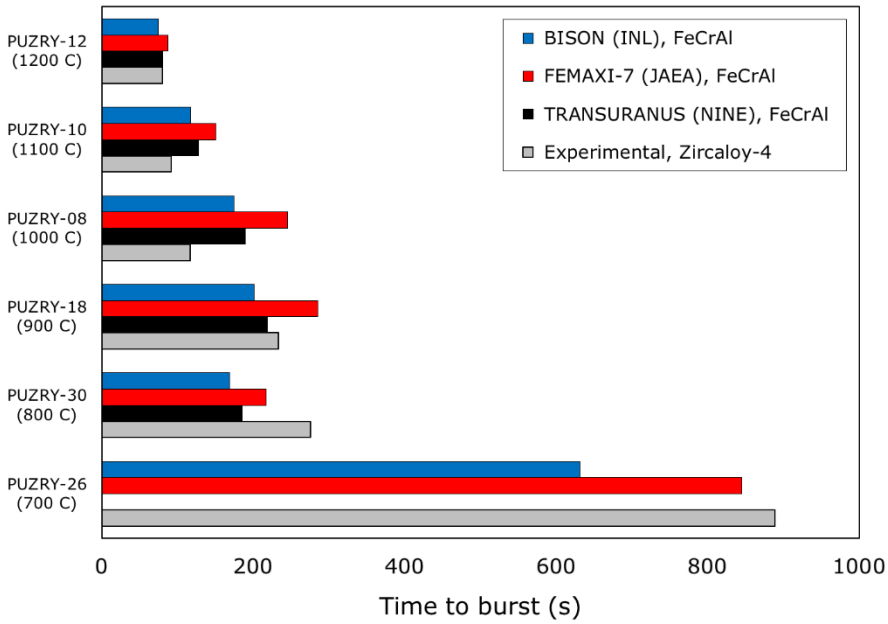


Figure A-7. Time to cladding burst failure for the loss-of-coolant cases (PUZRY cases) in the International Atomic Energy Agency benchmark. Code-to-code comparisons for FeCrAl and experimental data for Zircaloy-4 under the same conditions are illustrated.

Key Publications

- Cooper, M.W.D., Gamble, K.A., Matthews, C., Andersson, D.A., Capolungo, L., Beeler, B., Stanek, C. R., Metzger, K. E., "Irradiation-enhanced diffusion and diffusion-limited creep in U3Si2," https://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-20-24244
- Gamble, K.A., Pastore, G., Cooper, M.W.D., Beeler, B., Aagesen, L. K., Barani, T., Pizzocri D., "Integral validation of BISON U_3Si_2 modeling capabilities including multiscale improvements to modeling fission gas behavior," in progress.

Sponsor/Program

Nuclear Energy Advanced Modeling and Simulation

A.6. BISON Metallic Fuels Benchmark Simulations Based on the X430 Experiments

Report Participants

Ian Greenquist[1], Jeffrey Powers[1]

1 Oak Ridge National Laboratory

Scientific Achievement

To aid in the development of metallic fuel models in the BISON fuel performance code, Oak Ridge National Laboratory is developing a series of benchmark problems based on historical metallic fuels experiments. As part of that effort, Oak Ridge National Laboratory developed two benchmarks based on the X430 series of experiments in the Experimental Breeder Reactor-II (EBR-II).

The X430 experiment series was irradiated in EBR-II between 1987 and 1988 as part of the Integral Fast Reactor program. The experiments were designed to test the irradiation behavior of large-diameter fuel. There were three experiments in the series: X430, X430A, and X430B. After each experiment, the subassembly was disassembled, and postirradiation examination measurements were made on individual pins. Some pins were removed for destructive examination and replaced in the subassembly with fresh pins.

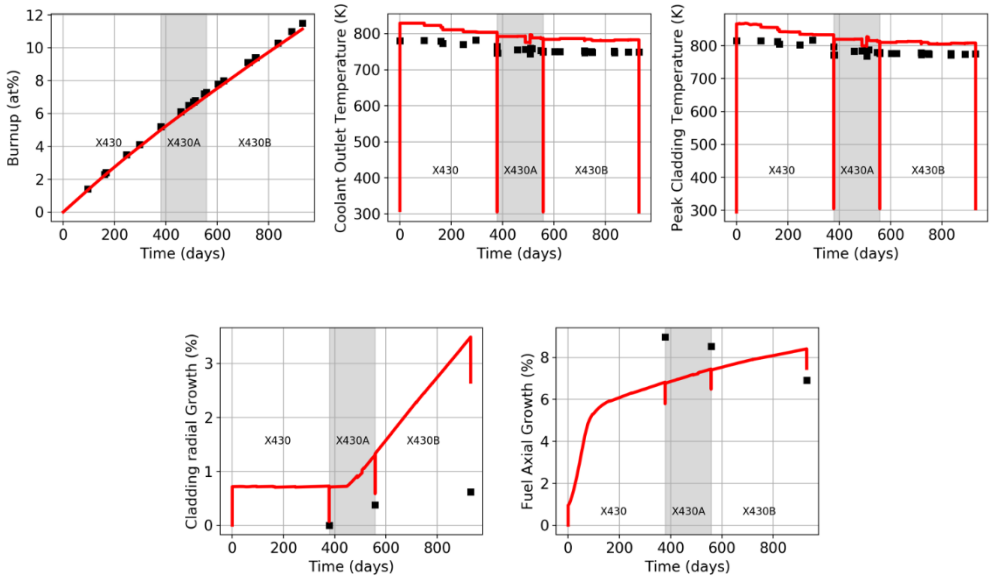


Figure A-8. Comparison of BISON simulation results (red) to experimental data (black) for X430 U-Zr fuel pin T651.

A benchmark problem is a simulation designed to recreate an experiment so that the simulation results can be compared directly against experimental data. The results are used to quantify the accuracy of computational models and to identify models that require additional development.

Significance

Two BISON metallic fuel benchmarks were developed based on pins irradiated in the X430 experiment series (T651, a U-Zr pin; and T654, a U-Pu-Zr pin). The benchmarks were developed using the available experimental data and publicly available materials properties. The BISON simulations accurately predicted the burnup and plenum pressure. The temperature profile was accurate for pins on the interior of the subassembly but was biased by about 35 K on the edge of the subassembly. The cladding radial growth was accurate at low burnup but became less accurate during the last experiment. The predicted fuel axial growth was accurate for U-Zr fuel but did not properly account for U-Pu-Zr fuel.

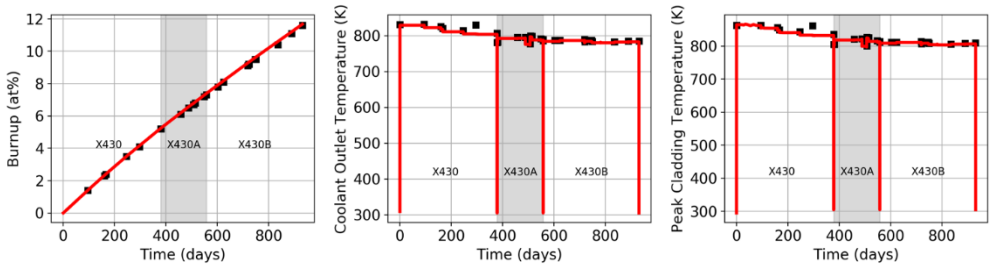


Figure A-9. Comparison of BISON simulation results (red) to experimental data (black) for X430 U-Pu-Zr pin T654.

The near-term development of BISON metallic fuel models should focus on improving the fuel swelling model's dependence on fuel composition. This may take the form of simple correction factors or the derivation of an entirely new correlation depending on the quality and availability of experimental data.

Key Publications

Greenquist, I., Powers, J., "Metallic Fuel Benchmark Simulations Based on the X430 Experiments," United States. https://doi.org/10.2172/1649124.

Sponsor/Program

Department of Energy Office of Nuclear Energy, Versatile Test Reactor Project

A.7. CASL VERA Applications to Departure from Nucleate Boiling Challenge Problem

Report Participants

Yiban Xu[1], Yixing Sung[1], Vefa Kucukboyaci[1], Robert Salko[2]

1 Westinghouse Electric Company LLC

2 Oak Ridge National Laboratory

Scientific Achievement

In support of industry's initiatives for safer and more efficient reactor operation and power generation, CASL has developed the multiphysics code system VERA that couples the neutron code MPACT with the thermal-hydraulic code CTF for addressing the departure from nucleate boiling (DNB) challenge problem. The VERA modeling and simulating capabilities have been demonstrated through the code applications to several DNB-limiting events in increasing complexity. Its results of the main steamline break DNB limiting scenario evaluation confirm the existing conclusion of the plant safety analysis. Its updated version can be used for analyzing DNB transients, such as a complete loss of flow or other flow reduction events.

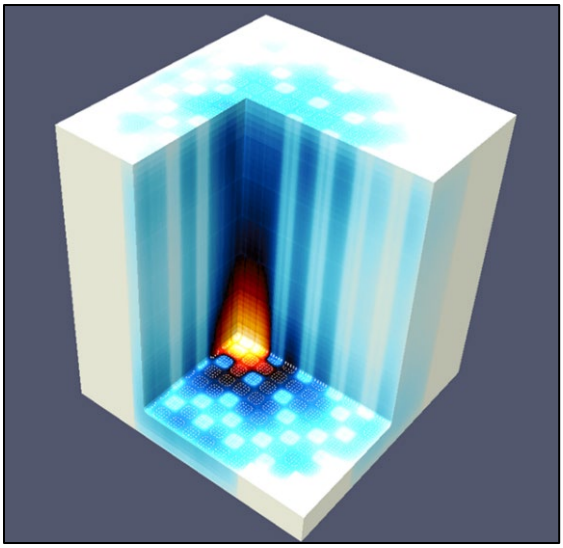


Figure A-10. VERA simulation of reactor core power distribution at DNB limit time step of a main streamline break high flow case.

Significance

As it is subject to continuous improvements and regulatory licensing, the VERA code system is CASL's solution to the DNB challenge problem and provides an advanced tool to the industry for PWR safety analysis and operational support. Based on the results of the study summarized in the paper, one of the potential applications of the VERA code system is to evaluate margin improvement from ATF features without DNB-induced fuel failure under non-loss-of-cooling accident conditions, such as a locked rotor event.

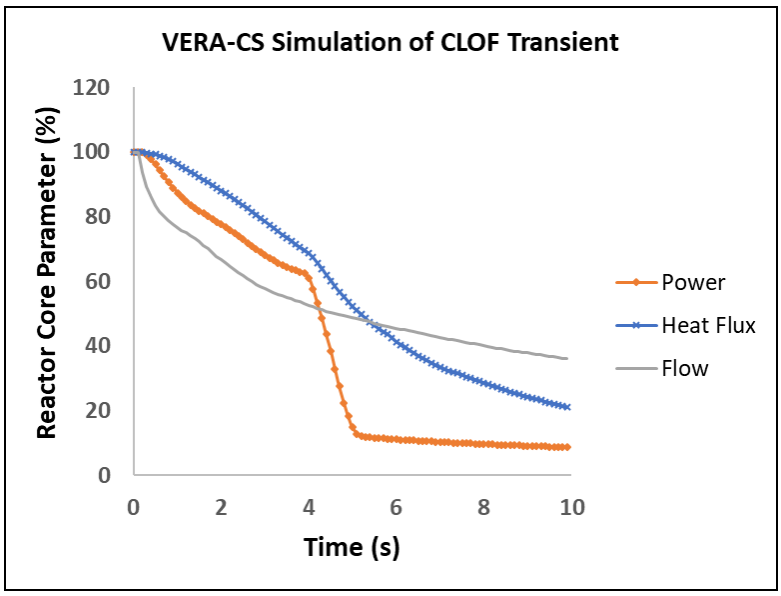


Figure A-11. VERA simulation of a reactor core response during a complete loss-of-flow transient.

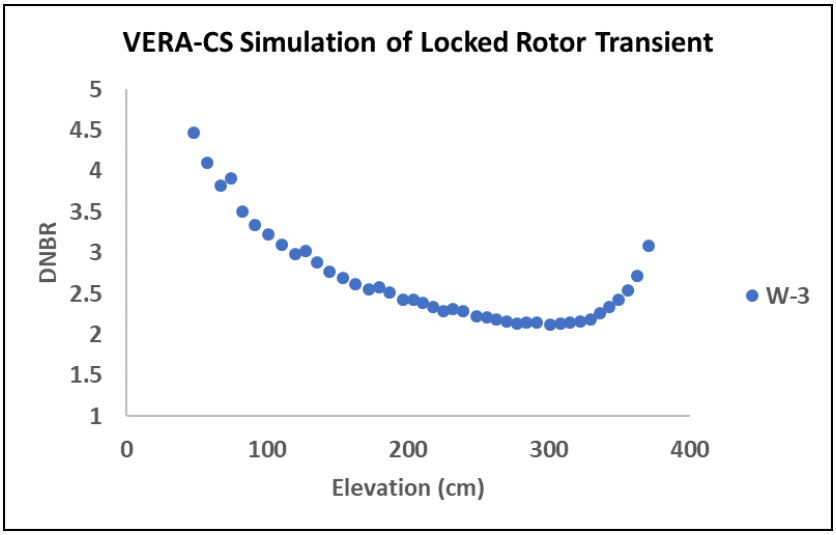


Figure A-12. VERA departure from nucleate boiling ratio vs. hot channel axial elevation at DNB limiting time step of locked rotor event.

Key Publications

- Brown, C. S., Zhang, H., et al., "Best estimate plus uncertainty analysis of departure from nucleate boiling limiting case with CASL core simulator VERA-CS in response to PWR main steam line break event," *Nuclear Engineering and Design*, vol. 309, pp.8-22, 2016. https://doi.org/10.1016/j.nucengdes.2016.09.006
- Xu, Y., Sung, Y. "Validation of Improved CTF Transient Fuel Rod Model, L3:AMA.CP.P18.07," CASL-U-2019-2865, 2019.
- Sung, Y., et al, "CASL VERA Applications to Departure from Nucleate Boiling Challenge Problem," 2020 ANS Winter Conference, CASL Symposium, (in progress).

Sponsor/Program

Consortium for Advanced Simulation of Light Water Reactors

A.8. CFD Modeling of Helium/Air Mixing of a Scaled-Down HTGR

Report Participants

Silvino Balderrama[1], Piyush Sabharwall[2], Richard Christensen[3], Joseph Hafen[3]

1 University of Idaho

2 Idaho National Laboratory

3 University of Idaho

Scientific Achievement

The objective of this work is to develop a CFD model of a scaled-down HTGR facility to perform an air/helium mixing analysis. The numerical data obtained from the simulation will be used to identify the optimal location for a venting system that will be employed during accident scenarios. The University of Idaho recently built a scaled-down HTGR facility to evaluate the performance of the venting system when it is placed at different locations on the containment section. The experimental data will thereafter be used to perform a verification and validation analysis of the CFD model. Once the CFD model has successfully completed the benchmark analysis, the model can be used to simulate other accident scenarios.

Figure A-13. Schematic of a scaled-down HTGR.

Significance

The CFD model obtained from this project is anticipated to provide valuable information about the gas dynamics that take place inside of the containment section of an HTGR. This CFD model, in addition to improving the visualization of helium and air flow patterns, will help identify the optimal position for the venting system.

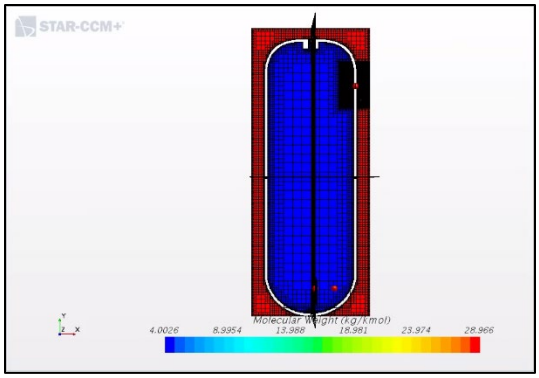


Figure A-14. Initial conditions of a CFD model HTGR.

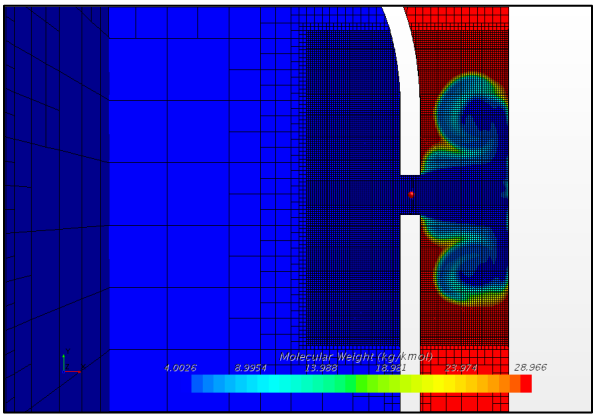


Figure A-15. Contour plot of helium/air mixing inside of containment.

Key Publications

Balderrama Prieto, S. A. (2019). CFD Modeling Update [PPT]. Idaho Falls: University of Idaho.

Sponsor/Program

Nuclear Energy University Program

A.9. Computational Analysis of Advanced Heat Exchanger Configuration for Nuclear Application

Report Participants

SuJong Yoon[1], Piyush Sabharwall[1], Scott Wahlquist[2], Amir Ali[2]

1 Idaho National Laboratory

2 Idaho State University

Scientific Achievement

The project objective is to numerically investigate a novel heat exchanger technology's thermal-hydraulic performance for diverse applications, including nuclear. The innovative technology is based on advancing the existing helical tube and twisted tube type heat exchanger, taking advantage of their established manufacturing capabilities. The innovative design combines both geometries into an oval-twisted helical tube heat exchanger. The modern geometry adds the twist velocity component to the secondary flow induced by the helical shape for a higher heat transfer performance with minimal stagnation points, which results in hot spots.

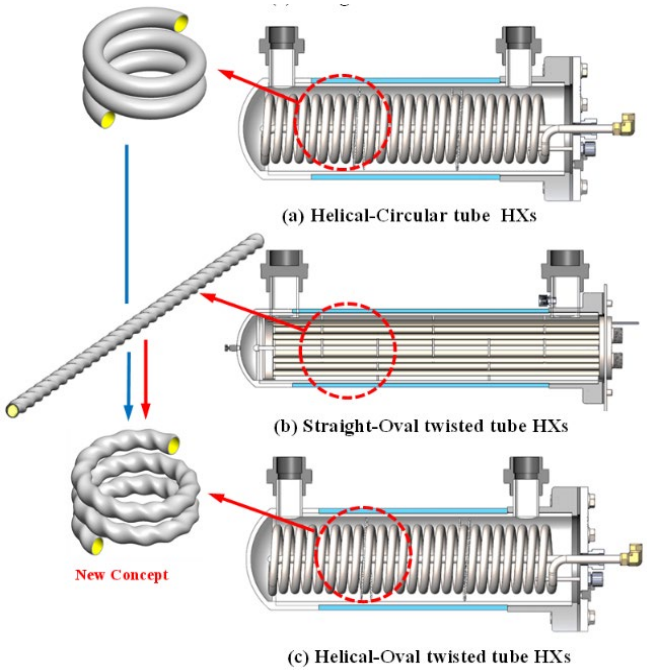


Figure A-16. The development of the new heat exchanger concept.

Significance

The initial results prove the concept, the oval twisted helical tube showed a 10–30% higher heat transfer performance than the individual twisted and helical tube heat exchangers as a passive device (no mechanical involvement is needed). The simplicity of the geometry does not add to the manufacturing cost, as it can be achieved using existing manufacturing tools. Additionally, the innovative technology's compactness seems to reduce the overall material and manufacturing cost by at least 10% compared to existing helical tube heat exchanger technology to achieve the same heat load. The pressure drop remains another concern when a new heat exchanger technology is proposed. The friction factor of the new heat exchanger is compared to the individual heat exchanger technologies available. The new heat exchanger experiences nearly the same pressure drop required to drive flow through the helical tube heat exchanger.

This project is expanding to conduct a parametric study, investigating the device performance and pressure drop's geometrical parameter effects. Advanced reactor prototypical conditions may be considered in further steps of the project and experimental activities, depending on the funding.

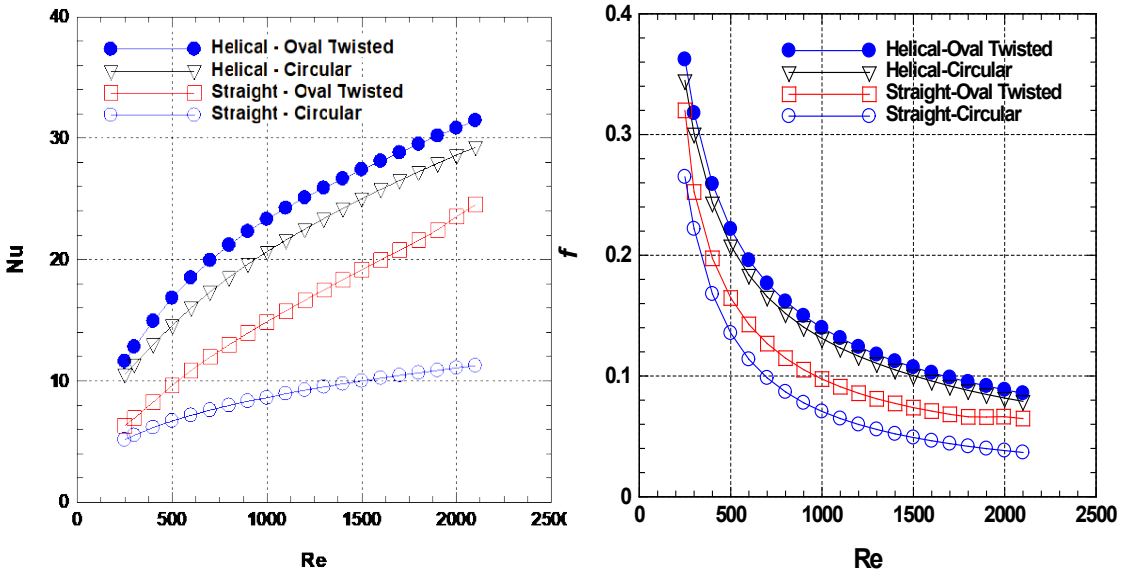


Figure A-17. The heat transfer performance and friction factor of different heat exchanger technologies.

Key Publications

Wahlquist, S., Yoon, S., Sabharwall, P, Ali, A.. "Novel Heat Exchanger Configuration for Enhanced Heat Transfer for Nuclear Applications," Accepted for publication in the American Nuclear Society (ANS), Winter Meeting (2020).

Sponsor/Program

Nuclear Energy

A.10. Computational Discovery of New Additive to Reduce Fuel-Cladding Interaction

Report Participants

Chao Jiang[1], Yi Xie[1], Michael Benson[1]

1 Idaho National Laboratory

Scientific Achievement

In this project, we have performed ab initio evolutionary searches using the variable-composition mode of the USPEX code to construct the state-of-the-art convex hulls for Zr-Bi-Nd and Zr-Se-Nd systems. All density functional theory (DFT) calculations are performed using the VASP code.

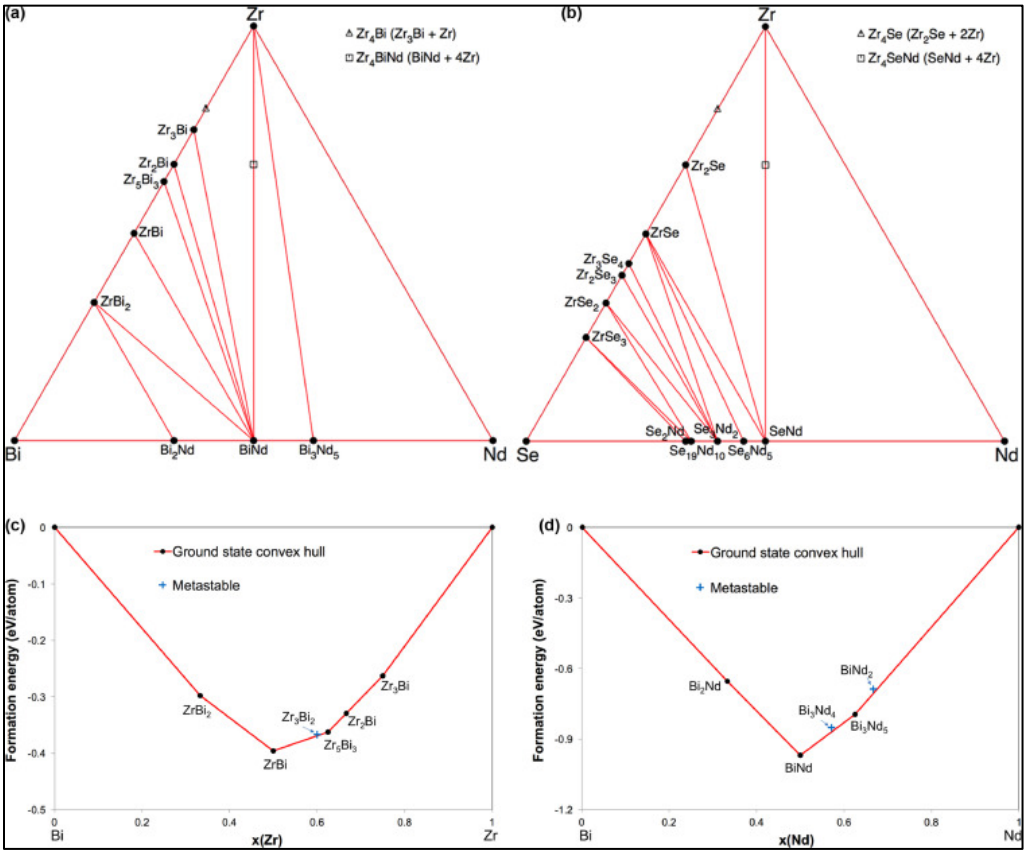


Figure A-18. The DFT predicted convex hulls of (a) Zr-Bi-Nd and (b) Zr-Se-Nd systems. The convex hulls of Bi-Zr and Bi-Nd are shown in (c) and (d), respectively. Filled circles indicate ground state structures that are stable at T = 0 K in these systems.

Significance

The chemical reactions between fission product lanthanides and Fe-based cladding, a phenomenon called fuel-cladding chemical interaction (FCCI), poses a long-standing issue that limits the lifetime and reliability of nuclear reactors. One way to reduce detrimental FCCI effects is by doping metallic fuels with additives that can strongly bind with lanthanides and reduce their mobility and chemical reactivity. Based on the DFT predicted convex hulls for Zr-Bi-Nd and Zr-Se-Nd systems (see Figure A-18), we have discovered Bi and Se as two highly effective lanthanide-binding elements for U-Zr based fuels. The effectiveness of the former has been corroborated by experiments.

Key Publications

Jiang, C., Xie, Y., Benson, M., (2020). "Efficient computational search for lanthanide-binding additive dopants for advanced U-Zr based fuels," *Materialia* 10, 100653. https://doi.org/10.1016/j.mtla.2020.100653

Sponsor/Program

Department of Energy, Office of Nuclear Energy

A.11. Computational Modeling Towards Accelerating Accident Tolerant Fuel Concepts and Determining In-Pile Fuel Behavior

Report Participants

Ember Sikorski[1,2]

1 Boise State University

2 Center for Advanced Energy Studies

Scientific Achievement

This work uses first-principles and AIMD to better understand nuclear materials. The majority of calculations are performed using VASP, and thermoelectric properties are obtained from the BoltzTraP program. Computations include atomic structure optimization, density of states, electron localization function, and partial charge density.

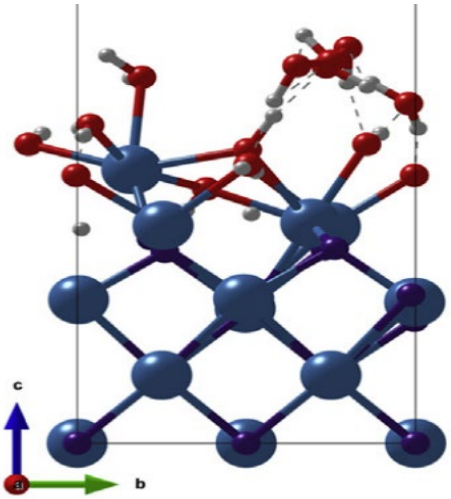


Figure A-19. Initial oxidation of the UN (110) surface.

Significance

This work comprises two main focuses: nuclear fuel and high-temperature irradiation-resistant thermocouples (HTIR-TCs). In nuclear fuel, first-principles work has focused on better understanding uranium nitride (UN) and uranium dioxide (UO_2). Published UN work has probed the starting mechanism of UN corrosion, which would occur in the event of a cladding failure. This work has been recognized by the 2020 Innovations in Nuclear Technology R&D Awards Program. Work is ongoing to determine the magnetic structure of the UN surface. As the magnetic structure treatment has varied across UN first-principles studies, this could lead to discrepancies in understanding corrosion mechanisms and inaccuracies as first-principles values are used to parameterize mesoscale and continuum-scale codes. This work seeks to unify the magnetic treatment in future work. Work is also ongoing in studying UN using AIMD. While first-principles can offer static views into UN corrosion, AIMD should elucidate more dynamic mechanisms as well as incorporate temperature. Work has been conducted in collaboration with experimentalists to better understand the structural properties when metallic additions are used in UN. For UO_2, we have studied amorphous cells to investigate their grain boundary behavior.

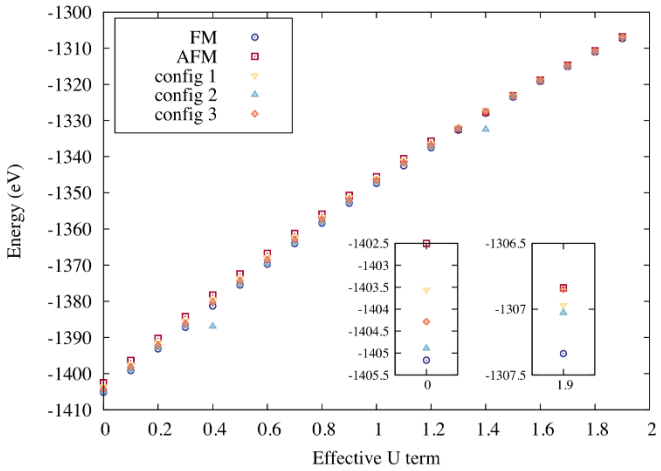


Figure A-20. UN magnetism study demonstrating that ferromagnetism is the most energetically favorable for the entirety of the Hubbard U ramp.

In HTIR-TCs, A collaboration is ongoing with researchers at INL's High Temperature Test Laboratory. We seek to use modeling to better understand the performance of HTIR-TCs in support of their use in research reactors and toward improving their durability and accuracy. Work is nearly complete in predicting the voltage produced by HTIR-TCs across the temperature range they will undergo in-pile. Once the model is complete, the predictive capability will be used to understand performance changes when using different alloys and during in-pile scenarios, such as oxidation, hydrogen uptake, and transmutation. This work should ultimately aid in the material design toward an improved HTIR-TC performance in research reactors, such as ATR and TREAT. This project has received an award for the Best Technical Presentation as part of the 2020 INL Intern Poster Session.

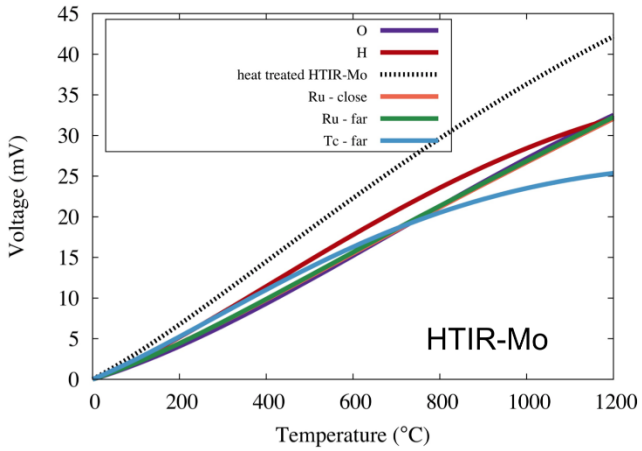


Figure A-21. Proof of concept of HTIR-TC model ability to compare performance of the HTIR-Mo thermoelement after oxidation, H pickup, and transmutation.

Key Publications

- E.L. Sikorski, E.B. Nelson, S.C. Middleburgh, L. Li, "Computational studies of amorphous UO_2 for grain boundary behavior," Top Fuel 2019, Seattle, WA, Sept. 22-27, 2019, Seattle, 2019: pp. 690–694.
- E.L. Sikorski, T.H. da Silva, L.K. Aagesen, B.J. Jaques, L. Li, "First-principles comparative study of UN and Zr corrosion," *J. Nucl. Mater*. vol. 523 pp. 402–412, 2019. doi:10.1016/j.jnucmat.2019.06.017.
- J.K. Watkins, E. Sikorski, L. Li, B.J. Jaques, "Improved Hydrothermal Corrosion Resistance of UN Fuel Forms Via Addition of Metallic Constituents," Top Fuel 2019, Seattle, WA, Sept. 22-27, 2019, pp. 1147–1156.

Sponsor/Program

Center for Advanced Energy Studies

Department of Energy, In-Pile Instrumentation Program

A.12. Computer Modeling of G Phase in Fe-Based Steels

Report Participants

Xianming Bai[1], Brent Hauser[2]

1 Virginia Tech

2 University of Illinois at Urbana-Champaign

Scientific Achievement

The Mn-Ni-Si based G phase is widely found in Fe-based steels during irradiation or thermal annealing. Recently, our experimental team found that a Mn-Ni-Si based G phase can form in δ Fe, which has a body-centered-cubic (bcc) structure, but not in γ Fe, which has a fcc structure. To understand the underlying mechanism, we have conducted density functional theory modeling to calculate the interface energies between the G phase and Fe of different phases.

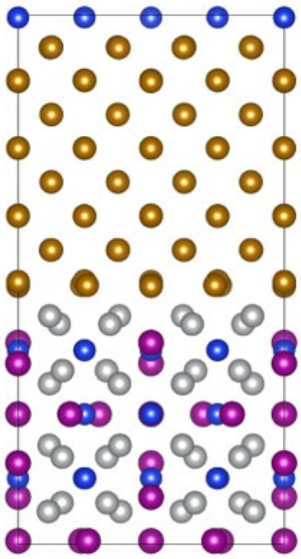


Figure A-22. Interface between Mn-Ni-Si based G phase (bottom) and bcc Fe (top).

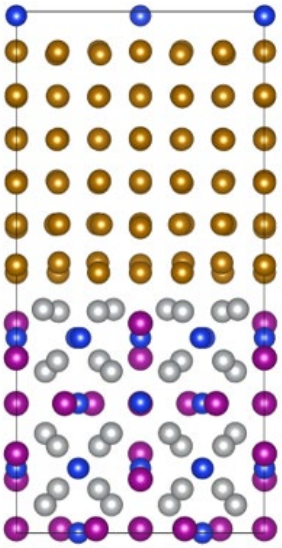


Figure A-23. Interface between Mn-Ni-Si based G phase (bottom) and bcc Fe (top).

Significance

G-phase precipitates play an important role in affecting the mechanical properties of steels. Understanding their formation mechanism is important for predicting their precipitation kinetics in Fe-based alloys. Using density functional theory modeling, our preliminary results show that the interface energy between the G phase and bcc Fe is lower than that between the G phase and fcc Fe. The results provide a science-based explanation for our experimental observations.

Key Publications

No publications yet. These are new and preliminary results.

Sponsor/Program

Nuclear Energy University Program and Idaho National Laboratory Joint Appointment Program

A.13. Consortium for Advanced Simulation of Light Water Reactors

Report Participants

Brendan Kochunas[1], Yuxuan Liu[1], Qicang Shen[1], Sooyoung Choi[1]

1 University of Michigan

Scientific Achievement

During FY20, the CASL project ramped down activities for the project closeout. Professor Kochunas performed calculations on Falcon and Sawtooth to perform full-core pressurized-water reactor assessments of decay heat physics, energy deposition models, more efficient multiphysics iteration schemes, and faster numerical methods for time integration for nuclear reactor applications. This study performed the first-of-a-kind validation of MPACT's pin-resolved solution.

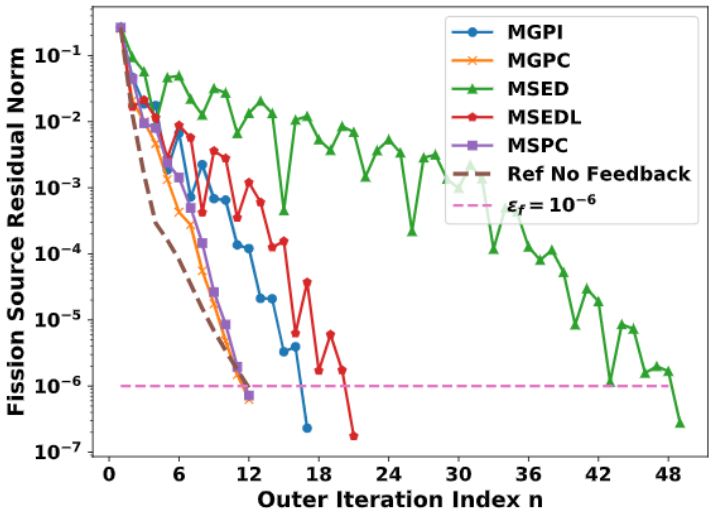


Figure A-24. Improved convergence of relaxation-free iteration schemes (MGPC and MSPC).

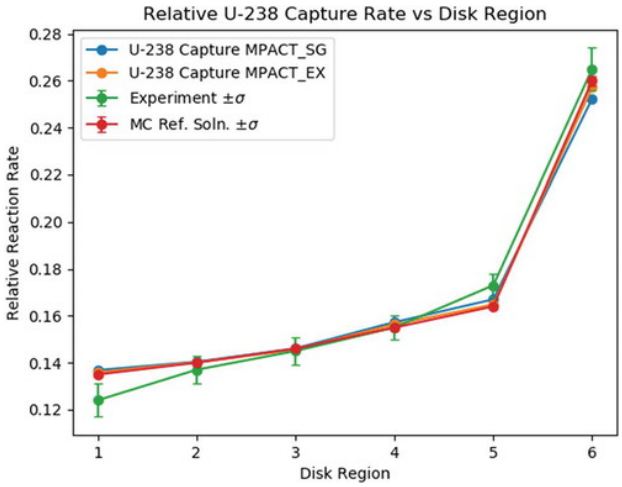


Figure A-25. Sub-pin reaction rate comparisons of MPACT, MCNP, and Experiment in UO2 Pellet.

Significance

This work allowed for reduced uncertainties and increased thermal margins in the analysis of pressurized-water reactor operational cycles and reactivity insertion accidents. Furthermore, the work on the numerical methods reduces the computational resource requirements for all future analyses with VERA. Lastly, VERA has been developed over the past 10 years of CASL and claimed a "pin-resolved" capability—however, this statement was not supported by validation before this work.

Key Publications

- Shen, Q. Kochunas B., (2021). "A Robust Relaxation-free Multiphysics Iteration Scheme for CMFD-Accelerated Neutron Transport k-eigenvalue Calculations I–Theory," *Nuclear Science and Engineering*, submitted.
- Shen, Q., Choi S., Kochunas B., (2021). "A Robust Relaxation-free Multiphysics Iteration Scheme for CMFD-Accelerated Neutron Transport k-eigenvalue Calculations II–Numerical Results," *Nuclear Science and Engineering*, submitted.
- Shen, Q., Kochunas, B., Xu, Y., Downar, T. (2021). "Transient Multilevel Scheme with One Group CMFD Acceleration," *Nuclear Science and Engineering*, in review.
- Liu, Y., Salko, R., Kim, K.S., Wang, X., Kabelitz, M., Choi S., Kochunas, B., Collins, B., Martin, W.R. (2021). "Improved MPACT Energy Deposition and Explicit Heat Generation Coupling with CTF," *Annals of Nuclear Energy*, in review.
- Liu, Y., Vaughn, K., Kochunas, B., Downar, T. (2020). "Validation of Pin-Resolved Reaction Rates, Kinetics Parameters, and Linear Source MOC in MPACT," *Nuclear Science and Engineering*, vol. 195, no. 1, pp. 50-68. https://doi.org/10.1080/00295639.2020.1780853
- Liu, Y., Kochunas, B., Martin, W., Downar, T. (2019). "Delayed fission energy effect on LWR normal operation and transients," *Annals of Nuclear Energy*, vol. 128, pp. 84–93. https://doi.org/10.1016/J.ANUCENE.2018.12.048

Sponsor/Program

Consortium for Advanced Simulation of Light Water Reactors

A.14. Control Rod Ejection Assessment for Limiting Plant

Report Participants

Brenden Mervin[1]

1 Electric Power Research Institute

Scientific Achievement

This work is evaluating a PWR plant that is considered limiting using the three-dimensional, coupled-multiphysics tools of VERA. This type of evaluation will be able to inform the industry and regulator of margins in demonstrating compliance to the proposed limit. In addition to the energy deposition calculations, the evaluation will also include an assessment of high temperature failure potential.

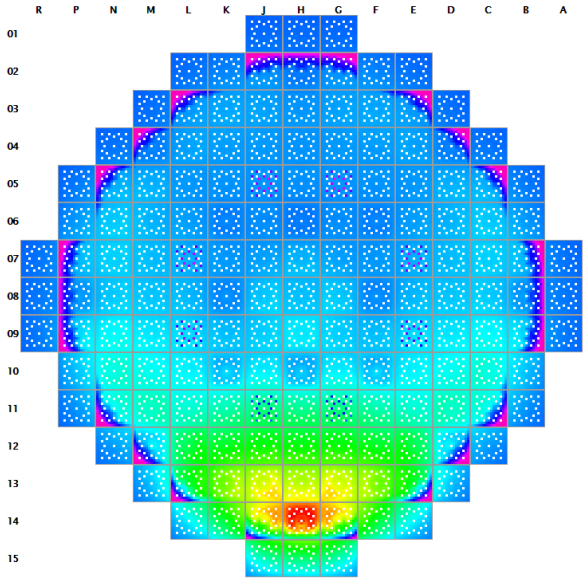


Figure A-26. Margin to fuel enthalpy limit.

Significance

The NRC has recently published a draft guidance on acceptable PWR limits on energy deposition at hot zero power and at power conditions. The proposed guidance includes lower limits on pellet cladding mechanical interaction and new limits on high temperature failure mechanisms relative to the limits based on fresh or low burnup datasets. The final guidance will be implemented on a forward-fit basis; thus, it would not automatically trigger a reanalysis at each plant. As the proposed limits represent a reduction in allowed energy deposition, a multireactor evaluation encompassing a range of plant design and operating parameters would be informative and useful to gauge the fleet performance relative to the proposed acceptance criteria and to inform other evaluations using licensed codes and methodologies.

Key Publications

In progress.

Sponsor/Program

Consortium for Advanced Simulation of Light Water Reactors

A.15. Core Safety Assurance Package Modernization Project—Cascade Reactivity Changes

Report Participants

Matthew Fransted[1]

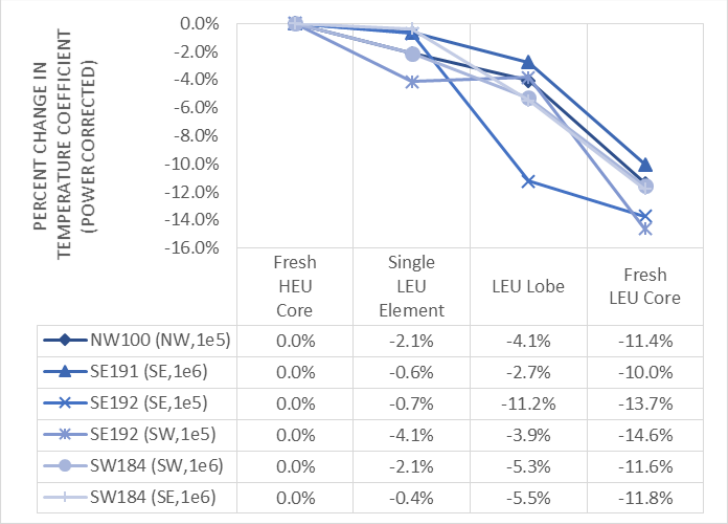
1 MPR Associates, Inc.

Scientific Achievement

This project assess the behavior of cascade reactivity within the Advanced Test Reactor (ATR) flux traps using Naval Nuclear Laboratories MC21 package.

Significance

Prior to every ATR cycle, a core safety assurance package (CSAP) is performed to ensure compliance with safety requirements. ATR reactor engineering (RE) is using MC21 to reassess all existing parts of the CSAP. Part of the CSAP requires the prediction of cascade reactivity worth during the cycle and compares that to the cascade reactivity limits. The changing fuel type in ATR requires a reevaluation of the cascade reactivity values for existing experiments. Initial efforts focused entirely on changes to the temperature coefficient of experiments in the flux traps. Figure A-27 shows that, in all cases, increasing the amount of low enriched uranium fuel elements in the core causes a decrease in the temperature coefficient. Figure A-28 shows the reason for this decrease, where the changes in reactivity due to temperature and density are plotted against each other for a low-enriched uranium fuel and full high-enriched uranium core. The temperature reactivity stays roughly the same, but the density reactivity makes up the full difference between the two. Future work will focus on the changing temperature increases between low-enriched uranium and high-enriched uranium that contribute to the cascade reactivity.



	Fresh HEU Core	Single LEU Element	LEU Lobe	Fresh LEU Core
NW100 (NW,1e5)	0.0%	-2.1%	-4.1%	-11.4%
SE191 (SE,1e6)	0.0%	-0.6%	-2.7%	-10.0%
SE192 (SE,1e5)	0.0%	-0.7%	-11.2%	-13.7%
SE192 (SW,1e5)	0.0%	-4.1%	-3.9%	-14.6%
SW184 (SW,1e6)	0.0%	-2.1%	-5.3%	-11.6%
SW184 (SE,1e6)	0.0%	-0.4%	-5.5%	-11.8%

Figure A-27. Percent change in power corrected temperature coefficients for various experiments within the ATR.

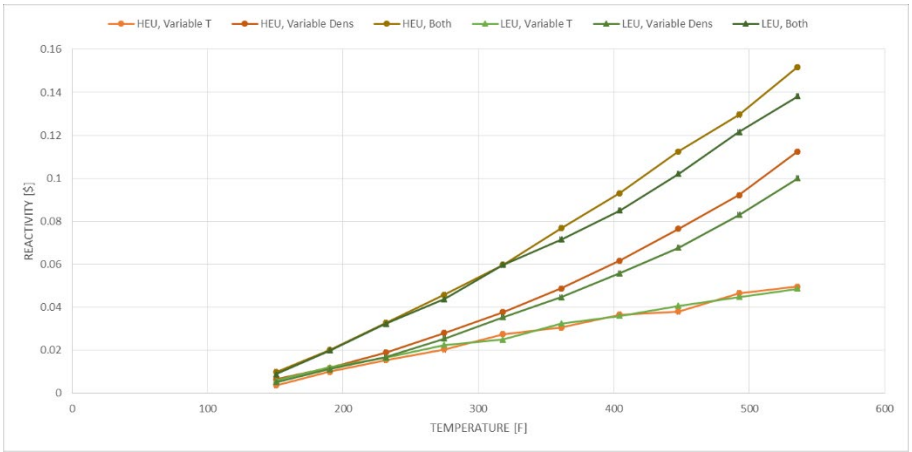


Figure A-28. Reactivity Values used to calculate temperature coefficient using only variable density versus variable temperature.

Key Publications

Expected publication in 2021.

Sponsor/Program

Department of Energy Office of Material Management and Minimization

Idaho National Laboratory's Advanced Reactor Technologies Reactor Engineering Group

A.16. Core Safety Assurance Package Modernization Project– Xenon Behavior Quantification

Report Participants

Douglas Hardtmayer[1]

1 MPR Associates, Inc.

Scientific Achievement

This project assess the behavior of xenon within the core of ATR using Naval Nuclear Laboratories MC21 package.

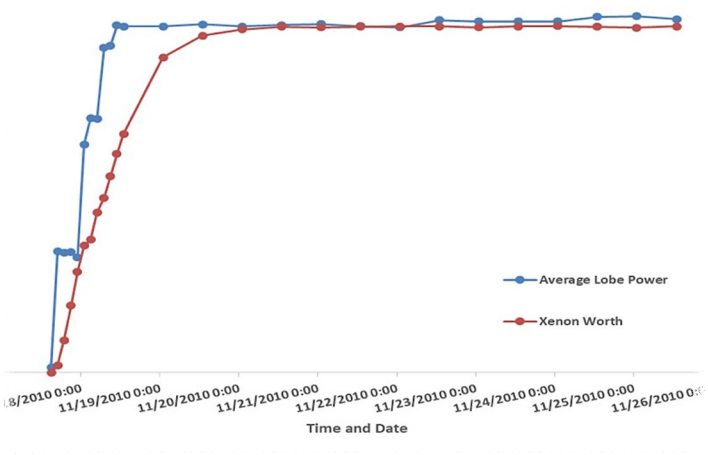


Figure A-29. Xenon worth in the ATR core as a function of time and power (Y-axis labels intentionally removed).

Significance

Prior to every ATR cycle, a CSAP is performed to ensure compliance with safety requirements. ATR RE is using MC21 to reassess all existing parts of the CSAP. Part of the CSAP requires the methodology to predict shim position if xenon is present in significant quantities within the core (called “xenon restarts”). Before MC21 results can be used to justify new methodologies for xenon restarts, MC21 must first be validated. This work justifies MC21’s accuracy when quantifying xenon behavior for the ATR base model. This is shown in Figure A-29, where xenon worth lags behind power increases, which matches physical expectations.

Key Publications

None.

Sponsor/Program

Department of Energy’s Office of Material Management and Minimization

Idaho National Laboratory’s Advanced Reactor Technologies Reactor Engineering Group.

A.17. Davis-Besse Dosimetry Benchmark Using VERA and Shift

Report Participants

Herschel Smith[1,2], Greg Hobson[1], Justin Thomas[1]

1 Framatome

2 BHI Energy

Scientific Achievement

This study evaluated and benchmarked VERA and Shift for use in commercial nuclear reactor *ex* core fluence analysis.

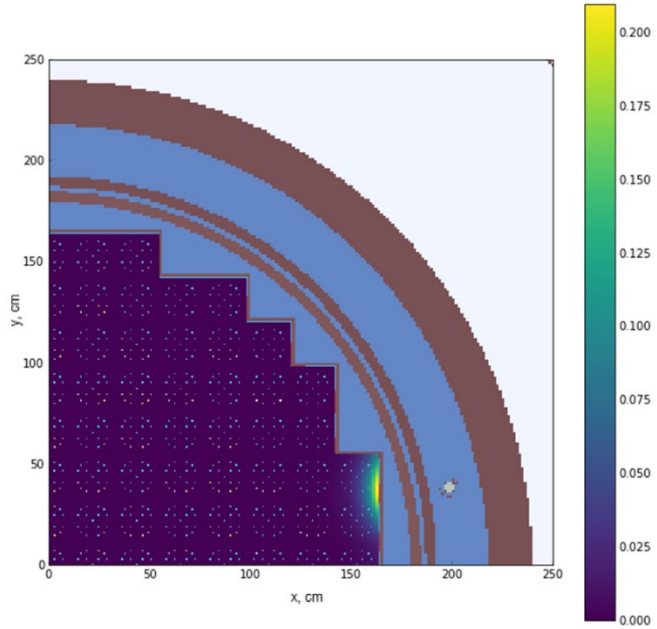


Figure A-30. Shift adjoint flux calculation results.

Significance

VERA provides accurate results for the incore power distributions, core reactivity calculations, and *ex* core analysis neutron source terms of an operating commercial nuclear power plant in the United States. When coupled with the Shift Monte Carlo code, the simulation suite was found to provide accurate predictions of *ex* core dosimeter fluences relative to measured data. An accurate prediction of e*x* core fluence is of continual importance as the US nuclear fleet begins to apply for further life extensions.

Key Publications

H. Smith and G. Hobson, "Davis-Besse dosimetry benchmark using VERA and Shift," ANS 2020 Winter Meeting, The Consortium for Advanced Simulation of Light Water Reactors Virtual Meeting. November 2020.

Sponsor/Program

Consortium for Advanced Simulation of Light Water Reactors

A.18. Determining Local Coordination Environments of Chlorocomplexes in LiCl-KCl Eutectic Mixture Using QMD and Computational Optical Absorption/Raman Spectra

Report Participants

John Fuller[1], Ruchi Gakhar[2], Qi An[1]

1 University of Nevada Reno

2 Idaho National Laboratory

Scientific Achievement

Understanding the coordination environments of transition metals in the LiCl-KCl binary molten-salt system is important for determining the chemical behavior for processes relevant to molten-salt reactors and the electrorefining of spent fuel. In this project, we have applied density functional theory quantum molecular dynamics simulations in conjunction with optical absorption spectra calculations using the HSE-06 hybrid functional to predict the local coordination environment of several 3D and 4D transition metals, which were then compared to experimentally obtained spectra to determine the validity of the calculation method.

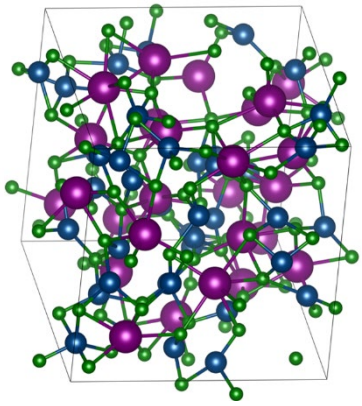


Figure A-31. The computationally obtained LiCl-KCl eutectic composition at 500 C. Blue spheres, green spheres and purple spheres represent Li, Cl, and K atoms, respectively.

Significance

The LiCl-KCl eutectic composition is an important and relatively well researched molten-salt system for both molten-salt reactors and electrorefining applications. Understanding the coordination chemistry of various species introduced via corrosion, contamination, or as fission products in the melt helps to influence more effective material designs for future molten-salt reactors as well as facilitating a better understanding of the electrorefining behavior for pyroprocessing. Several experimental techniques, such as Raman spectral analysis and optical absorption analysis, are well known methods of analyzing the local coordination environment; however, computational methods for determining this coordination behavior are less extensively researched. Experimental research into coordination chemistry in molten salts requires the use of protective equipment, such as gloveboxes, precise temperature control in furnaces, and expensive analytic equipment, while computational analysis provides an attractive alternative to bypass these requirements. Excitonic effects on the absorption spectra and the complexity of molten-salt systems make accurate calculations to determine the optical absorption spectra for molten-salt systems difficult to obtain computationally, while computational Raman spectra require extremely well optimized systems to accurately calculate. However, the use of novel computational techniques here allows for the qualitative identification of the local coordination of chlorocomplexes in the LiCl-KCl eutectic mixture, which

provides an invaluable insight into the structure and coordination environment across extended wavelength and temperature ranges.

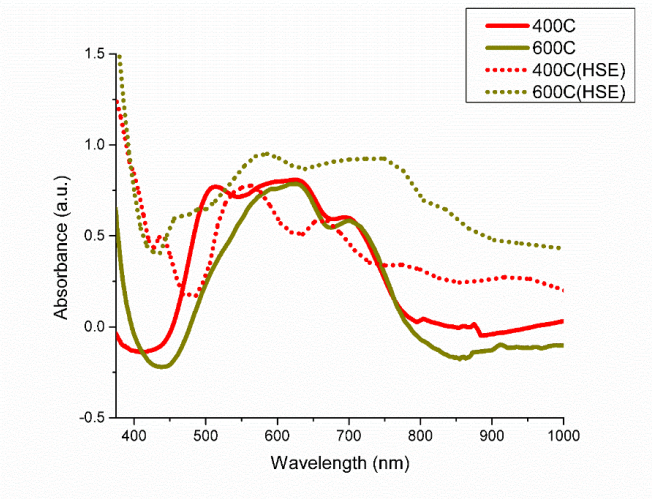


Figure A-32. Experimental and computationally obtained optical absorption spectra of Ni2+ in a LiCl-KCl eutectic melt as a function of temperature. Computational spectra at 400°C and 600°C show moderate correlation with experimental results, with an expected blue shift in the peak location.

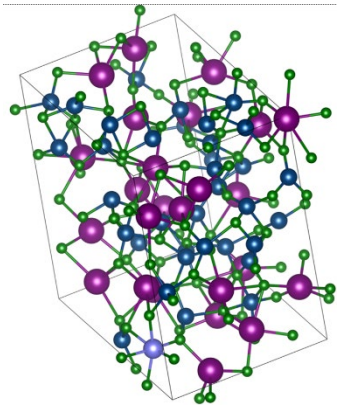


Figure A-33. CeCl3 in a LiCl-KCl eutectic composition; the expected octahedral CeCl63-chlorocomplex is shown in the bottom section (silver sphere is Ce3+) with blue, green, and purple spheres representing Li, Cl, and K atoms.

Key Publications

J. Fuller, W. Phillips, Q. An, R. Gakhar. “Local Coordination Environment of 3D and 4D Transition Metal Ions in LiCl-KCl Eutectic Mixture,” in progress.

Sponsor/Program

Nuclear Energy University Program

A.19. Development of a Mechanistic Hydride Behavior Model for Spent Fuel Cladding Storage and Transportation

Report Participants

Edward M. Duchnowski[1], Seokbin Seo[1], Miles O'Neal[1], Nicholas Brown[1]

1 University of Tennessee, Knoxville

Scientific Achievement

This study demonstrated the implementation of a hydrogen migration and redistribution model in BISON. Two main components, hydrogen diffusion and precipitation kinetics, are assessed using separate effect test simulations. Using the BISON predictions, we retrieved the concentration-penetration curve of hydrogen and estimated the diffusion coefficient.

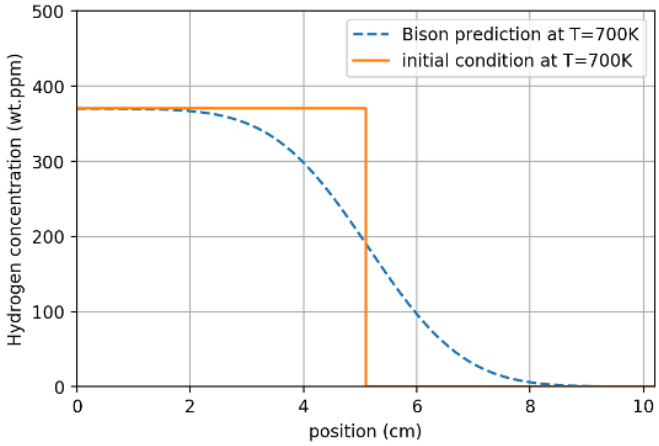


Figure A-34. BISON prediction of hydrogen concentration evolution as function of the position.

We validated the prediction of hydrogen distributions using historical experiments and ongoing experiments conducted within the scope of project. We tested both the existing and the improved hydrogen models using the same simulations under both experimental conditions.

Significance

The study found that the BISON predictions of the diffusion behavior of hydrogen in zirconium is in reasonable agreement with the experimental data. The BISON prediction of the precipitation kinetic parameters in comparison with experimental data shows that BISON closely follows the historical data. BISON accurately predicts the total hydrogen distribution along the sample where the concentration increases towards the colder regions.

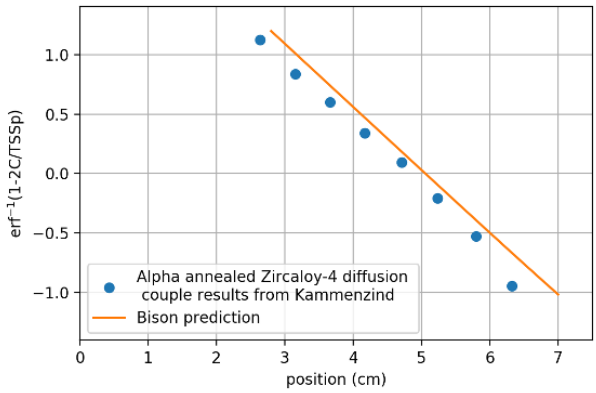


Figure A-35. BISON prediction of hydrogen diffusion in solid solution.

The improvement in the precipitation and dissolution kinetics of the BISON model, referred to as the hydride nucleation-growth-dissolution model, appeared in the prediction of hydrogen distribution during historical and ongoing experiments, showing that the new model was successfully implemented into BISON.

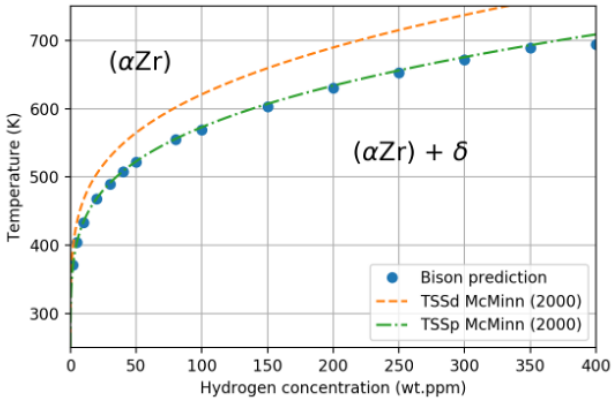


Figure A-36. BISON predictions of the precipitation behavior.

Key Publications

- Aly, Z., Casagranda, A., Pastore, G., Brown, N. R. (2019). "Variance-based sensitivity analysis applied to hydrogen migration and redistribution model in Bison. Part I: Simulation of historical experiments," *Journal of Nuclear Materials*, vol. 524, pp. 90-100. https://doi.org/10.1016/j.jnucmat.2019.06.035
- Aly, Z., Casagranda, A., Pastore, G., Brown, N. R. (2019). "Variance-based sensitivity analysis applied to the hydrogen migration and redistribution model in Bison. Part II: Uncertainty quantification and optimization," *Journal of Nuclear Materials*, vol. 523, pp. 478-489. https://doi.org/10.1016/j.jnucmat.2019.06.023
- Seo, S., Duchnowski, E.M., Brown, N.R. (2020). "The Impact of Model Parameters and Local Conditions on the Hydrogen Migration and Redistribution Model in Bison," Proceedings of ANS Annual Meeting 2020, June 8–11.

Sponsor/Program

Department of Energy

A.20. Diffusion of Lanthanides Elements in the Metallic Nuclear Fuel

Report Participants

Fergany Badry[1], Yipeng Gao[1], Larry Aagesen[1]

1 Idaho National Laboratory

Scientific Achievement

A computational approach that combines finite element and phase-field methods was developed to determine effective diffusion coefficients for lanthanide elements in metallic fuel.

The developed model is applied to some simple cases, mainly, one, four, and sixteen bubbles with periodic distribution. According to the produced results, the effective diffusion coefficients increase as the gas bubble volume fractions increase. Based on the obtained results, the increasing trend is nonlinear where it is identical to the increasing behavior of the gas bubbles surface area fraction; which means that the effective diffusion coefficients' behavior is dominated by the surface area.

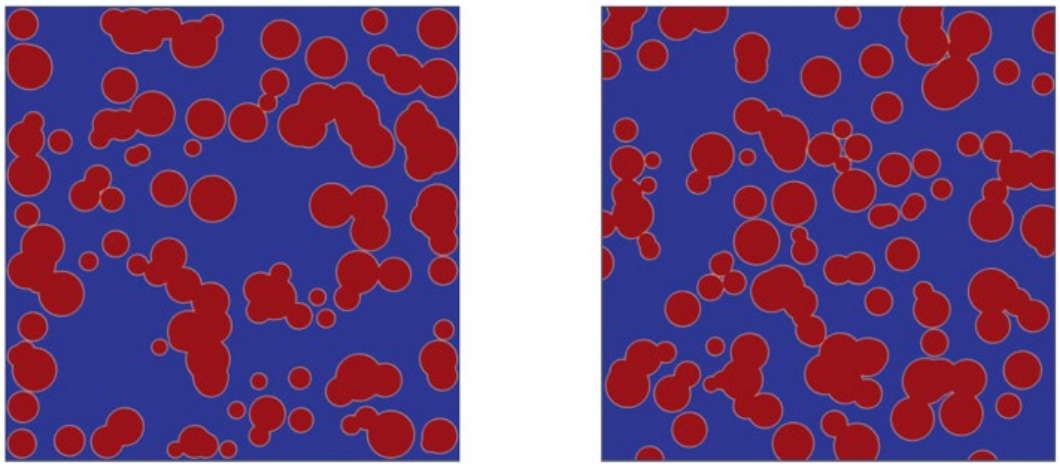


Figure A-37. Snapshots for the dispersed random bubbles without (left image) and with (right image) alignment with the domain boundaries, respectively.

The simulations were expanded to include gas bubbles with random distributions with and without alignment with the domain boundaries. Additionally, a comparison between three different approaches (a direct method based on Dirichlet boundary conditions, a direct method based on Neumann boundary conditions, and a homogenization method) was completed. Based on this comparison, the direct method based on the Dirichlet boundary conditions was proven to be the most reliable and accurate approach of the three.

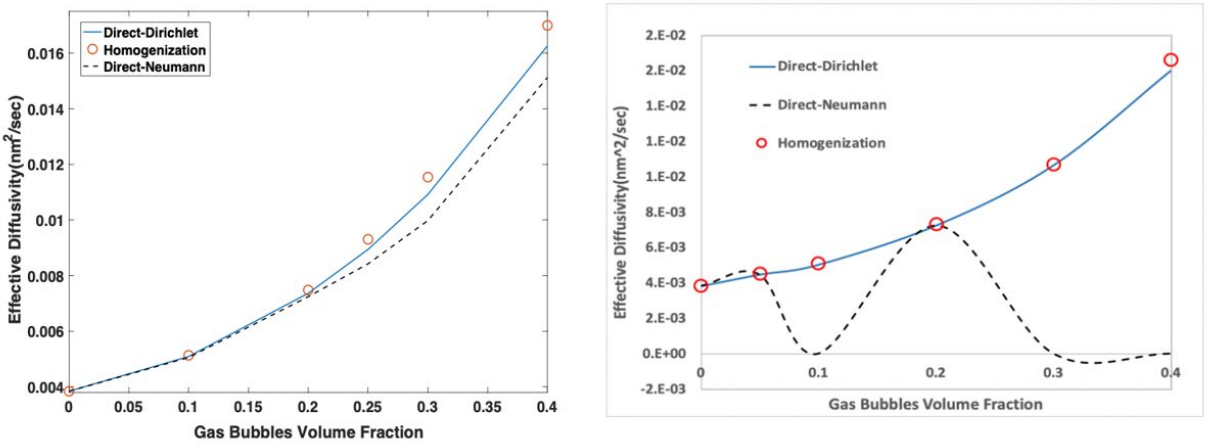


Figure A-38. Effective diffusivity coefficients based on different methods for random distributions of gas bubbles with (left image) and without (right image) alignment with the domain boundaries, respectively.

Significance

One of the main challenges of using metallic fuels is the fuel-cladding chemical interaction, which can trigger when the fuel swells and contacts with the cladding. As the fuel swells during burnup, the interdiffusion between the fuel and cladding materials leads to the formation of a complex multiphase interaction region on the fuel-clad interface, which brittles the cladding and reduces the melting point of the fuel periphery. To mitigate the fuel-cladding chemical interaction and enhance the stability and the accident tolerance of the fuel system, a fundamental understanding of lanthanide diffusion in metallic fuels is essential.

Key Publications

Badry, F., Gao, Y., and Aagesen, L. (2020). "Mesoscale modeling of effective diffusion coefficients of lanthanides in the alpha phase of U-Zr fuel," in progress.

Sponsor/Program

Nuclear Energy Advanced Modeling and Simulation

A.21. Evaluation of Metal Fuel for Use in Light Water Reactors Utilizing the BISON Code

Report Participants

Wenfeng Liu[1]

1 Structural Integrity Associates, Inc.

Scientific Achievement

The nuclear industry wants to enhance the accident tolerance and improve the fuel utilization of LWRs. This could be achieved through innovative fuel designs. One proposed fuel concept is the use of metallic fuel (uranium zirconium alloy) in LWRs. The desired characteristics of high flow rate, low operating temperature, and fewer modifications to power plants make this attractive for near-term deployment. However, it may take decades to generate data from experimental irradiation programs to qualify the use of metal fuel and even longer to find out performance issues from operation. Therefore, it is important to develop analytical tools for the utility customers and the nuclear regulators to perform quantitative evaluations to foresee potential problems, which in turn may improve the fuel designs.

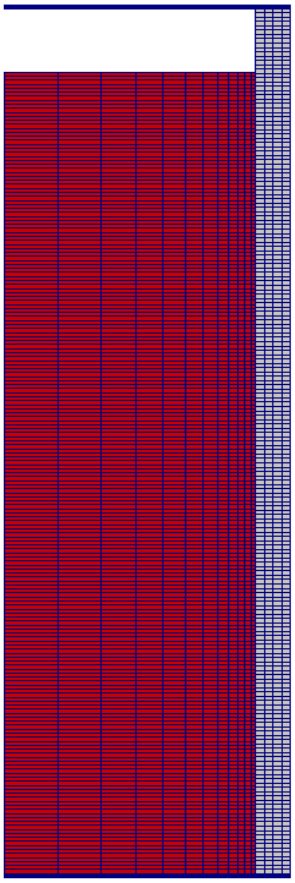


Figure A-39. Finite element mesh used for the PWR REA case.

Significance

This project would leverage the modeling and simulation capabilities developed from the NEAMS and CASL programs to assist fuel qualification and licensing activities. In particular, the BISON fuel performance code developed at INL, with participation from participants in this FOA proposal, will be used as an analytical simulation of metal fuel behavior in an LWR environment. New material and behavior models will be developed and implemented in BISON to provide the needed capabilities for the high-fidelity performance evaluation of metal fuel under normal operations, anticipated operational occurrences and accident conditions. The models and general methodology will be documented in a detailed report.

Key Publications

W. Liu, A. Mai, J. Alvis, J.Y.R. Rashid, C. Folsom, Richard L. Williamson, “Bison Application to the Analysis of LWR Fuel Responses Under Accident Conditions,” Global Top Fuel, 2019.

Sponsor/Program

Industry

A.22. High-Enrichment Fuel Simulations and Benchmarks

Report Participants

Gary Mangham[1], Fausto Franceschini[1], David Salazar[1]

1 Westinghouse Electric Company, LLC

Scientific Achievement

The goal of this project is to benchmark Westinghouse tools to MPACT, SHIFT, and SERPENT for standard fuel lattices with 235U enrichments greater than 5%.

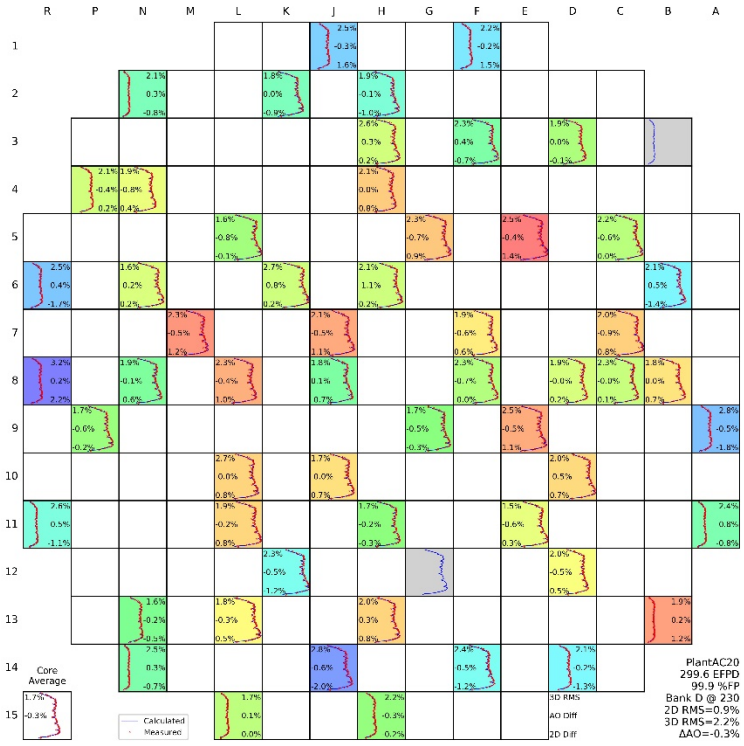


Figure A-40. Comparison of full power measured-to-predicted 2D and 3D reaction rates for plant A.

Significance

This study demonstrated, using the INL HPC resources, the ability of the VERA code suite to accurately predict key physics parameters in currently operating PWRs of various types loaded with a variety of fuel designs. Favorable comparisons between predictions and plant measurements are essential in promoting the uptake of these advanced tools by the industry. Current work extends this benchmarking to investigate the code-to-code comparisons of future novel ATF and high-burnup, high-enrichment fuel applications. The results of these calculations are expected to support the implementation of advanced nuclear fuel products to benefit the U.S. commercial nuclear industry through an improved safety performance and economic efficency.

Key Publications

Gary Mangham et. al. “VERA Benchmarking of PWR Startup and Steady State Operation,” 2020 ANS Virtual Winter Meeting

Sponsor/Program

Consortium for Advanced Simulation of Light Water Reactors

Nuclear Energy Advanced Modeling and Simulation

Light Water Reactor Sustainability

Industry

A.23. Improving the Fission Gas Release Prediction of Doped UO_2 Fuel in BISON Using Variational Bayesian Monte Carlo

Report Participants

Yifeng Che[1], Koroush Shirvan[2]

1 Massachusetts Institute of Technology

Scientific Achievement

Dopants in UO_2 fuel can effectively promote grain growth and suppress the fission gas release (FGR) under transients, reducing the failure risk of fuel rods. Accurate modeling of doped UO_2 fuels requires the accurate prediction of FGR, which is an essential part of the fuel performance analysis for its feedback on the overall fuel rod thermomechanical behavior. The current work improves the BISON FGR model for chromia/alumina-doped UO_2 fuel by statistical calibration with in-reactor experimental data. Due to the complicated operating condition of the Halden data and correspondingly high computational cost in BISON, we introduced Variational Bayesian Monte Carlo (VBMC) as a low-cost nonintrusive approach. VBMC achieves a similar accuracy to the conventional statistical methods but has a far superior efficiency.

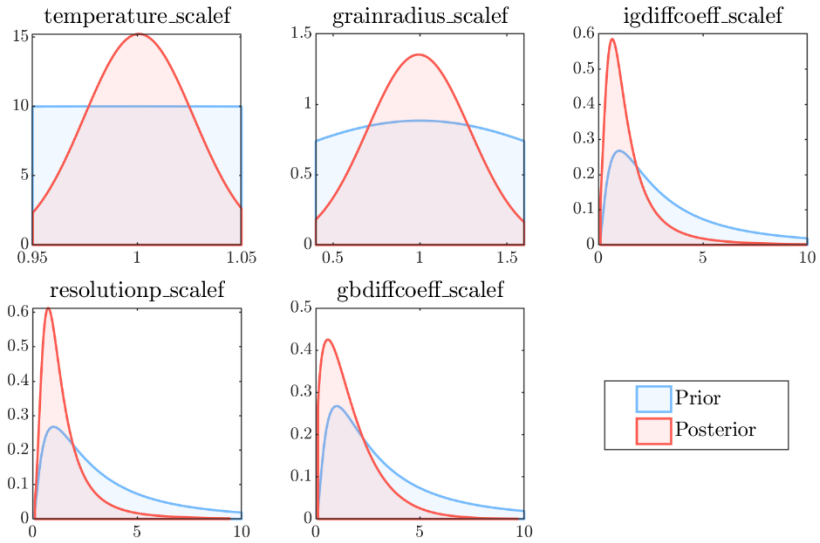


Figure A-41. Comparison of priors and posteriors obtained from VBMC.

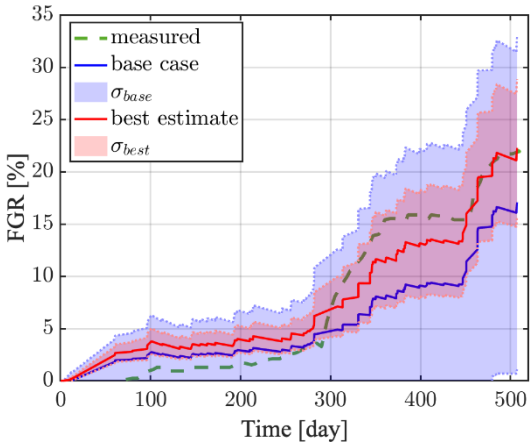


Figure A-42. BISON prediction of an FGR time-series using the nominal values (blue) and calibrated values (red).

Significance

This work not only provides a best-estimate of the uncertain parameters in the FGR model, but also updates the uncertain ranges for each uncertain parameter during the inverse-UQ process, which benefits the future uncertainty quantification for the overall fuel performance analysis. Such information becomes especially useful to demonstrate the enhanced safety for accident-tolerant fuels. This work also provides a demonstration of VBMC as an effective Bayesian inference method for computationally expensive black-box codes like BISON.

Key Publications

- Che, Y., Wu, X., Pastore, G., Li, W., Shirvan, K. (2020). "Application of Kriging and Variational Bayesian Monte Carlo Method for Improved Prediction of Doped UO_2 Fission Gas Release," *Annals of Nuclear Energy*, under review.
- Che, Y., Wu, X., Pastore, G., Li, W., Shirvan, K. (2020) "Application of Variational Bayesian Monte Carlo Method for Improved Fission Gs Release (FGR) Prediction of Doped UO_2 Fuel," oral presentation at TMS 2020, San Diego, February 23-27.

Sponsor/Program

Nuclear Energy University Program

A.24. IRC Reactor Metrology

Report Participants

Tommy Holschuh[1], Scott Watson[1], David Chichester[1]

1 Idaho National Laboratory

Scientific Achievement

This study aims to accurately model a high-purity germanium (HPGe) detector in support of the Transient Reactor Test (TREAT) facility and ATR experiments. The fission product and activation product analyses are integral to understanding the power coupling factor in TREAT and the neutron energy spectrum in TREAT and ATR. The INL HPC resources enable the use of high-fidelity Monte Carlo N-Particle (MCNP) simulations to determine the absolute detector efficiency to correct for geometric differences between samples during the measurement of an irradiated material. The development of accurate HPGe models will allow for the full simulation of an experimental measurement prior to an execution of the work.

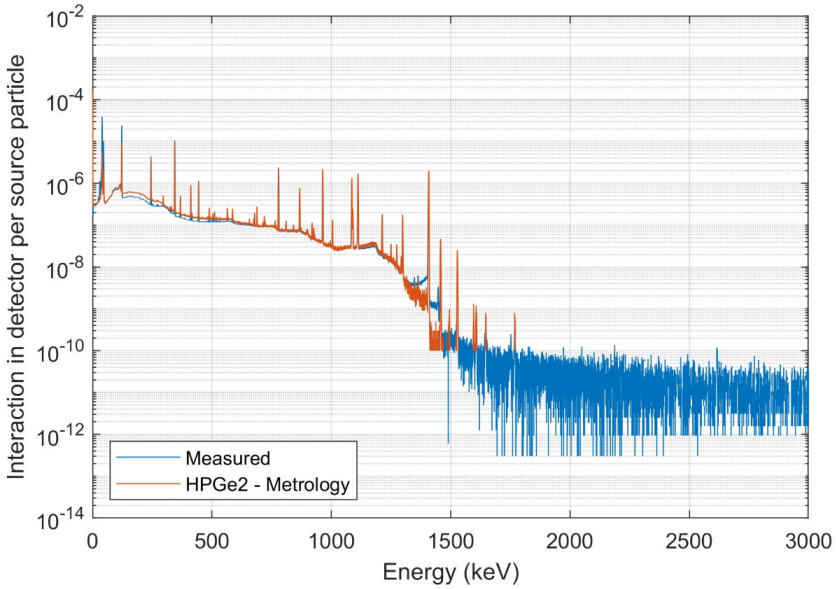


Figure A-43. Measured 152Eu spectrum compared to an HPGe simulation of the calibration source.

Significance

The MCNP model of the HPGe detector is used in conjunction with TRYC, a code that provides fission product concentrations from an irradiated sample. As part of the development of a quality reactor metrology program, substantial effort went toward creating radiation transport models, using the MCNP code, to provide geometric correction factors for capsule and wire measurements, since the form factor is different from the calibration source. A ^{152}Eu check source was simulated and compared with experimental data. When determining an efficiency for irradiated fuel samples, such as SETH-A (irradiated in TREAT), the measured efficiency curve for the detector must be corrected to account for geometric differences, and an accurate detector model is essential for this purpose. Since the time between irradiation and measurement of the SETH-A rodlet was approximately 4.5 months, there are only a few contributing isotopes to the majority of the rodlet's fission product inventory and total activity, including ^{95}Zr, ^{95}Nb, ^{103}Ru, ^{137}Cs, and ^{144}Pr. The ^{235}U and ^{238}U photopeaks are visible in the simulated data, though only ^{234m}Pa was used in the ^{238}U decay series.

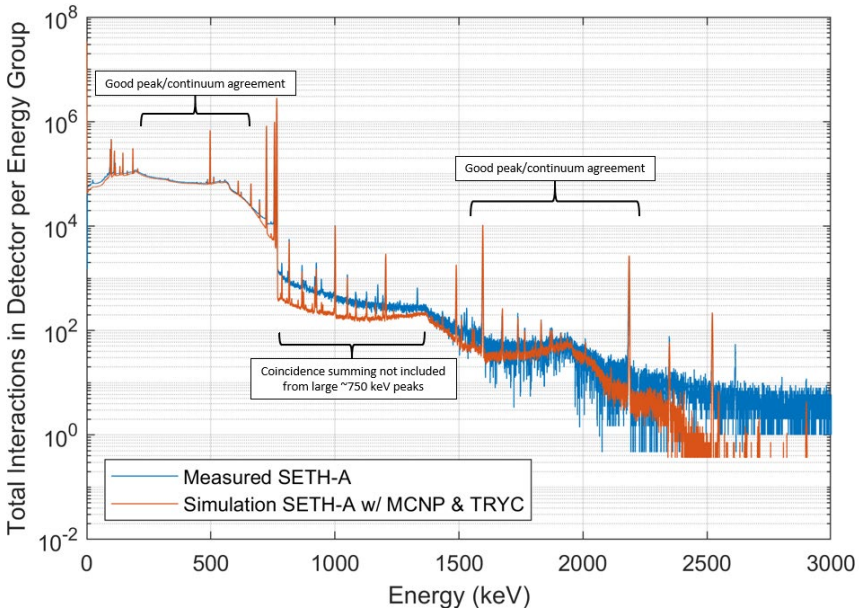


Figure A-44. Measured and simulated fission product spectra for SETH-A UO_2 pellet.

Key Publications

- Woolstenhulme, N., Fleming, A., Holschuh, T., Jensen, C., Kameraman, D., Wachs, D., "Core-to-specimen energy coupling results of the first modern fueled experiments in TREAT," *Annals of Nuclear Energy*, vol. 140, 2020. https://doi.org/10.1016/j.anucene.2019.107117
- Holschuh, T., Watson, S., Chichester, D., "TREAT Reactor Metrology Results from CTFW-4 and CTFW-5," INL/EXT-20-57177, March 2020, Idaho National Laboratory.
- Holschuh, T., Watson, S., Johnson, J., Chichester, D., "Reactor Metrology for TREAT Experiments," INL/MIS-20-57521, March 2020, Idaho National Laboratory.
- Holschuh, T., Watson, S., Chichester, D., "Metrology for Transient Reactor Characterization Using Uranium Wires," *Nuclear Technology*, vol. 205, No.10, pp. 1-10, 2019. https://doi.org/10.1080/00295450.2019.1599613
- Holschuh, T., Watson, S., Chichester, D., "TREAT Reactor Metrology Program Status–FY2019," INL/EXT-19-55987, September 2019, Idaho National Laboratory.

Sponsor/Program

Transient Reactor Test Facility

Advanced Test Reactor

A.25. Machine Learning Analysis of MCO and Hot K-Effective

Report Participants

Phil McCalley[1], John Gruenwald[1], Jonathan Nistor[1], Jordan Heim[1]

1 Blue Wave AI Labs

Scientific Achievement

In this project, we are modeling moisture carryover (MCO) and hot k-effective in the General Electric Type-4 BWR using machine-learning methods and data from operating plants. These machine-learning techniques make use of unsupervised learning in the variable-reduction phase of the program and complex supervised learning networks for the actual model development. Understanding MCO and the conditions that give rise to an elevated value is important since excessive MCO can damage critical turbine components, result in elevated dose levels to onsite personnel, and interfere with late-cycle power management. The analysis of MCO takes into account simplifying reactor symmetries and important geometric dependencies. The plant data are taken from several reactors and were collected over multiple years and multiple fuel cycles. A machine-learning model is constructed from the data using applicable algorithms and data-reduction techniques. Matching model complexity with available data is one of the more challenging machine-learning tasks. Too many features and too little data will lead to overfitting. The data for each fuel cycle included over 6,876 original features, nine for each fuel bundle. Various approaches were used to reduce the data set into a manageable number of features. Even with these simplifications, the endeavor is computationally intensive, as thousands of models are developed for each fuel cycle in order to pick models closet to the global minimum for the cost function.

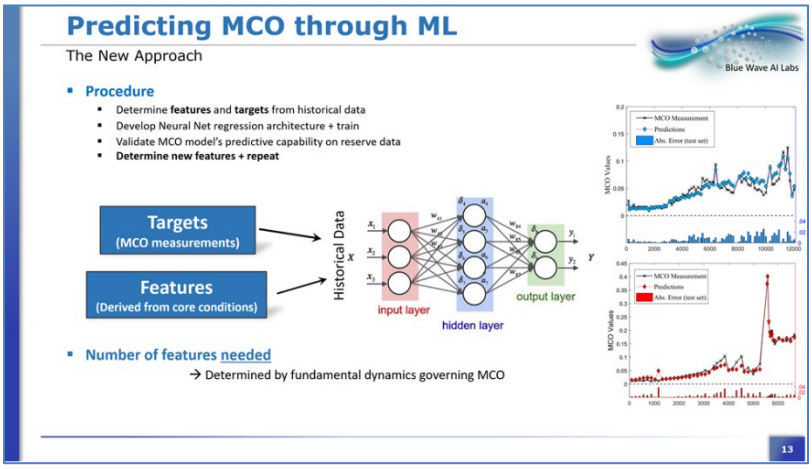


Figure A-45. Predicting MCO through ML.

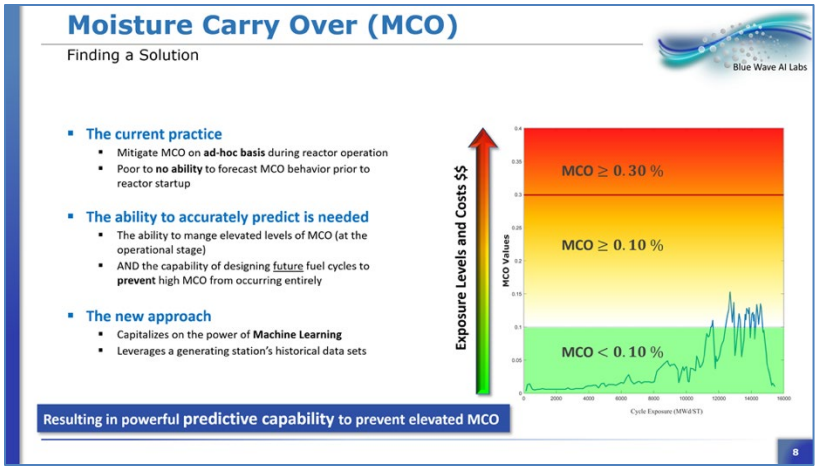


Figure A-46. MCO data structures,

The BWR operates on a saturated steam cycle relying on mechanical equipment to remove liquid moisture from a two-phase mixture that exits the core. Excess MCO can lead to both the intergranular stress corrosion cracking of turbine blades and an increase in the exposure levels of maintenance personal to ^{60}Co that is carried over in the liquid droplets that leave the steam dryers. While the BWR in the United States was originally designed to achieve MCO levels that are acceptable from a plant economic performance perspective, changes in recent years in the way these plants are operated and in the reactor core design efficiencies have led to increased MCO levels. Specifically, new fuel management strategies and the use of an increased core flow (>100%) to extend the cycle aimed at minimizing fuel costs have led to a greater fraction of liquid reaching the turbine as a consequence of the increased load on the steam separators and steam dryers.

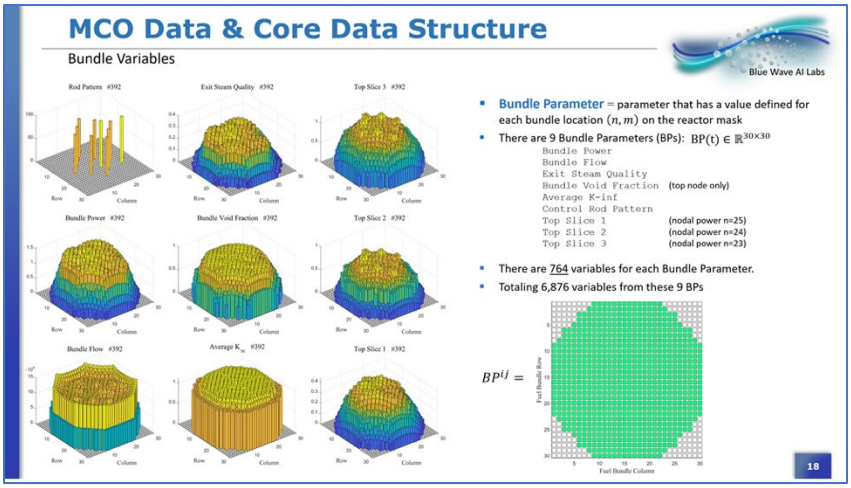


Figure A-47. Predicting MCO through ML.

Most of the analytical software is written in Python running in a Linux environment. We sometimes make use of the container software Singularity to aid portability.

Significance

The prediction of MCO values as reactor burnup progresses is an important operational issue with significant economic impacts to power generation. It depends on a very complex set of operating conditions, and the electric utility has limited ways to control and manage MCO while keeping power at planned levels. Having a useful predictive model of MCO is thus of high importance. Given the large amount of data collected over the years of nuclear reactor operation, machine learning presents itself as a very promising way to model MCO. Machine learning is based on rigorous mathematical theory and, in simple terms, posits that the function governing the system's evolution is in the data and can be approximated if enough data are available. Of course, the data also contain noise and so appropriate care was taken in this paper to avoid fitting the noise.

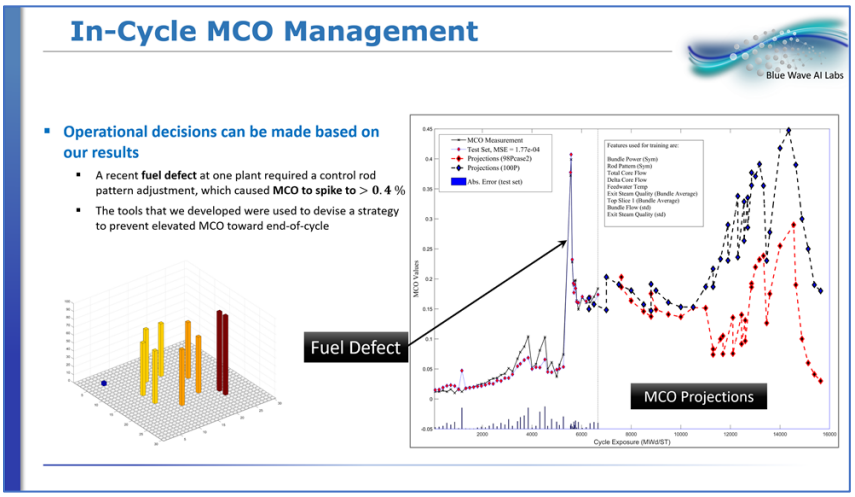


Figure A-48. MCO data structures.

This work has the potential to save the nuclear industry tens of millions of dollars per reactor if used to manage fuel planning decisions.

Key Publications

Publications in progress.

Sponsor/Program

Department of Energy, Moisture Carryover and K-Effective Investigation

A.26. Material Model and Ease-of-Use Improvements in BISON or Application to BWRs

Report Participants

Aysenur Toptan[1], Kyle A. Gamble[1]

1 Idaho National Laboratory

Scientific Achievement

The main focus of this work is to develop and document required material models that would aid in predicting cladding failure with a specific hydride distribution to be investigated for BWR applications in the next fiscal year. In terms of materials, the primary differences between a BWR and PWR is the use of gadolinia doping of the UO_2 fuel, the use of Zircaloy-2 for the cladding, and the addition of a liner on the inner surface of the cladding for improved pellet-clad mechanical interaction performance. The liner is typically made of pure zirconium or a lower tin content zirconium alloy (e.g., Zr-0.3%Sn). This work details the development and documentation of material and behavioral models for BWR analysis, such as the addition of material and behavior models for gadolinia doped UO_2, pure zirconium, Zr-0.3%Sn, and Zircaloy-2 to the BISON fuel performance code as well as the ease-of-use additions to allow internal meshing capabilities to include liners. Another important aspect affecting cladding performance is the hydrogen diffusion and hydride precipitation in the cladding. A model was added previously for unlined, homogeneous claddings. In this work, instructions are provided on how to apply the model to the BWR liner cladding. Representative experimental values are provided for the hydrogen diffusion parameters and precipitation-dissolution kinetics for typical liner materials of interest. The validation of the new thermal conductivity model for gadolinia-doped UO_2 was verified as part of this study to the IFA-681 experiments.

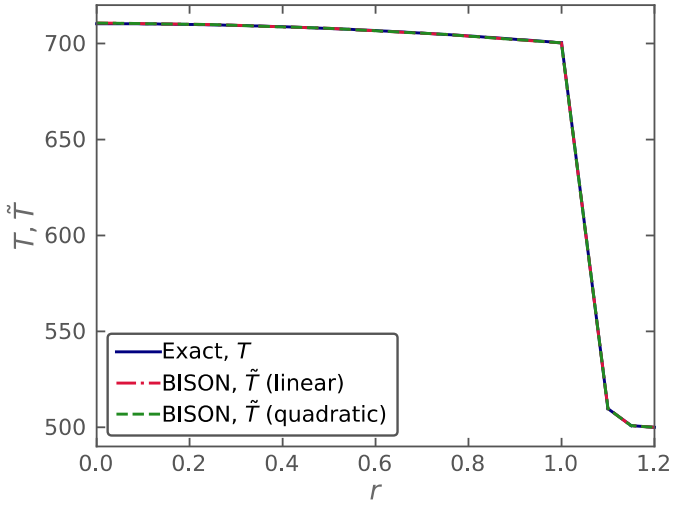


Figure A-49. Temperature distribution for the verification problem. Exact and finite element solutions are obtained using one-dimensional elements to show proper implementation of liner meshing capabilities.

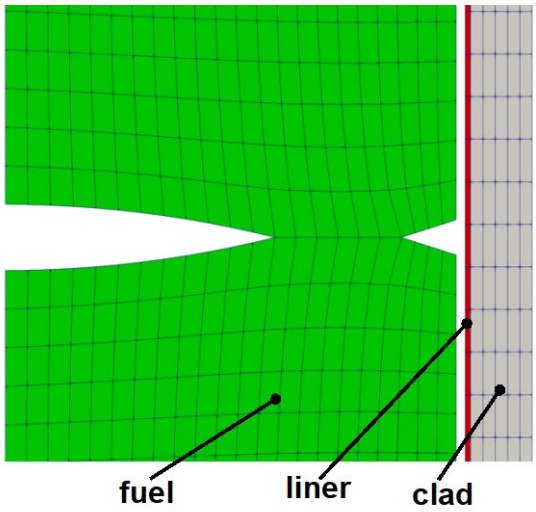


Figure A-50. Discrete pellet mesh containing dishes and chamfers with a lined cladding.

Significance

The new thermal conductivity model provides improved confidence in its predictions of the temperature of gadolinia-bearing fuels due to the fact that the uncertainty in its creation has been reduced. Both Exelon and General Electric plan to use the gadolinia fuel and liner capabilities through VERA tool developed out of Oak Ridge National Laboratory to analyze their BWR systems.

Key Publications

Toptan A., Gamble K. A., "FY20 BISON BWR Fuel Modeling Capability: Material Models," INL/EXT-20-59936, 2020.

Sponsor/Program

Consortium for Advanced Simulation of Light Water Reactors

A.27. Modeling and Analysis of Exelon Boiling-Water Reactors (VERA-BWR)

Report Participants

Brendan Kochunas[1], Sooyoung Choi[1]

1 University of Michigan

Scientific Achievement

This is an ongoing project that has completed its first year. The first year milestone for which we were responsible was the development of geometric capabilities for modeling boiling-water reactors and to support the evaluation of MPACT to compute solutions robustly for boiling-water reactors.

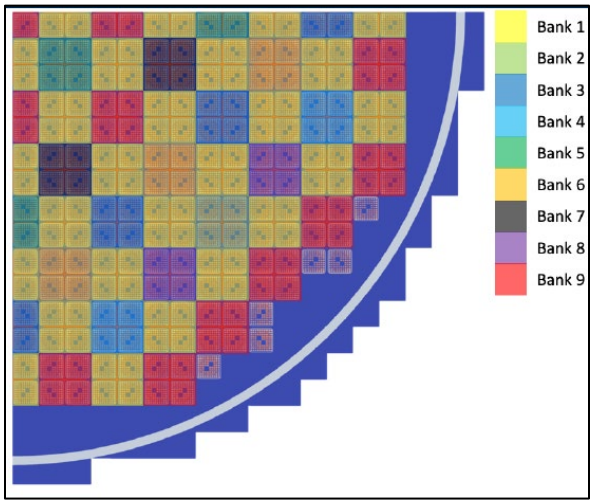


Figure A-51. Full Core BWR MPACT Model.

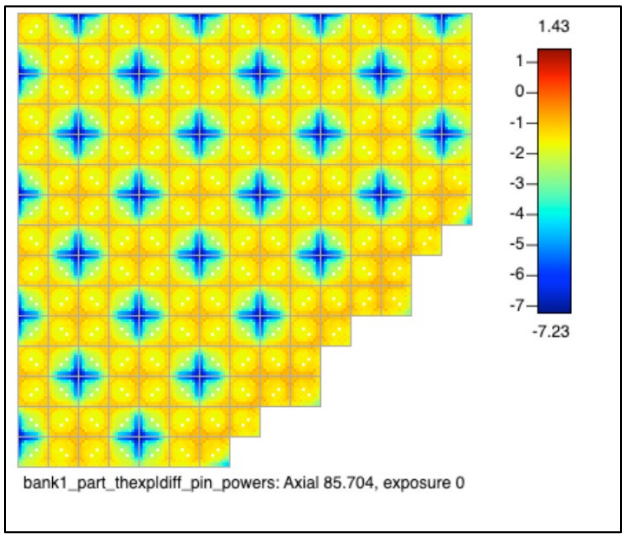


Figure A-52. Pin power distribution with checkboard control blade insertion.

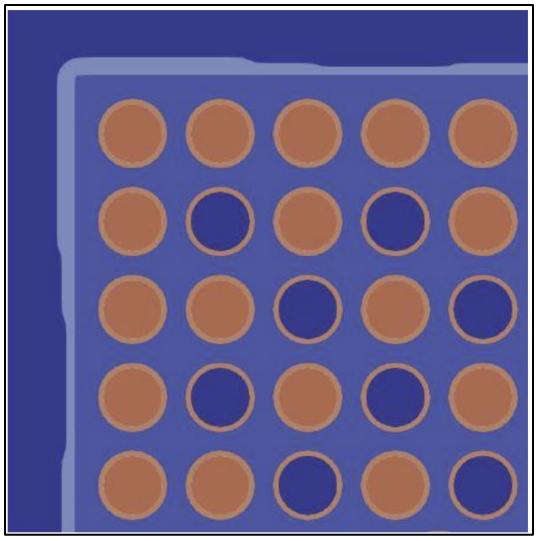


Figure A-53. Thick-thin-thin channel box geometry in MPACT model.

Significance

Thus far, the capabilities of MPACT were successfully extended to model nearly all geometric features of BWRs. This includes control blades, detectors, and channel boxes Thus enabling year two milestones to perform calculations on real plants and for comparison to their data.

Key Publications

Kochunas, B., Choi, S., Dodson, Z., Folk, T., Jabaay, D., Kabelitz, M., Jeon, B.K., Liu, Y., Downar, T. (2020). “MPACT Development Progress for Full-Core BWR Modeling,” NURAM-2020-001-00, University of Michigan.

Sponsor/Program

Department of Energy

A.28. Modeling Reactivity Insertion Experiments of TRISO Particles in NSRR Using BISON

Report Participants

Daniel Schappel[1], N. R. Brown[1,2], K. A. Terrani[1]

1 Oak Ridge National Laboratory

2 University of Tennessee, Knoxville

Scientific Achievement

Models and methodology for calculating failure probability of ceramics were implemented by researchers in BISON. This is part of the Transformational Challenge Reactor Program to inform the design process. This has reduced the amount of fracture testing that is required during the conceptual design stage.

Significance

BISON was used to simulate the stresses and temperatures of TRISO particles during transients at Nuclear Safety Research Reactor (NSRR). A good agreement with experimental results was obtained in both temperature and failure fractions. This provides some confidence in using BISON in a predictive capability for future transient testing.

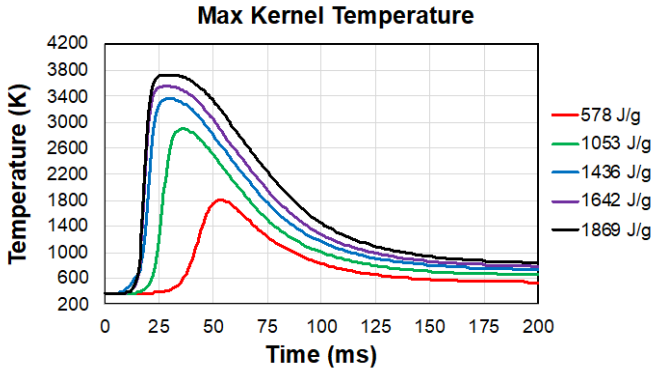


Figure A-54. Predicted maximum fuel temperatures.

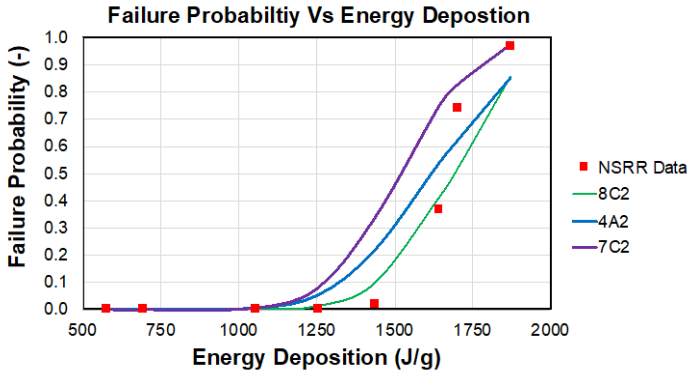


Figure A-55. Predicted failure probabilities temperatures.

Key Publications

- D. Schappel, N. R. Brown, T. A. Terrani, "Modeling reactivity insertion experiments of TRISO particles in NSR using BISON." *Journal of Nuclear Materials*, vol. 530, no. 151965. https://doi.org/10.1016/j.jnucmat.2019.151965
- D. Schappel, K. Terrani ,L.L. Snead, B.D. Wirth. "Modeling radionuclide release of TRISO bearing fuel compacts during post-irradiation annealing tests," *Nuclear Engineering and Design*, vol. 357, no. 110428. https://doi.org/10.1016/j.nucengdes.2019.110428

Sponsor/Program

Department of Energy, Transformation Challenge Reactor (TCR) program

A.29. Multiphysics Fuel Performance Modeling of TRISO-Bearing Fuel in Advanced Reactor Environments

Report Participants

Emily Stirrup[1]

1 University of Tennessee

Scientific Achievement

The purpose of this research is to target the thermomechanical behavior of nuclear fuel rods according to the needs of various DOE-affiliated entities and programs. In support of this effort, this research used and modified the source code of BISON to include more thorough constitutive properties for proposed coating materials for fuel rod cladding. It will further utilize BISON to provide an engineering analysis for various fuel designs and coating performance.

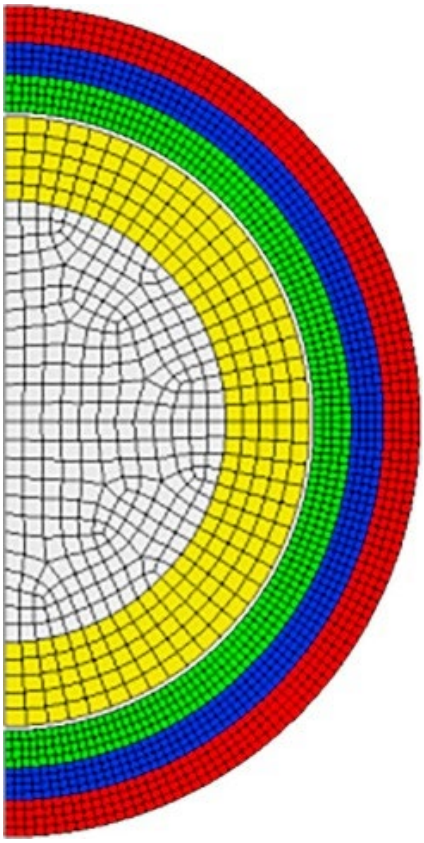


Figure A-56. A representation of the mesh used for the single TRISO particle analysis. This 2D representation has its centerline on the left.

Significance

This research is important for the advancement and possible deployment of coated nuclear fuel rods, which are designed to enhance the safety of operating nuclear reactors. This work seeks to evaluate the viability of these coating based on their mechanical response. To date, work has been done by researchers to benchmark and confirm previous work completed by D. Schappel modeling TRISO-based fully ceramic matrix fuels in an LWR environment. An advanced gas reactor irradiating TRISO pellets will validate predictions made by this and following works—including a UQ assessment of the radiological source term during accident scenarios.

Key Publications

None.

Sponsor/Program

Nuclear Energy Advanced Modeling and Simulation

A.30. Multiscale Thermal-Fluids of Pebble Bed Reactors

Report Participants

April Novak[1]

1 Argonne National Laboratory

Scientific Achievement

The core regions of pebble-bed reactors (PBRs) is a complex fluid-solid structure consisting of hundreds of thousands of centimeter-sized pebbles around which coolant flows to remove fission heat. Each pebble itself consists of tens of thousands of millimeter-sized multilayered fuel particles that enclose a fissile kernel in protective layers to reduce the release of radioactive material. Thermal-hydraulic models of these systems must be able to predict both core-level phenomena, such as the feasibility of natural circulation, as well as particle-level phenomena, such as particle integrity and fission product diffusion to the coolant. In this work, we have continued the development of thermal-hydraulic models in a multiscale computational tool built on MOOSE, named Pronghorn. This work enables the prediction of intermediate-resolution thermal-hydraulic models in PBRs with a vastly reduced computational effort compared to full-scale simulations for a fast-turnaround design and analysis.

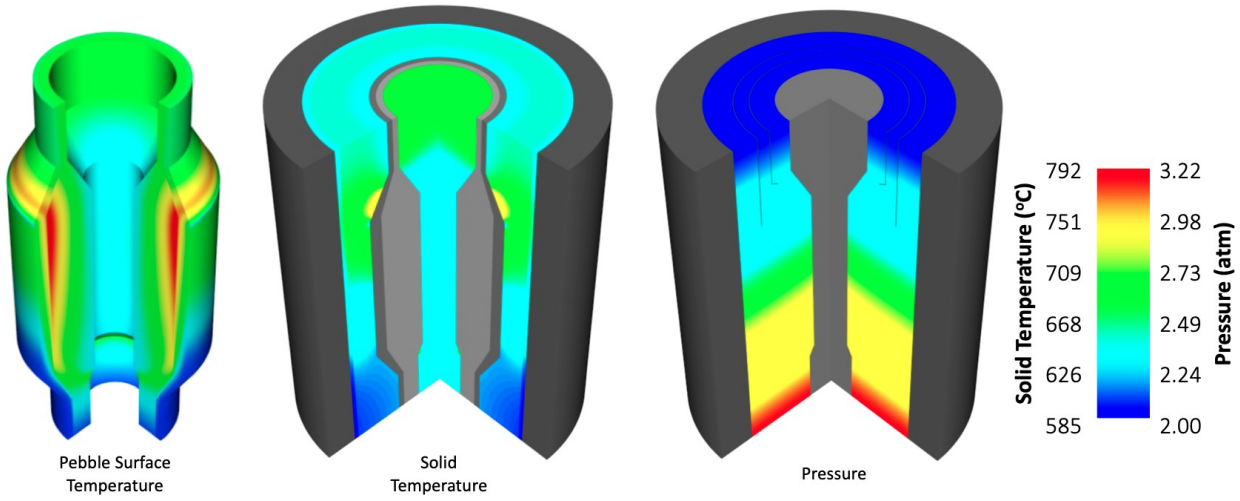


Figure A-57. Pronghorn predictions of pebble temperature, ex-core structural temperature, and pressure in the Mark-1 Pebble-Bed Fluoride-Salt-Cooled High-Temperature Reactor (PB-FHR), a novel salt-cooled PBR concept.

Significance

PBRs are expected to display excellent heat removal characteristics due to the large quantities of graphite in most core designs, the high failure temperatures of particle fuel, and the low reactor power densities involved. Modeling of PBRs is needed to facilitate rapid design and scoping studies, support licensing activities, and assess differences between designed and as-built systems. PBRs constitute one category of the six most promising future reactor development areas identified by the Generation IV International Forum and, as such, have the potential to contribute significantly to reducing carbon emissions in both the electricity and high-temperature process heat sectors. The development of thermal-hydraulic models in Pronghorn and the seamless multiphysics coupling capabilities shared by applications developed on the MOOSE framework brings complex interphysics predictions to the analyst's toolset.

Key Publications

- A.J. Novak, R.W. Carlsen, S. Schunert, P. Balestra, D. Reger, R.N. Slaybaugh, and R.C. Martineau. "Pronghorn: A Multidimensional Coarse-Mesh Application for Advanced Reactor Thermal Hydraulics." *Nuclear Technology*. https://doi.org/10.1080/00295450.2020.1825307
- R.C. Martineau, D. Andrs, R. Carlsen, D. Gaston, J. Hansel, F. Kong, A. Lindsay, C. Permann, A. Slaughter, E. Merzari, R. Hu, A. Novak, R. Slaybaugh. "Multiphysics for nuclear energy applications using a cohesive computational framework." *Nuclear Engineering and Design,* vol. 367, no. 110751, 2020. https://doi.org/10.1016/j.nucengdes.2020.110751
- A.J. Novak, J.W. Peterson, L. Zou, D. Andrs, R.N. Slaybaugh, R.C. Martineau. "Validation of Pronghorn friction-dominated porous media thermal-hydraulics model with the SANA experiments," *Nuclear Engineering and Design*, vol. 350, pp. 182-194, 2019. https://doi.org/10.1016/j.nucengdes.2019.04.037

Sponsor/Program

Nuclear Energy Advanced Modeling and Simulation

A.31. Multiscale-Informed Modeling of High-Temperature Component Response with Uncertainty Quantification

Report Participants

Lynn Munday[1], Som Dhulipala[1], Albert Casagranda[1], Stephanie Pitts[1], Benjamin Spencer[1]

1 Idaho National Laboratory

Scientific Achievement

Finite element simulations were used to predict the lifetime of components subjected to the high-temperature environments typical of those that structural components in advanced nuclear reactors would experience. These simulations used two new material models developed at Argonne National Laboratory and Los Alamos National Laboratory that account for both the uncertainty in material properties based on experimental measurements and a reduced-order model created from microscale deformation mechanisms for the Grade 91 alloy. The input parameter sensitivity for the two constitutive models on the high-temperature creep of an engineering scale component was simulated using the MOOSE stochastic tools module in Grizzly.

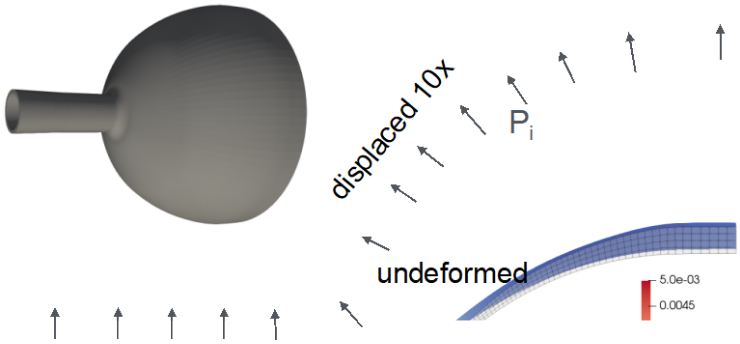


Figure A-58. The inset shows the sphere nozzle component used for the engineering-scale material uncertainty simulations. A 2D cross section of the component is shown in the color contour plot displaying the maximum principal strains that develop in a pressurized component over 20 years. The initial undeformed sphere nozzle is shown by the gray mesh and the colored mesh has been displaced by the creep simulation.

Significance

The first Grade 91 material model developed by Argonne National Laboratory fit the uncertainty in material parameters of a phenomological material model from the Nuclear Engineering Material Modeling Library (NEML) to historical Grade 91 experimental data using a Bayesian approach. This model with uncertainty was then used to run Monte Carlo realizations of a component-level finite element model in order to determine the sensitivity of the material parameters on the component's predicted life. The second material model developed at Los Alamos National Laboratory used the Los Alamos Reduced Order Models for Advanced Nonlinear Constitutive Equations (LaRomance) to create an engineering-scale constitutive model from a mechanism-based crystal plasticity model of Grade 91. We used Monte Carlo sampling of the microstructural input parameters to quantify the sensitivity of the mechanistic input parameters in the LaRomance material model, such as dislocation density, and the secondary phase content on the evolution of creep in an engineering scale componenent over an expected lifetime of 20 years. Large amounts of HPC resources were required to adequately sample the range of input parameters, environmental conditions, and expected mechanical loads on the simulated structural component in order to determine the sensitivities of the input parameters on the expected long term creep and to determine the low probabilities of failure over the 20-year lifetime of the component.

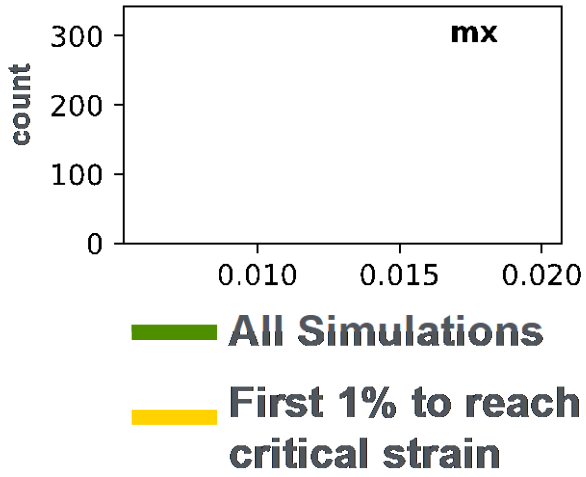


Figure A-59. Normal distributions showing the sensitivity of the secondary phase content in the LaRomance model on increased creep. The green distribution is the Monte Carlo sampling of a normal distribution of valid input parameters and the yellow distribution are those samples that resulted in the largest amount of creep. A higher secondary phase content was shown to increase creep.

Key Publications

Munday, L.B., Dhulipala, S.L., Casagranda, A., Pitts, S.A., Spencer, B.W., Capolungo, A., et al., "Multiscale-Informed Modeling of High Temperature Component Response with Uncertainty Quantification" (No. INL/EXT-20-59795-Rev000). Idaho National Laboratory (INL), Idaho Falls, ID (United States), 2020.

Sponsor/Program

Nuclear Energy Advanced Modeling and Simulation

A.32. NEUP Project 17-12939: Expansion of BISON Capabilities to Predict the Dynamic Response of Irradiated Fuel Rods

Report Participants

Christopher Wong[1]

1 University of Utah

Scientific Achievement

Researchers will expand the capabilities of BISON and MOOSE to simulate the structural dynamic responses of fuel rods and fuel assemblies during handling (wet and dry storage) and transportation.

Significance

Expanding the capabilities of BISON and MOOSE to facilitate the evaluation of the dynamic response of fuel rods and assemblies is important for conducting a more reliable risk assesment of fuel assemblies as well as storage and transportation casks.

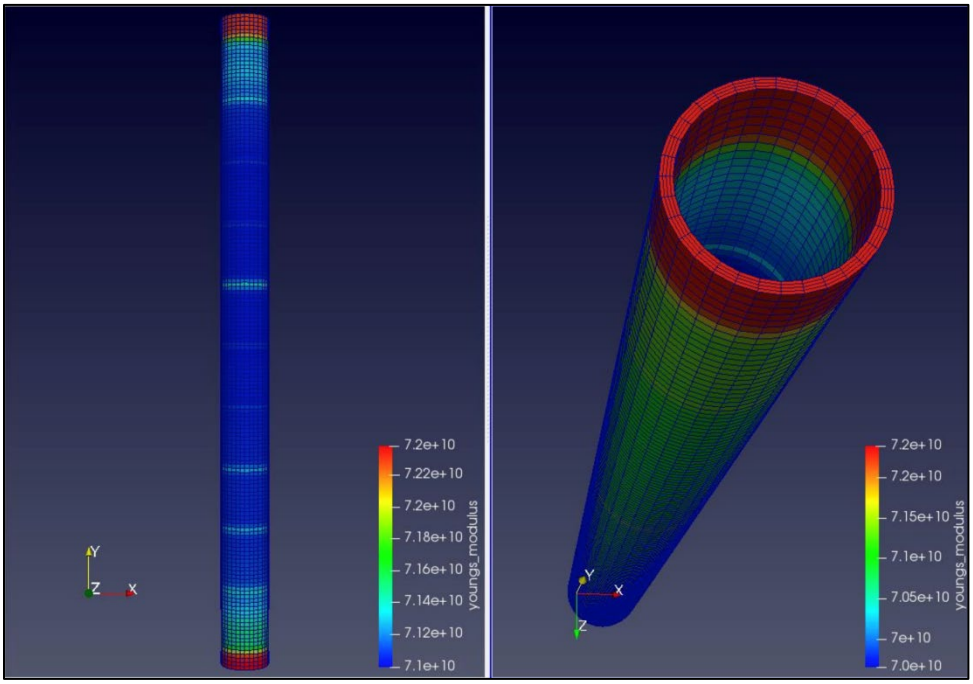


Figure A-60. Young's modulus as a function of burnup computed using the MATPRO model on an axisymmetric mesh in BISON and then mapped to a 3D equivalent mesh for a subsequent structural analysis.

Key Publications

In progress.

Sponsor/Program

Nuclear Energy University Program

A.33. NEUP Project 18-15602–Thermal Energy Storage

Report Participants

Richard Christensen[1], Amey Shigrekar[1], Piyush Sabharwall[2], Trevor Casper[1], Jan Lambrechtsen[1], Matthew Memmott[3]

1 University of Idaho

2 Idaho National Laboratory

3 Brigham Young University

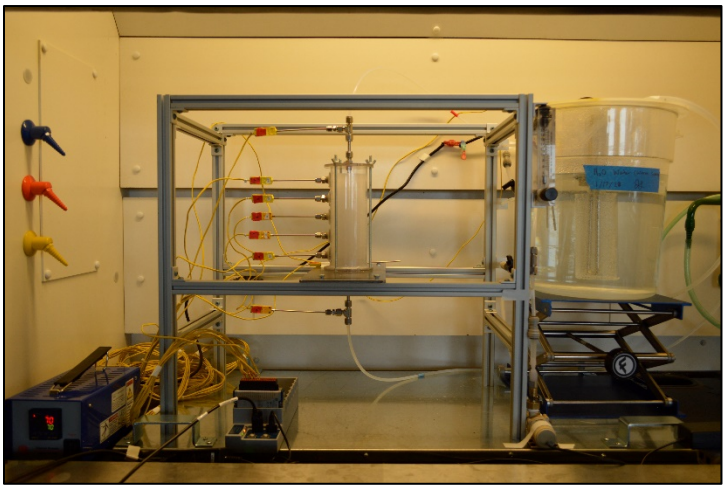


Figure A-61. An experimental TES setup utilizing wax for heat storage.

Scientific Achievement

Conducting modeling and experimental studies to aid in the design and testing of a thermal energy storage (TES) system and computational models to model the behavior of the system. This modular TES design chiefly utilizes the latent heat of nitrate salts to store energy and is designed to be part of an integrated system where it might store energy from a nuclear reactor to better enable load following. For this project, the Nuclear Energy University Program requires a validated computational model in Modelica and Raven. The validation of the models in these systems requires experimental data on salt properties and lab-scale thermal energy storage charging and discharging cycles.

Significance

This work will seek to demonstrate the feasibility of a latent-heat thermal energy storage system utilizing molten salts. Renewable energy sources present many advantages, but their increasing use in energy markets can present a challenge to base-load power technologies like nuclear that perform most efficiently at a constant output. Most research into energy storage has studied its integration with renewable technologies like solar power, but relatively little research has been done on integrating energy storage with nuclear power, despite the significant potential economic advantages. This project seeks to further research in this area, meeting a current need.

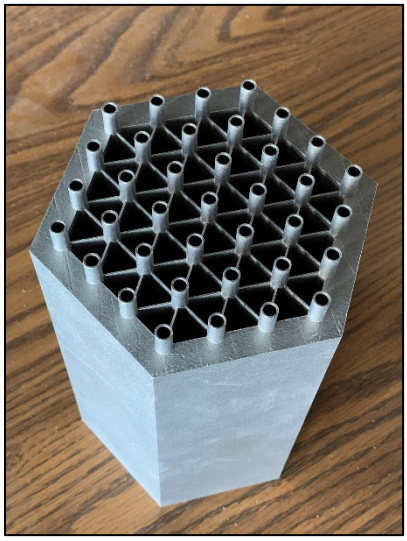


Figure A-62. A 3D-printed model of a potential TES design.

Key Publications

In progress.

Sponsor/Program

Nuclear Energy University Program

A.34. Neutronic Uncertainty Quantification for Advanced Graphite Creep Program

Report Participants

Vishal Patel[1], Will Windes [2], Jason Brookman[2]

1 Ultra Safe Nuclear Corporation

2 Idaho National Laboratory

Scientific Achievement

This study enables the uncertainty quantification of the flux that Advanced Graphite Creep Program graphite experiment experiences in ATR. MCNP is used, along with python-based wrappers, to perform an uncertainty quantification by varying the MCNP inputs.

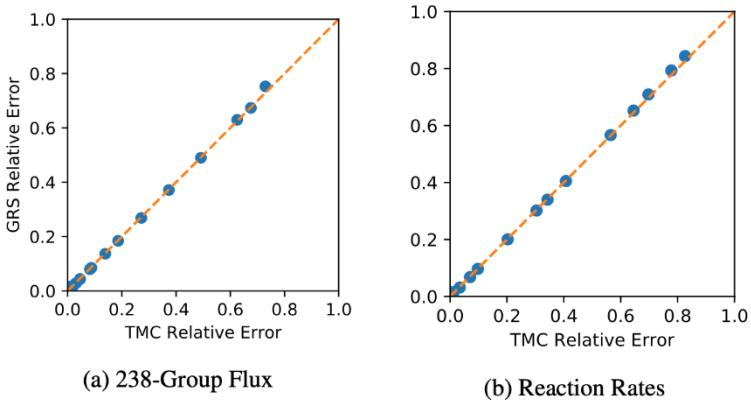


Figure A-63. Fast MC UQ Method Agrees Very Well with Traditional Brute Force Method.

Significance

A rigerous approach to calculating uncertainties has allowed for a better understanding of neutron fluence within the Advanced Graphite Creep Program graphite experiments. This work is still in progress but has already had an impact for the sponser in terms of increasing the confidence of their models.

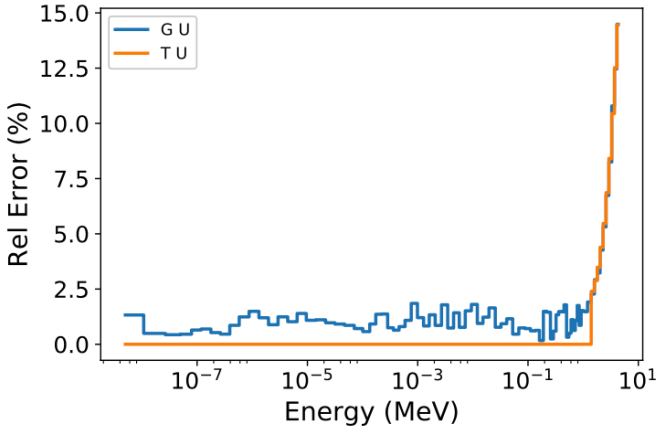


Figure A-64. Flux Uncertainties Compared within Graphite (G-GRS T-TMC).

Key Publications

- P.W. Humrickhouse, V. Patel, J. Navarro, J. Brookman, W. Windes, “Reactor dosimetry and uncertainty quantification in support of the AGC Experiments, “ INGSM-18 (2017)
- Several internal INL deliverables.
- More publications in progress.

Sponsor/Program

Advanced Test Reactor

A.35. Phase-Field Modeling of Zirconium Hydrides

Report Participants

Pierre-Clément Simon[1], Larry Aagesen[2], Andrea Jokisaari[2], Michael Tonks[3], Arthur Motta[1]

1 Pennsylvania State University

2 Idaho National Laboratory

3 University of Florida

Scientific Achievement

During normal operations in LWRs, the zirconium cladding picks up a fraction of the hydrogen produced by waterside corrosion. Once the hydrogen concentration reaches the solubility limit, it precipitates into brittle hydrides. However, cladding embrittlement largely depends on hydride morphology. Understanding the mechanisms governing zirconium hydride microstructure is thus important to assessing the cladding integrity during operation, transportation, and storage. We have developed a quantitative phase-field model to predict the hydride morphology and investigate different precipitation mechanisms.

Significance

In this project, we coupled a quantitative phase-field model with an elastic scheme. The model showed the importance of the elastic anisotropy in predicting the elongated shape and circumferential stacking of nanoscale hydrides. Figure G-67 shows the most favorable nanoscale hydride configurations, including a single hydride or a circumferential stacking of two hydrides. This insight provides a better understanding of zirconium hydride morphology and contributes to the assessment of LWR cladding integrity. Our future work will involve understanding the mechanisms behind the hydride reorientation from circumferential to radial under external stress.

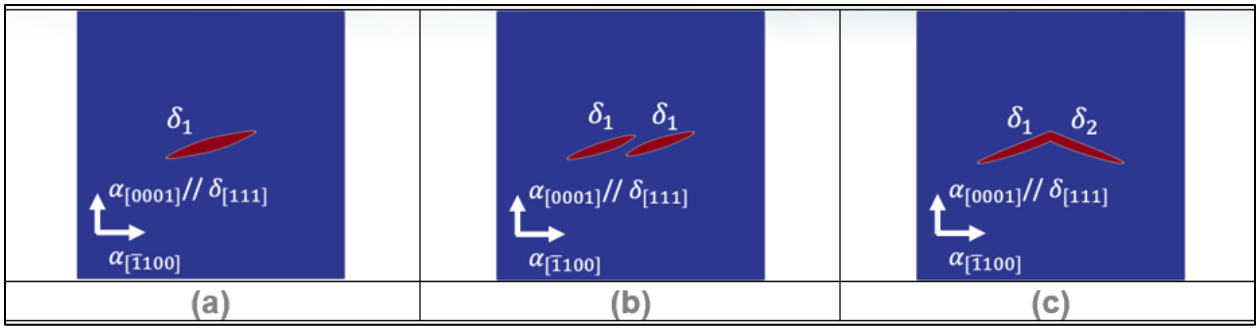


Figure A-65. Hydride morphologies predicted by the phase-field model with (a) one hydride, (b) two hydrides from the same variant, and (c) two hydrides from two different variants. The elongated growth of the hydrides and the circumferential stacking of nanoscale hydrides are predicted by the phase-field model. Domain size is 400 nm × 400 nm.

Key Publications

- P.-C. A. Simon, L.K. Aagesen, A.M. Jokisaari, E. Lacroix, A.T. Motta, M.R. Tonks, "Investigation of the orientation of δ zirconium hydrides using quantitative phase field simulations supported by experiments," (May 8, 2019). Available at SSRN: https://ssrn.com/abstract=3384332
- P.-C. A. Simon, L. K. Aagesen, A. T. Motta, M. R. Tonks, "The effects of introducing elasticity using different interpolation schemes to the grand potential phase field model," *Computational Materials Science*, vol. 183, no. 109790, 2020. https://doi.org/10.1016/j.commatsci.2020.109790

Sponsor/Program

Nuclear Energy University Program

A.36. Power Maneuvering Analysis for PWR Flexible Power Operations

Report Participants

Brenden Mervin[1], Dylan Wray[1]

1 Electric Power Research Institute

Scientific Achievement

Operators are evaluating extending this strategy to power reductions to 60%, 40% and even 20% of rated power. These reductions are expected to occur over periods as short as 6 hours to as long as 28 days. Fuel reliability restrictions are one consideration for utilities' determination of a specific flexible operations strategy. This project will address potential restrictions due to pellet-cladding interaction fuel reliability considerations.

Currently we are testing the execution of this project using VERA. The project is still in its early phase.

Significance

Work is just beginning. We have yet to get the VERA/BISON one-way coupling calculation to work on the INL HPC machines.

Key Publications

In progress.

Sponsor/Program

Consortium for Advanced Simulation of Light Water Reactors

A.37. Pronghorn Fully Compressible Equation Set Validation Against SANA Open Plenum Experiments

Report Participants

Jieun Lee[1], Paolo Balestra[2], Sebastian Schunert[2]

1 Texas A&M University

2 Idaho National Laboratory

Scientific Achievement

The verification and validation of Pronghorn porous media models are important for predicting the fluid behavior and heat transfer in advanced reactors, specifically HTGRs. The implementation of fully compressible equations in Pronghorn (modern Pronghorn) and its verification with StarCCM+ is performed by observing fluid velocity, temperature, and pressure fields in the SANA experiments.

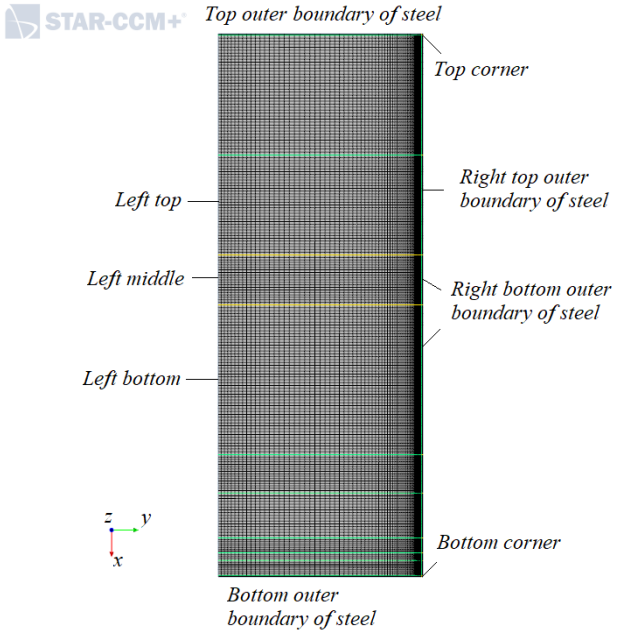


Figure A-66. Geometry and fine mesh of the StarCCM+ model.

Significance

Preliminary results show excellent agreement between both the friction-dominated (legacy Pronghorn) and modern Pronghorn porous media flow models with StarCCM+ for solid and fluid temperatures in the pebble bed. The computed results agree well with experimental data at the outer wall of the SANA facility but disagree by less than 100 K close to the heater. This discrepancy is at least partially caused by a lack of information about the total amount of fluid in the closed system. In addition, the predicted flow pattern in the upper plenum is similar for modern Pronghorn and StarCCM, but significantly different for legacy Pronghorn, confirming the unsuitability of legacy Pronghorn's approximation for open plenums. Nevertheless, fluid and solid temperatures in the bed are in good agreement across all three simulations.

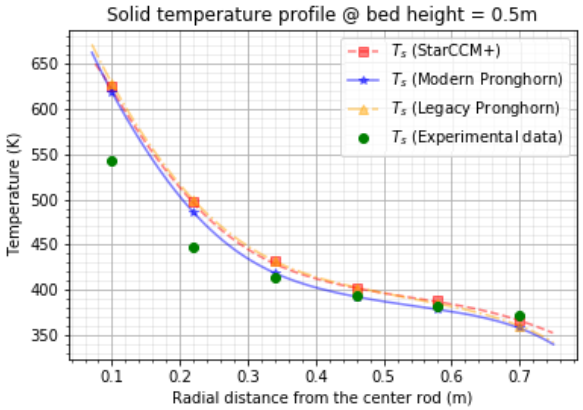


Figure A-67. Solid temperature profile at a 0.5 m bed height.

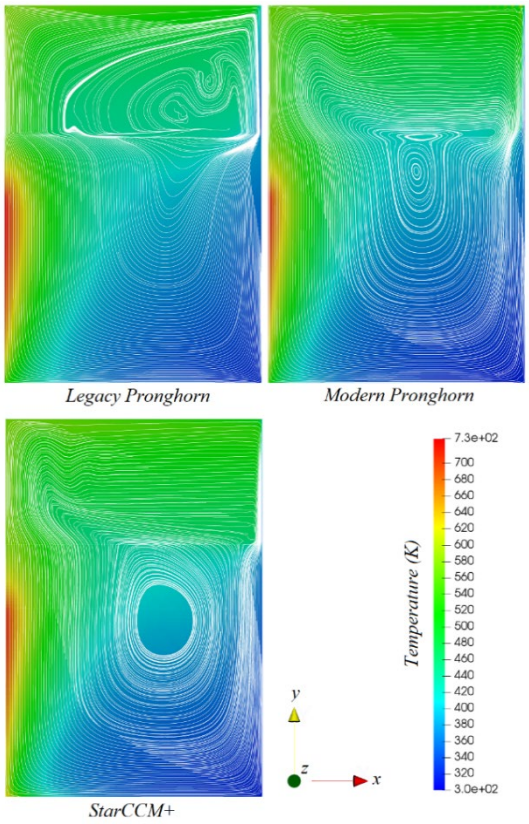


Figure A-68. Velocity streamlines and fluid temperature profile.

Key Publications

J. Lee, P. Balestra, S. Schunert, A. Novak, Y. Hassan, M. DeHart, R. Martineau. "Pronghorn fully compressible equation set validation against SANA open plenum experiments" *High Temperature Reactor Technology* 2021, under review.

Sponsor/Program

Nuclear Energy Advanced Modeling and Simulation

A.38. RCCS Modeling and Validation for High-Temperature Gas Reactors

Report Participants

Ramiro Freile[1], Sebastian Schunert[2], Paolo Balestra[2]

1 Texas A&M University

2 Idaho National Laboratory

Scientific Achievement

This work aims at providing natural convective heat transfer correlations between the reactor pressure vessel (RPV) and reactor cavity cooling system (RCCS) adapted to high-temperature gas reactors (HTGR) designs. Thus, we strive toward enhancing the accuracy in modeling the natural convection heat transfer in the HTGR RCCS using Pronghorn while still maintaining a low computational cost as compared to full-scale models. In order to provide the data to fit the correlations, we use computational fluid dynamics (CFD) RANS models. To account for the Nusselt number dependency on the Rayleigh number and on the nonisothermal boundary condition at the RPV wall, we performed simulations of a HTGR cavity at different high Rayleigh numbers ∈ [6.1×10^11,2.9×10^13] to encompass several HTGR designs and performed simulations of a PBMR 400 HTGR cavity with several temperature profiles on the RPV wall, which are obtained after a simulation of a PLOFC using the MOOSE-based app Pronghorn. To obtain the Nusselt number correlations, the data is then fitted by using the sparsity promoting least-squares method. The correlations include both local and average Nusselt numbers as a function of the global Rayleigh number, local Rayleigh number, and temperature profile at the hot wall of the RCCS.

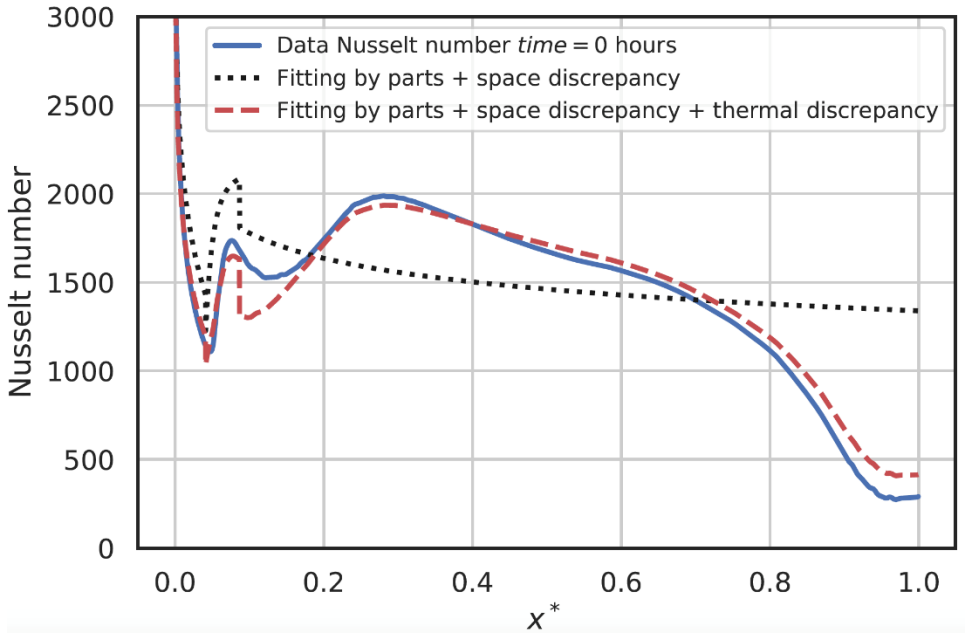


Figure A-69. Local Nusselt number correlation at the RPV hot wall as a function of dimensionless height.

Significance

The RCCS represents the ultimate heat sink for HTGRs. Therefore, the RCCS design must ensure the integrity of the nuclear fuel, structures, and critical equipment by extracting the decay heat passively through natural convection or with the use of redundant forced-convection cooling systems.

Modeling the natural convection heat exchange at the RPV wall is very challenging because of the high Rayleigh number turbulent phenomena in the RCCS. An accurate characterization of heat transfer between the RPV and the RCCS is of great importance for the design of HTGRs, especially in accident scenarios.

The correlations developed in this work enable Pronghorn to perform reliable simulations while maintaining a low computational cost.

Key Publications

Freile R., Tano M., Balestra P., Schunert S., Kimber M., "Improved Natural Convection Heat Transfer Correlations for Reactor Cavity Cooling Systems of High Temperature Gas Cooled Reactors: from CFD to Pronghorn," July 2020, in progress.

Sponsor/Program

Nuclear Energy Advanced Modeling and Simulation

A.39. Secondary Source Core Reload Modeling with VERA

Report Participants

Cole Gentry[1], Benjamin Collins[1], Eva Davidson[1], Gregory Davidson[1], Thomas Evans[1], Andrew Godfrey[1], Shane Hart[1], Germina Ilas[1], Seth Johnson[1], Kang Seog Kim[1], Scott Palmtag[2], Tara Pandya[1], Katherine Royston[1], William Wieselquist[1], Gary Wolfram[3]

1 Oak Ridge National Laboratory

2 Tennessee Valley Authority

3 North Carolina State University

Scientific Achievement

VERA was used to perform high-fidelity simulations of ex-core source range detector responses during core loading. This was a benchmarking exercise to demonstrate the performance of the recently added MPACT external source solver capability and MPACT-Shift coupling to transfer the MPACT calculated fission source to Shift for detector response simulations.

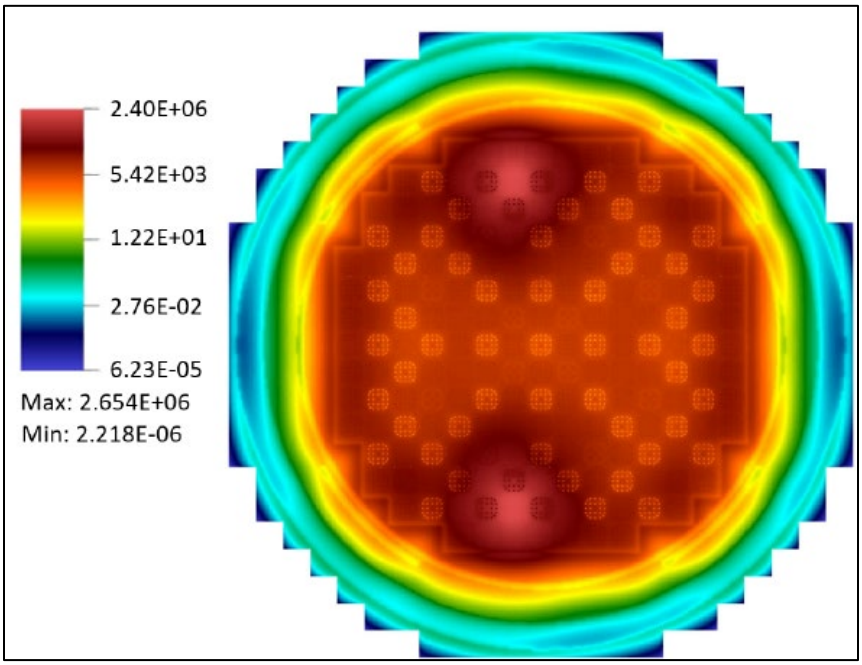


Figure A-70. Example of fine-mesh thermal neutron flux with secondary sources at core midplane in n/(cm^2·sec).

Significance

The accurate modeling of the source range detector response is crucial for ensuring proper light-water reactor (LWR) core loadings to prevent an adverse detector response. An adverse detector response here could mean a low signal during refueling, which can prevent continued fueling until resolved, or through nonlinear inverse count rate ratio (ICRR) behaviors, which lead to the mispredictions of critical configurations and potentially delayed operator detection of adverse plant conditions.

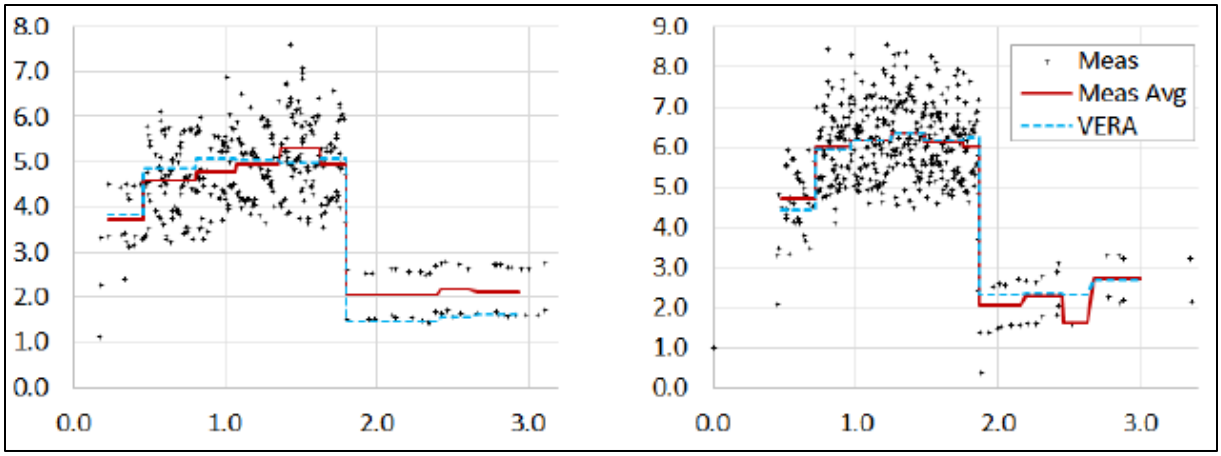


Figure A-71. Example of detector signal (counts per second) vs. measurement time plots (hrs) Cycle A (left) and Cycle B (right).

Key Publications

- C. Gentry, et al., "Secondary Source Core Reload Modeling with VERA", *Nuclear Science and Engineering*. https://doi.org/10.1080/00295639.2020.1820797
- T. Pandya, et al. "High-Fidelity Ex-core Capabilities with VERA", Physor 2020 proceedings, 1398, (2020). https://www.osti.gov/biblio/1619040
- E. Davidson, et al. "Benchmarking of Source Range Detector Responses During Watts Bar Unit 1 Refueling," ANS Winter 2020.
- C. Gentry et al., "Modeling of Subcritical PWR with Fixed Neutron Source Using MPACT", *Transactions of the American Nuclear Society*, 117, 1227 (2017)

Sponsor/Program

Consortium for Advanced Simulation of Light Water Reactors

A.40. Subchannel Code Development within the MOOSE Computation Framework

Report Participants

Vasileios Kyriakopoulos[1], Mauricio Tano Retamales[1], Jean Ragusa[1], David Andrs[2]

1 Texas A&M University

2 Idaho National Laboratory

Scientific Achievement

The aim of this project is the development of a subchannel capability within the MOOSE framework. A novel iterative solution technique is utilized that involves solving for (axial and cross) mass flow and enthalpy in the downstream direction. A back pressure solve is employed as a second step. Upon completion, the code will be able to model two-phase flows of various fluids and is going to be validated with an appropriate benchmark data set.

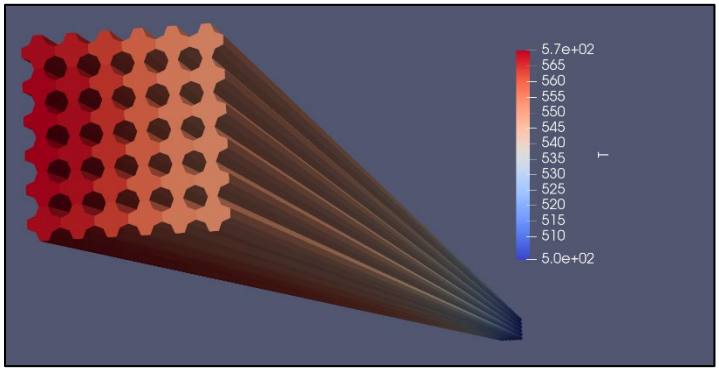


Figure A-72. Temperature contour for representative 5 × 5 bundle.

Significance

Subchannel codes are important tools in the analysis of core thermal hydraulic phenomena in nuclear reactors. Although not as detailed as Computational Fluid Dynamics (CFD) codes, they allow for a relatively fast and reasonable estimation of the flow, enthalpy, and void distributions. During routine operations and accidental conditions in LWRs, the coolant exits the subchannel as a two-phase mixture of liquid and vapor. Knowing the flow rate of the coolant subchannel and the manner in which the two phases are distributed provides a realistic basis for the evaluation of thermal performance parameters, such as the critical heat flux or departure from nucleate boiling.

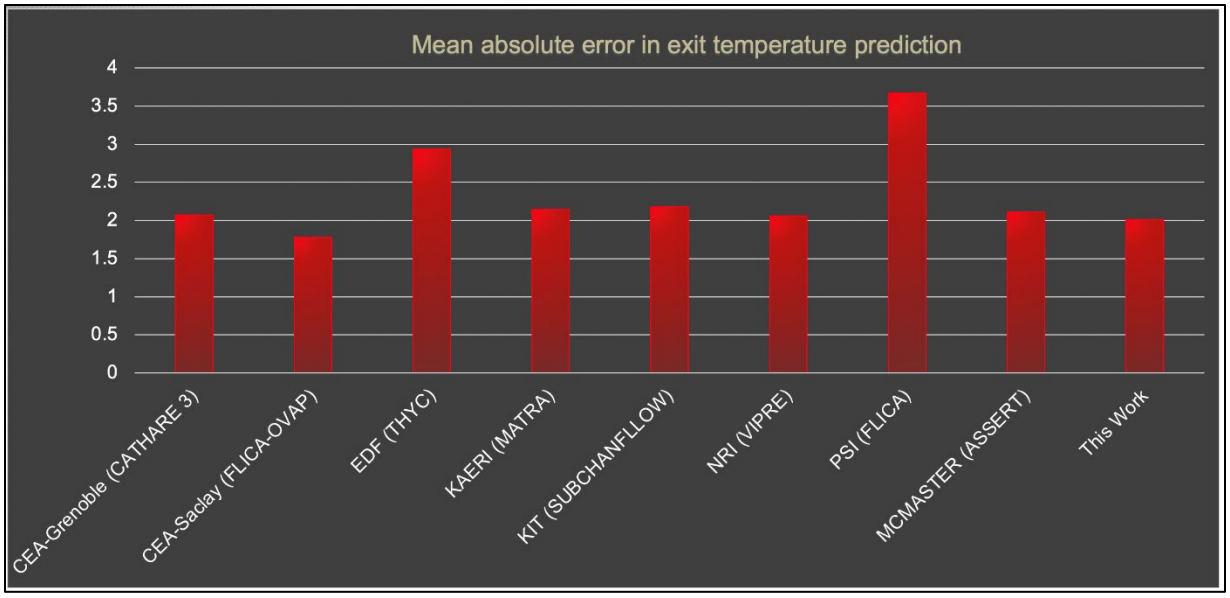


Figure A-73. Comparison of PSBT benchmark mixing test results.

Until now there hasn't been a subchannel capability within MOOSE. This project aims to demonstrate how MOOSE can integrate such a code in its arsenal. The established international Organization for Economic Cooperation and Development and NRC PWR Subchannel and Bundle Tests benchmark, based on the NUPEC database, is used to advance the subchannel analysis of fluid flow in rod bundles, which is important to the nuclear reactor safety margin evaluation. This benchmark was chosen for validation purposes. Initial results of the single phase steady-state version of the subchannel code, were validated with the steady-state fluid temperature benchmark of the PWR Subchannel and Bundle Tests and compared against results of other participants of said benchmark.

Key Publications

V. Kyriakopoulos, M.T. Retamales, J. Ragusa, "ANS M&C 2021—The International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering" Raleigh, North Carolina April 11–15, 2021, in progress.

Sponsor/Program

Nuclear Energy Advanced Modeling and Simulation

A.41. Uncertainty Quantification of BWR Progression Problems for the VERA Core Simulator

Report Participants

Travis Mui[1], Dean Price[1], Tomasz Kozlowski[1]

1 University of Illinois at Urbana-Champaign

Scientific Achievement

The objective of this project is to enhance the capabilities of the state-of-the-art advanced modeling and simulation code package VERA (Virtual Environment for Reactor Applications), developed under CASL (a Department of Energy innovation hub), to support the detailed modeling and simulation of BWRs. Such capabilities will play a vital role not only for improved reactivity and thermal margin predictions but also for the continued advancement of new fuel products and designs, such as ATF and their deployment to current operating BWRs. A set of progression problems will be developed to define a set of technical achievements in which the code capability will be demonstrated and validated. Our work will supplement verification and validation activities with additional uncertainty quantification and sensitivity analysis to assess the need for further model development.

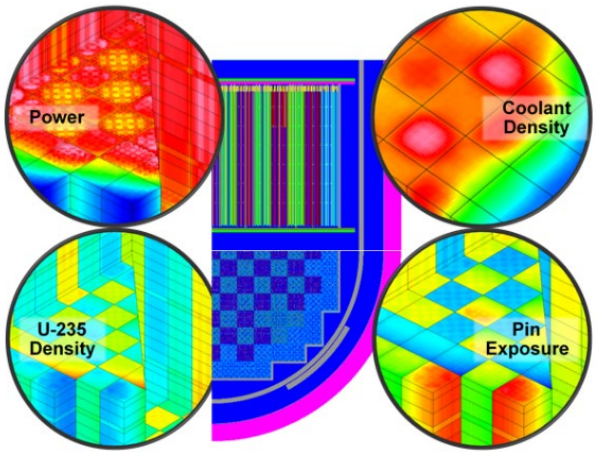


Figure A-74. Graphical representation of high-fidelity simulation capability of VERA-CS.

Significance

This project will provide a key assessment of the baseline simulation capability to perform high-fidelity modeling of BWR core designs. There will be a significant additional contribution of uncertainty attributed to two-phase flow modeling and its converse effects on simulating the neutronics and fuel performance physics. This work will also identify possible deficiencies in the physics models. This work in progress was recently started in Q2 of 2020 and is currently in the preliminary stages of the project. Work is underway to adapt and deploy the Python-based Transient Analysis Package, developed at the University of Illinois at Urbana-Champaign (UIUC) for use with VERA-CS, to allow for an uncertainty quantification and sensitivity analysis study.

Key Publications

In progress.

Sponsor/Program

Consortium for Advanced Simulation of Light Water Reactors

A.42. Use of RELAP5-3D and Machine Learning to Detect Drywell Cooling Fan Failure at a Nuclear Power Plant

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.

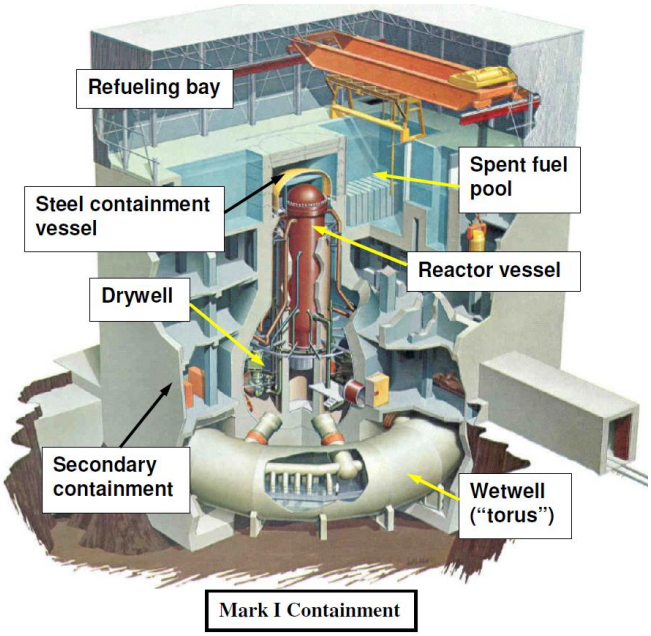


Figure A-75. BWR containment structure (Lochbaum, 2014).

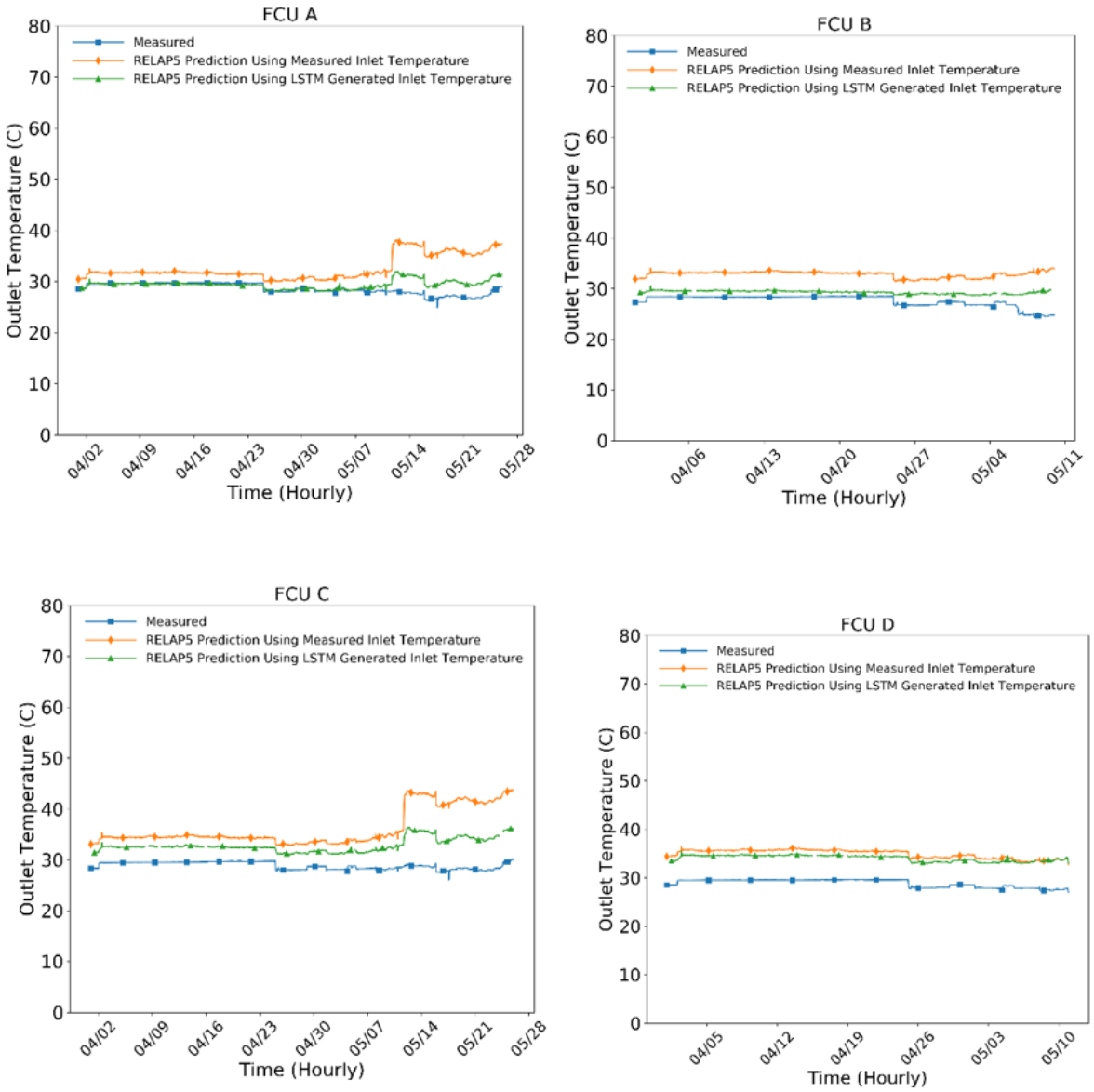


Figure A-76. Predicted and measured nitrogen outlet temperature for each of the four FCUs.

Significance

A physics-informed machine-learning model was created to analyze the failures of two drywell cooling fan coil units (FCUs) at a BWR nuclear power plant. A RELAP5 thermal hydraulic model was created to simulate the steady-state normal operation of the fans. The use of RELAP5 was used with a recurrent neural network model to prototype a physics-based anomaly detection model for the drywell FCUs in a BWR. This hybrid approach can be useful for anomaly detection using data from existing plant sensors. The ultimate 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 failures. 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 LWRs.

Key Publications

- D.P. Guillen, N. Anderson, C. Krome, R. Boza, L.M. Griffel, J. Zouabe, A. Al Rashdan, "A RELAP5-3D/LSTM model for the analysis of drywell cooling fan failure," *Progress in Nuclear Energy* vol. 130, no. 103540, 2020. https://doi.org/10.1016/j.pnucene.2020.103540
- A.Y. Al Rashdan, K.M. Giraud, L.M. Griffel, D.P. Guillen, M.R. Kunz, H.S. Abdel-Khalik, A. Varuttamaseni, "An Applied Strategy for Using Empirical and Hybrid Models in Online Monitoring," Idaho National Laboratory Report EXT-20-00556.

Sponsor/Program

Department of Energy, Light Water Reactor Sustainability Program

DOE Office of Science, Office of Workforce Development for Teachers and Scientists, Science Undergraduate Laboratory Internship Program

A.43. Validation of Coupled Moltres, SAM, and BISON for the MPCMIV Benchmark Exercise

Report Participants

Travis Mui[1], Dean Price[1], Tomasz Kozlowski[1]

1 University of Illinois at Urbana-Champaign

Scientific Achievement

A problem of significant interest in the nuclear industry is pellet cladding interaction, a fuel failure mode that can significantly limit the performance and marketability of a reactor by reducing the extension of power uprates with higher burnup fuels. With all this in mind, the multiphysics pellet cladding mechanical interaction validation (MPCMIV) benchmark was organized under the Organization for Economic Cooperation and Development Nuclear Energy Association Expert Group on Multi-Physics Experiment Data, Benchmarks, and Validation through the efforts of N.IN.E in collaboration with Studsvik. The goal of the MPCMIV benchmark is to investigate a suitable experiment that calls for the tight coupling of reactor physics, thermal-hydraulics, and fuel performance tools to obtain a high-fidelity result. Our team at the UIUC will leverage the MultiApps capability of MOOSE to couple Moltres (reactor physics), SAM (thermal-hydraulics), and BISON (fuel performance) to validate against this benchmark problem.

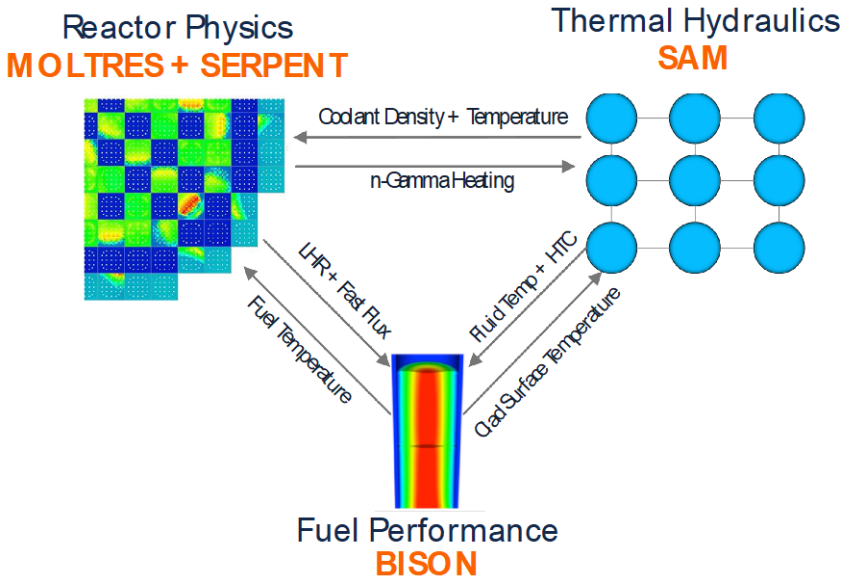


Figure A-77. Coupling scheme of Moltres + Serpent, SAM, and BISON codes that will be used in the UIUC effort.

Significance

Preliminary work has begun with the coupling of SAM with BISON as a novel demonstration to simulate the in-core domain of the experiment loop in this benchmark exercise. This capability was verified and assessed for conservativity and validated against transient benchmark measured data (fuel rodlet elongation and ramp rig outlet flow temperature). The restart capability was also leveraged to perform an initial base irradiation of the fuel rodlet in BISON before modeling the cold ramp experiment transient with both coupled codes. This work is in progress.

Key Publications

Mui, T. Kozlowski, T. (2020) “Preliminary Fuel Performance and Thermal Hydraulic Modeling of the MPCMIV Benchmark,” *Transactions*, vol. 123, no. 1, PP. 1583-1586, 2020.

Sponsor/Program

Nuclear Energy

A.44. VERA Users Group

Report Participants

Brendan Kochunas[1]

1 University of Michigan

Scientific Achievement

This project provided support to VERA users on the reactivity insertion accident application through debugging models, developing code improvements, and performing analyses.

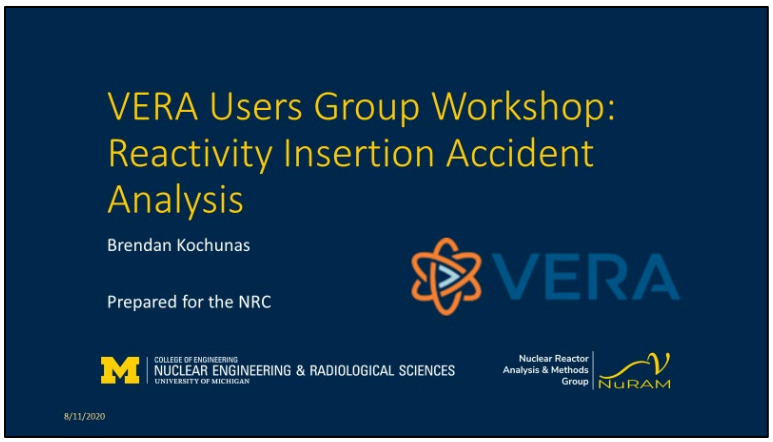


Figure A-78. VERA Users Group Workshop for U.S. NRC on RIA applications with VERA.

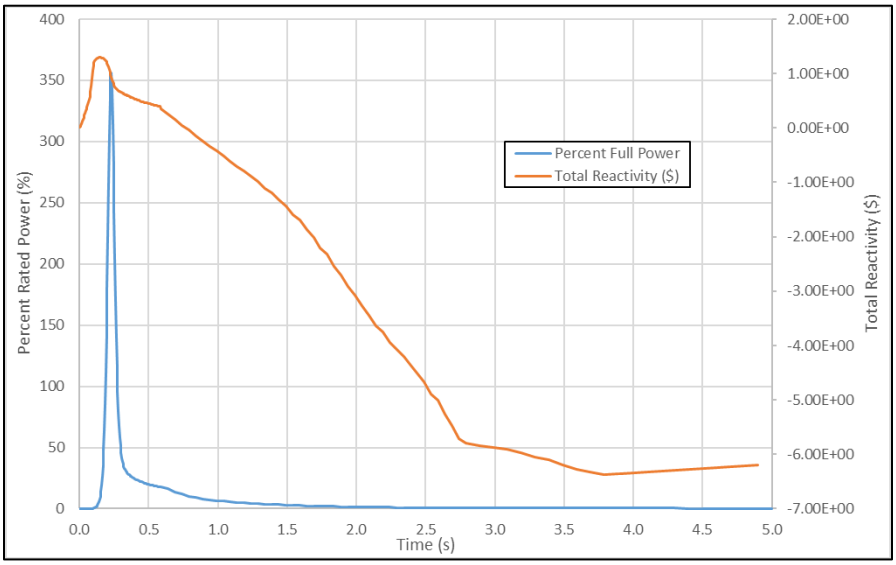


Figure A-79. Reactivity insertion accident results from VERA for VERA benchmark problem 9 at HZP.

Significance

The impact of this work was to allow users at the Electric Power Research Institute and Westinghouse to successfully run reactivity insertion accident calculations for analysis and comparison to their existing reports and methods. This project also supported the development of a workshop on reactivity insertion accident applications for VERA given to the U.S. Nuclear Regulatory Commission.

Key Publications

- Kochunas, B. (2020) “VERA Users Group Workshop: Reactivity Insertion Accident Analysis,” presentation, Aug. 11, 2020.
- Kochunas, B. (2020) “VERA-CS Analysis of CNN-MK-ADJ,” Technical Report CASL-P-2018-1546-001, Revision 1, Consortium for Advanced simulation of Light Water Reactors.

Sponsor/Program

VERA Users Group

A.45. Westinghouse VERA Licensees, CASL AMA Lead and VERA Industry User, VERA User Group Steering Committee Member

Report Participants

Fausto Franceschini[1]

1 Westinghouse

Scientific Achievement

As the CASL Advanced Modeling Application Focus Area Lead and as a member of the VERA User Group Steering Committee, I routinely apply Virtual Environment for Reactor Analysis (VERA) to perform reactor analysis to improve reactor operation by analyzing and resolving operational issues that challenge the current industry reactor simulation toolkit. The scientific and industrial relevance of the simulations performed can be ascertained in the publications listed below. The greatest majority of the VERA simulations that I have been performing have been run on the INL HPC.

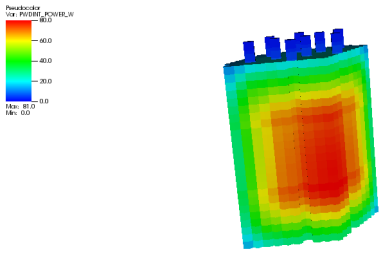


Figure A-80. AP1000 Startup: VERA Predicted Fission Source Distribution.

Significance

VERA applications over the course of the year have enabled the successful development of a high-fidelity multiphysics tool to perform reactor analysis at a resolution that cannot be achieved by the tools developed by and available to industry. This successful development has been achieved thanks to the VERA code testing, validation, and application by accessing INL HPC resources. VERA has now been successfully employed to simulate the core operation of around 250 reactor cycles from decades of commercial reactors of different types, including the AP1000, where VERA had been employed in a "blind" benchmark to simulate the reactor startup with its predictions in outstanding agreement with the measurements. VERA will also be applied to advanced fuel simulations for licensing support, ATF, and high-burnup high-enrichment fuel. Its continued application, together with access to INL HPC resources to effectively perform these advanced simulations, will continue to make a difference in the nuclear industry.

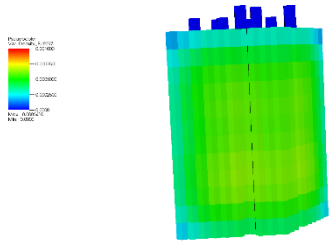


Figure A-81. AP1000: VERA Predicted Power Distribution (EOC).

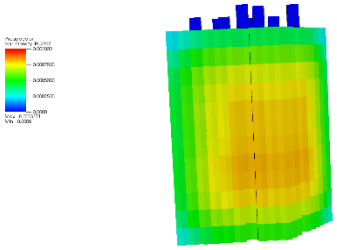


Figure A-82. AP1000: VERA Predicted Power Distribution (MSHIM).

Key Publications

- F. Franceschini et. al., “Results of VERA Application to the AP1000® PWR Startup”, *Physor*, Cambridge, United Kingdom, March 29th–April 2nd, 2020.
- F. Franceschini et. al. “Modeling of Westinghouse Advanced Fuels EnCore and ADOPT with the CASL Tools,” Top Fuel, Seattle, WA, Sept. 2019 (USA).
- F. Franceschini et. al., “Implementation of Westinghouse ATF into PWRs: Fuel Cycle Economics and Operational Flexibility Improvements”, Top Fuel, Prague (Czech Republic), Sept. 30–Oct. 4, 2018.

Sponsor/Program

Consortium for Advanced Simulation of Light Water Reactors

Nuclear Energy Advanced Modeling and Simulation

Light Water Reactor Sustainability

Industry

Appendix B

NUCLEAR REGLUATORY COMMISSION

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B.1. DOE/NEAMS Tools–Advanced Non-Light-Water Reactors

Report Participants

Joseph Kelly[1]

1 US Nuclear Regulatory Commission

Scientific Achievement

This research uses DOE and Nuclear Energy Advanced Modeling and Simulation (NEAMS) tools that are part of BlueCRAB for the analysis of non-light-water reactors. For example, they could be used to develop a reference plant model for heat-pipe cooled microreactors.

Significance

This study demonstrated the ability to use DOE/NEAMS tools for advanced non-light-water reactor licensing calculations.

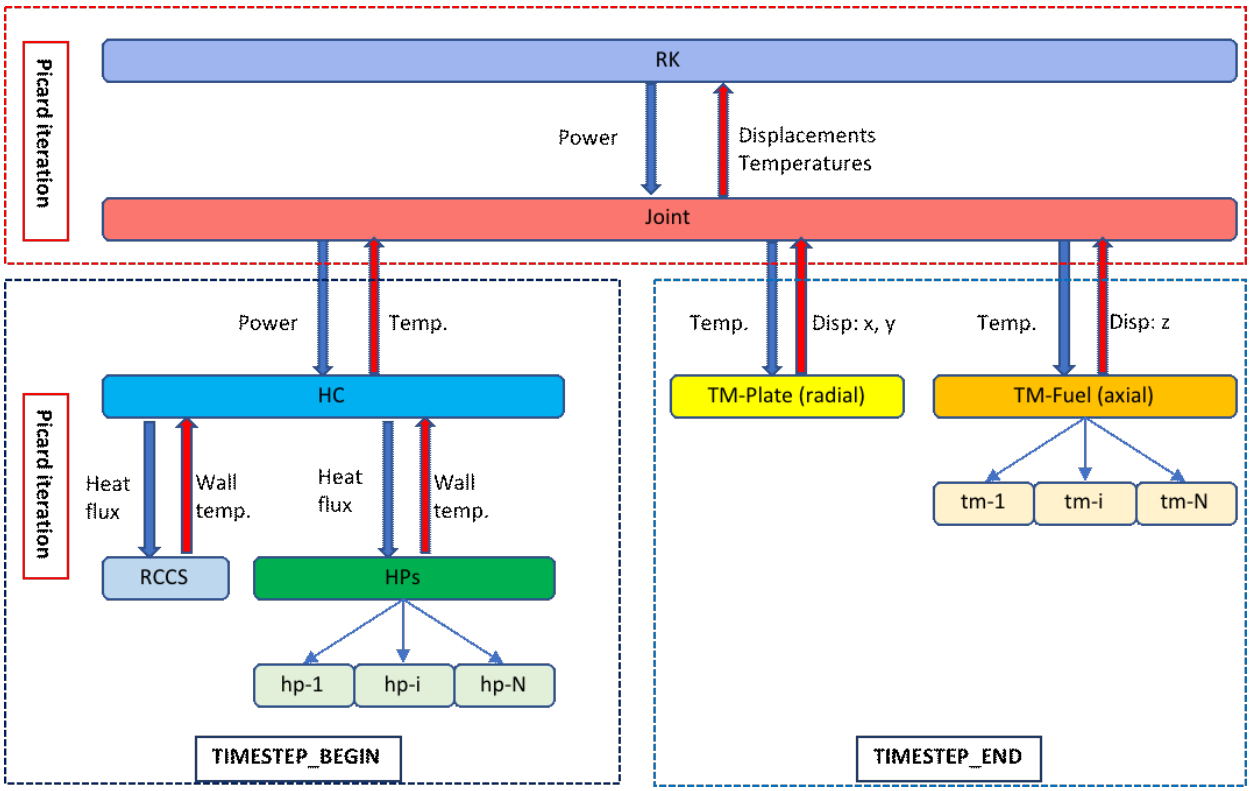

Figure B-1. Schematic of the multiphysics coupling method for heat-pipe microreactors.

Key Publications

G. Hu, R. Hu, J.M. Kelly, J. Ortensi, "Multiphysics Simulations of Heat Pipe Micro-Reactors" ANL-NSE-19-25, https://doi.org/10.2172/1569948. https://www.osti.gov/servlets/purl/1569948.

Sponsor/Program

Nuclear Regulatory Commission

Appendix C

LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

Table of Contents

C.1. AB Initio Modeling of Molten Salts

Report Participants

Benjamin Beeler[1,2], Ruchi Gakhar[2] , Gorakh Pawar[2], Yuxiao Lin[2]

1 North Carolina State University

2 Idaho National Laboratory

Scientific Achievement

Calculated the density of the LiCl-KCl pseudobinary molten-salt system over the entire range of compositions for a variety of temperatures in the liquid phase. In this project, ab initio molecular dynamics (AIMD) simulations were performed to establish equilibrated liquid structures, obtain the equilibrium volume, and determine the bulk modulus at each individual temperature and composition. This work provides a basis for a wide swath of thermophysical property investigations via AIMD into the LiCl-KCl molten-salt system.

Significance

Each unique molten-salt system possesses different properties and interactions and thus must be modeled uniquely. One such area for computational implementation that includes this individuality is in the selection of the van der Waals (vdW) dispersion interaction. Within the Vienna ab initio Simulation Package (VASP), there are a number of modifications to the exchange correlation energy to account for dispersion; however, there are also individual vdW exchange correlation functionals. Both types of vdW inclusions have been previously utilized to study ionic liquids, but no standards have been developed specifically for molten salts or for the LiCl-KCl system. Establishing a given dispersion interaction was undertaken by calculating the equilibrium volume for the LiCl, LiCl-20KCl (mol percent), and KCl systems at 1100 K. A comparison of the selected vdW dispersion interactions is included in Figure C-1.

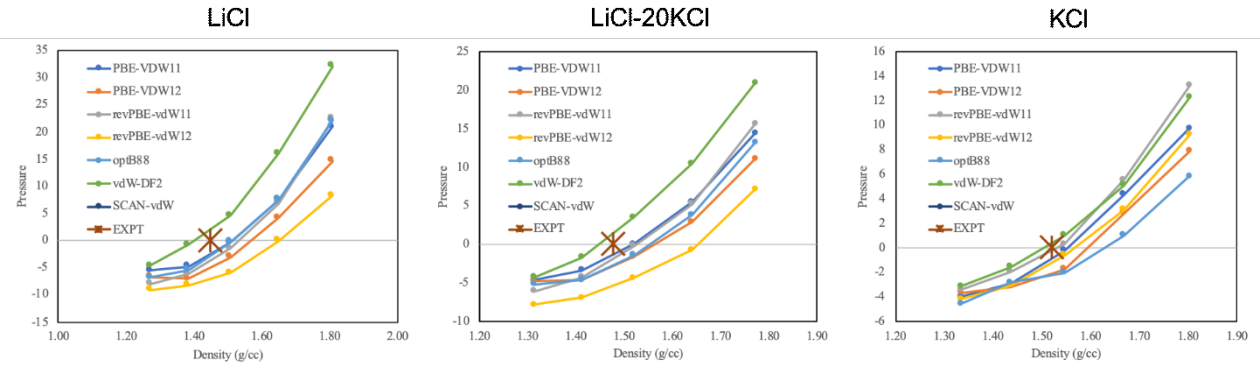

Figure C-1. Comparison study of different van der Waals dispersion formulations within the density functional theory for predicting density of the LiCl-KCl system.

This study pointed us towards the DF2 van der Waals functional, as this implementation most accurately predicted the general trends in density as a function of composition. Subsequently, the densities for the entire compositional and temperature phase space were calculated and are displayed in Figure C-2. There is some noise within the data, but this is to be expected, as these are systems of approximately 200 atoms equilibrated over a period of a few picoseconds. However, this provides an excellent qualitative aggreement with experimental densities, consistently slightly underpredicting the density. The work can now serve as the basis to determine fundamental thermophysical properties of the LiCl-KCl system, such as heat capacity, themal conductivity, melting point, and viscosity.

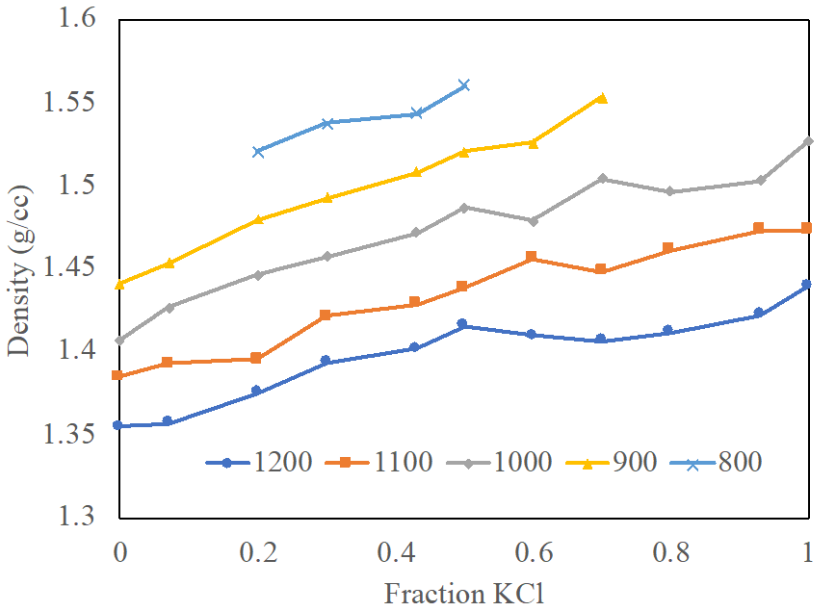

Figure C-2. Density of LiCl-KCl as a function of composition and temperature.

Key Publications

Publications to be submitted.

Sponsor/Program

Laboratory Directed Research and Development

C.2. Atomic Kinetic Monte Carlo Simulations of the Effects of Additives on Radiation-Induced Segregation in Fenicr Alloys

Report Participants

Yongfeng Zhang[1], Anus Manzoor[2], Dilpuneet Aidhy[2]

1 University of Wisconsin-Madison

2 University of Wyoming

Scientific Achievement

Radiation-induced segregation (RIS) in austenitic steels causes a redistribution of alloying elements, such as the depletion of Cr from grain boundaries, and degrades the corrosion resistance, potentially facilitating irradiation-assisted stress corrosion cracking. Previous research indicates that RIS in austenitic steels can be effectively mitigated by introducing minor additives that trap point defects, but with discrepancies in the experimental measurements. Taking atomic scale inputs on the interaction between vacancy and additives in this project, atomic kinetic Monte Carlo (AKMC) simulations are carried out to study the effect of additives on RIS in FeNiCr alloys. An AKMC model for RIS in ternary alloys is developed using the SPPARKS framework in FY19, and we studied the effects of temperature, dose rate, grain size, and additives in FY20.

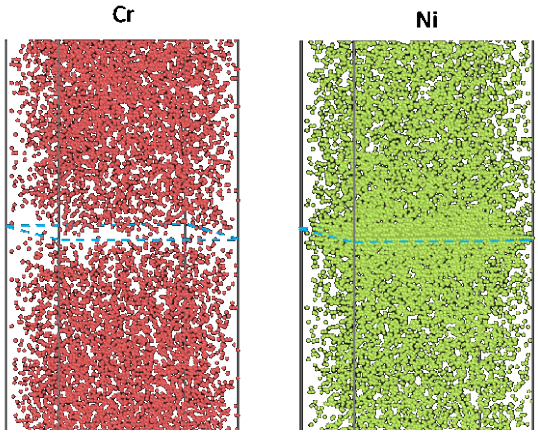

Figure C-3. Atomic configurations showing Cr depletion and Ni enrichment at a grain boundary (enclosed by the blue dash line).

Significance

Using the Fe12Ni18Cr model alloy, the effects of temperature, dose rate, and grain size are studied using AKMC simulations with a bi-crystal model. As shown in Figure C-3, in austenitic steels, Cr depletes and Ni enriches from grain boundaries under irradiation, primarily due to the inverse Kirkendall effect. The total amount of Cr depletion increases with a decreasing dose rate (dpa/s) and with an increasing grain size (see Figure C-4) and initially increases and then decreases with an increasing temperature. The effects of additives, such as Y and Hf, are studied using the Fe18Cr model alloy. Although both Y and Hf are found to be effective in delaying Cr depletion, the beneficial effect is found to be effective only at low doses. On the one hand, the strong binding between vacancy and additives suppresses the RIS of Cr and Ni. On the other hand, it also leads to the RIS and precipitation of the additives themselves (see Figure C-5 for the results for Y as an example). As such, additives become depleted from the matrix, thereby losing the effectiveness of suppressing the RIS. This new finding explains the inconsistent experimental data in the literature. The AKMC results have two important indications. First, this suggests our experimental collaborators within the same LDRD project to

characterize RIS and precipitation of additives, to confirmation the modeling findings. Second, there may exist a combination of vacancy-additive binding, additive diffusivity, and additive concentration that maximizes the beneficial effect. Different amounts of additives may be added based on the total dose of irradiation an alloy may receive during its lifetime in service. This will be searched for using AKMC simulations to guide the future design of modified steels. The combination of modeling and experiments may accelerate the development of modified autenitic steels with additives that are resistant to RIS, thereby mitigating the detrimental effect of irradiation-assisted stress corrosion cracking.

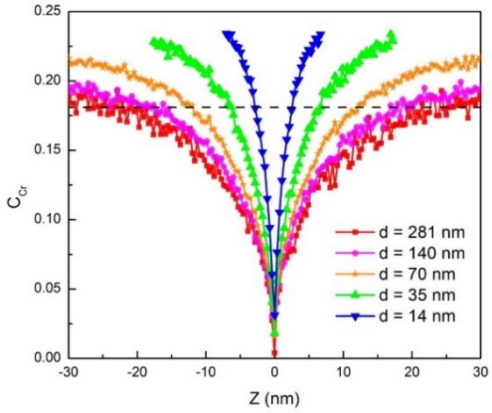

Figure C-4. Cr concentration profile near a GB with different grain sizes.

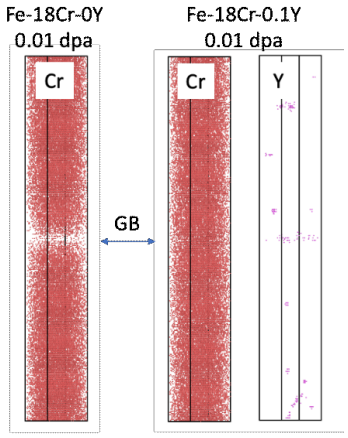

Figure C-5. Atomic configuration showing Y segregation and precipitation.

Key Publications

- D. Morgan and Y. Zhang, 2020. Comment on “Thermal vacancies in random alloys in the single-site mean-field approximation”, Phys. Rev. B 101, 136101.
- A. Manzoor, Y. Zhang, and D. Aidhy, 2020. “Factors affecting the vacancy formation energy in Fe70Ni10Cr20 random concentrated alloy,” under review.
- Y. Zhang, A. Manzoor, D. Aidhy, M. Song, X. Lou, and L. He, “The Effect of Minor Additives on Radiation Induced Segregation in Austenitic Steel Alloys,” TMS 2020, San Diego, CA, Feb 23—27, 2020.

Sponsor/Program

Laboratory Directed Research and Development

C.3. Atomistic Investigation of the Thermal Stability of Silica Nanofiber

Report Participants

Rajni Chahal[1], Gorakh Pawar[2], Bjorn Vaagensmith[2]

1 The University of Texas at Arlington

2 Idaho National Laboratory

Scientific Achievement

The amorphous silica (SiO_2) nanowires of two different diameters (D=1.75 nm and 2.85 nm) are used to study the thermal stability of the nanofibers (NFs). Single-phase step-heating method is used to slowly heat the NFs using the reactive force-field potential in LAMMPS. A sudden increase in the potential energy curve is observed at the start of the melting of the NF (marked as Point A in Figure C-6).

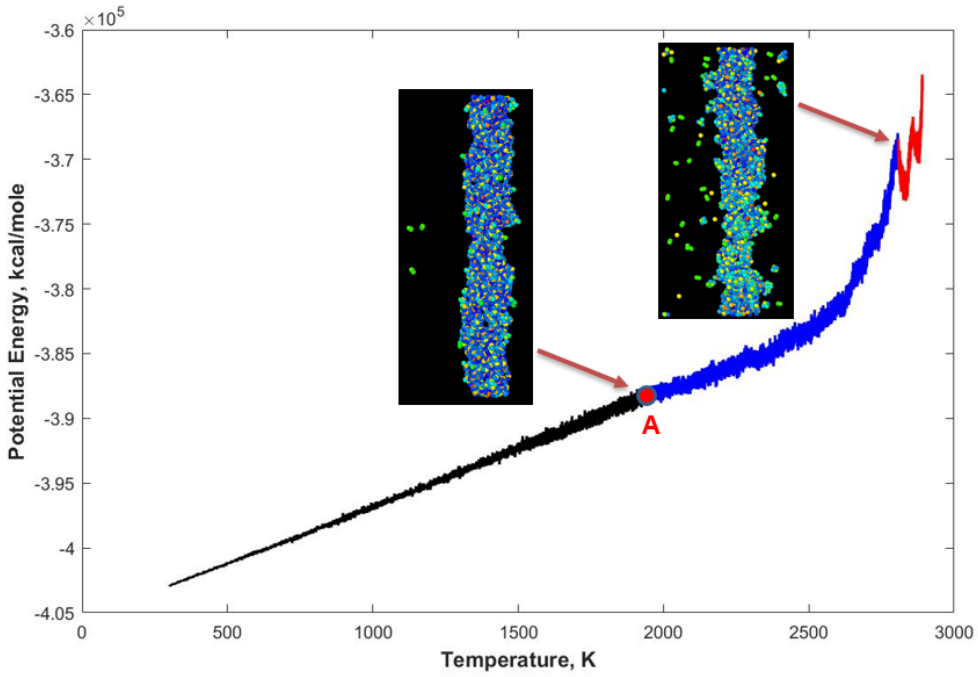

Figure C-6. Variation in potential energy during the NF heating process (NF diameter = 1.75 nm).

Figure C-7 shows the change in the NF microstructure as the NF starts to melt at nearly 1957 K. After adjusting for the superheating of the material in the molecular modeling, the melting temperature (Tm) for NF can be adjusted as Tm=TA/1.23. For NF of D=1.75 nm, the Tm is approximately 1590 K. The values calculated using molecular simulations using INL HPC resources are in good agreement with the experimental values obtained at INL. A melting point depression is observed as the NF diameter decreases, which indicates that, due to the increased surface energy, the Tm of the nanostructures tends to be lower than that of the bulk material.

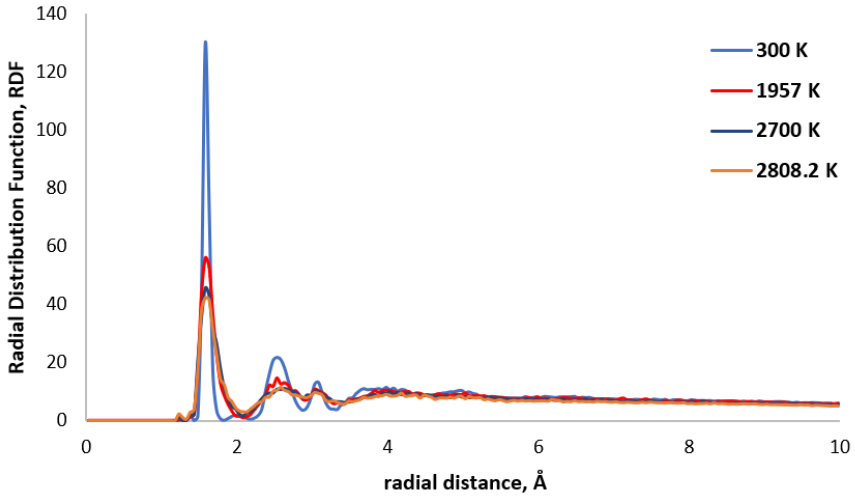

Figure C-7. Comparison of RDF during NF heating process (NF diameter=1.75 nm).

Significance

SiO_2 NF is a popular material used in the micro- and nanoelectronic devices, optical fibers for telecommunications, and the glass fibers that form fiber-reinforced polymer composites. A fundamental understanding of the thermal stability of silica NFs would facilitate increasing their reliability when integrated into functional nanodevices. The molecular simulations conducted using INL HPC resources have confirmed the melting point depression phenomenon in the SiO_2 NFs.

Key Publications

- Chahal, R., Pawar, G., Adnan, A., Vaagensmith, B., Ring, T., Reeves, J. (2020). "Melting temperature calculation of Silica Nanofibers and their mats: A Molecular Dynamics and Experimental Study." in progress.
- Chahal, R., Pawar, G., Adnan, A., Vaagensmith, B., Ring, T., Reeves, J. (2020). "Three-Dimensional Stochastic Modelling of Silica Nanofiber Mats," in progress.

Sponsor/Program

Laboratory Directed Research and Development

C.4. Automated Fuel Performance Modeling with 1,977 EBR-II Metallic Fuel Pins Using BISON Code with FIPD and IMIS Databases

Report Participants

Kyle M. Paaren[1], Micah Gale[1], Matthew J. Kerr[1], Pavel Medvedev[1], Douglas Porter[1], Nancy Lybeck[1]

1 Idaho National Laboratory

Scientific Achievement

Using the BISON fuel performance code, we conducted simulations of an automated process to read initial and operating conditions from the Fuels Irradiation and Physics Database (FIPD) and Integral Fast Reactor Materials Information System (IMIS) databases, which contain metallic fuel data from the EBR-II. The work demonstrates an integrated framework to access the vast majority of EBR-II experimental fuel pin data to support the rapid development of fuel performance models for next-generation metallic fuel systems. Between IMIS and FIPD, there is enough information to conduct 1,977 unique EBR-II metallic fuel pin histories from 24 different experiments, at varying levels of details between the two databases (IMIS was originally developed during the Integral Fast Reactor program). Each of these histories includes a high-resolution power history, flux history, coolant channel flow rates, and coolant channel temperatures. FGR, cumulative damage fraction, fuel axial swelling, cladding profilometry, and burnup were all simulated in BISON. The results were compared to post-irratiated examination (PIE) results for the demonstration of automated BISON modeling and statistical fitting to PIE data. A generic BISON input file, coupled with IMIS and FIPD-simulated burnup results, was in agreement with the PIE measurements and calculations. Cladding profilometry, FGR, and fuel axial swelling were found to be in agreement with PIE measurements, depending on the physics used within the BISON input files. Cumulative damage fraction values were assessed to see if the pins may have failed by having a value above one. This work suggests that the continued development of an automation tool for BISON should focus on the inclusion of the Fast-Flux Test Facility experimental data for a larger database for metallic fuel, improved physical models to better capture physics, such as contact, and a more detailed comparison with available PIE data to further the BISON model development.

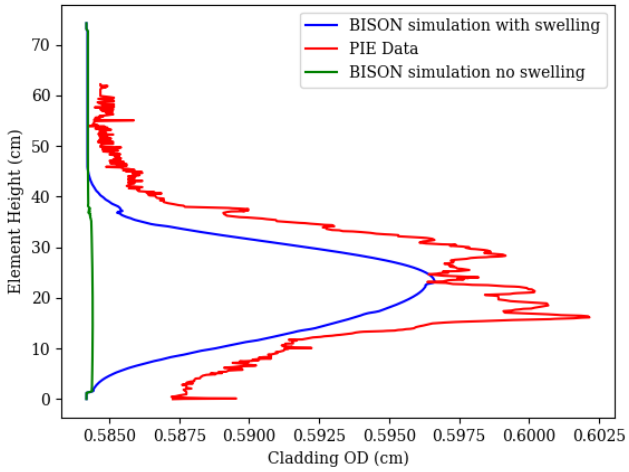

Figure C-8. X486 J651 (SS316 cladding) swelling comparison.

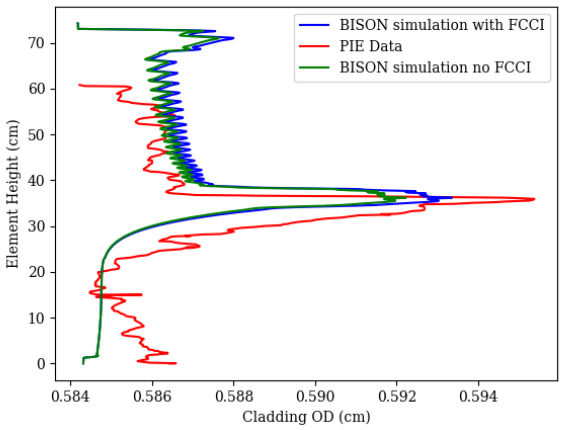

Figure C-9. X447A DP11 Cladding profilometry with 0.2 friction coefficient and 0.2 anisotropic swelling factor.

Significance

Metallic fuel models within BISON are able to be assessed using historic PIE data housed within the IMIS and FIPD databases. Initial conditions and boundary conditions within IMIS and FIPD were used to generate BISON fuel performance simulations for PIE comparison. This has led to to the creation of new BISON material objects to describe different phenomena seen in PIE data, but not currently represented in BISON simulations. The statistical fitting of modeling parameters to PIE data has been conducted to evaluate new and current models, such that a probabilistic risk assessment may be performed on new fuel designs. This is important, as fuel performance predictions are needed for next-generation reactor designs that are currenty undergoing licensing.

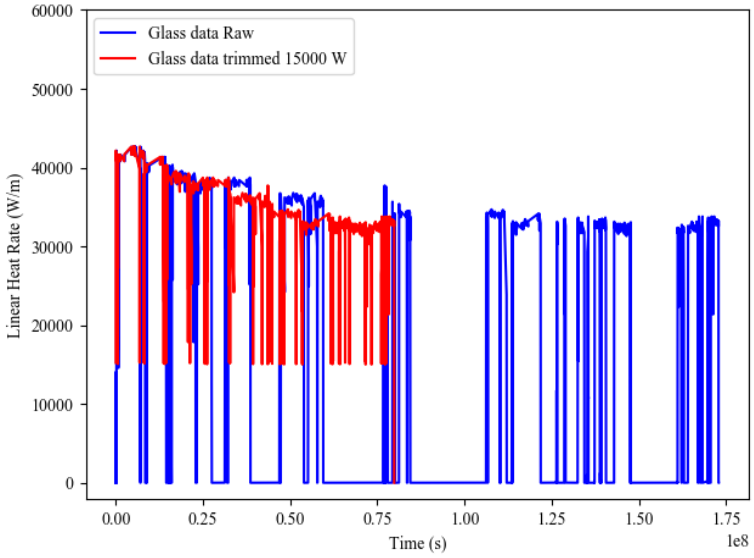

Figure C-10. T653 X430B Power History Raw and Trimmed.

Key Publications

- Paaren, K. M., Gale, M., Kerr, M. J., Medvedev, P. G., Porter, D. L. (2020). "Initial demonstration of Automated fuel performance modeling with 1,977 EBR-II metallic fuel pins using BISON code with FIPD and IMIS databases." *Journal of Nuclear Materials*, in progress.
- Paaren, K. M., Lybeck, N., Mo, K., Medvedev, P. G., and Porter, D. L. (2020). "Cladding Profilometry Analysis of EBR-II metallic fuel pins with HT9, D9, and SS316 cladding," *Journal of Nuclear Materials*, in progress.
- Paaren, K. M., Black, A., Lybeck, N., Mo, K., Medvedev, P. G., and Porter, D. L. (2020). "BISON Fuel Performance Optimization for Experiment X447 and X447A," *Journal of Nuclear Materials*, in progress.

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Laboratory Directed Research and Development

C.5. Development of a Genetic Algorithm to Facilitate EXAFS Data Analysis

Report Participants

Donna Guillen[1], Jeff Terry[2], Shlomo Argamon[2], Min Long[3], Miu Lun Lau[3]

1 Idaho National Laboratory

2 Illinois Institute of Technology

3 Boise State University

Scientific Achievement

The researchers developed a proof-of-concept for the automated processing of extended X-ray absorption fine structure (EXAFS) data using machine learning. A genetic algorithm, inspired by processes of biological evolution, was evaluated and showed success at determining the crystal structure of single component molecules and crystals. Analysis utilizing the genetic algorithm provides information on the local atomic structure of the material around the absorber of interest. A genetic algorithm was developed to expedite the processing of synchrotron EXAFS data.

Significance

The ability to automatically analyze experimental data is essential to support the analysis of scientific measurements from high-throughput data generators, such as in a synchrotron facility where large amounts of data are collected at extremely fast rates. The ability to process such data in situ would optimize the use of these user facilities and enable the user to rapidly adjust data collection parameters and automate the data collection process. EXAFS has been shown to be extremely useful in understanding the local atomic structure of materials of interest in myriad applications, such as materials the synthesis and design of batteries, assessment of material performance for energy materials, and evaluation of radiation damage for nuclear energy applications.

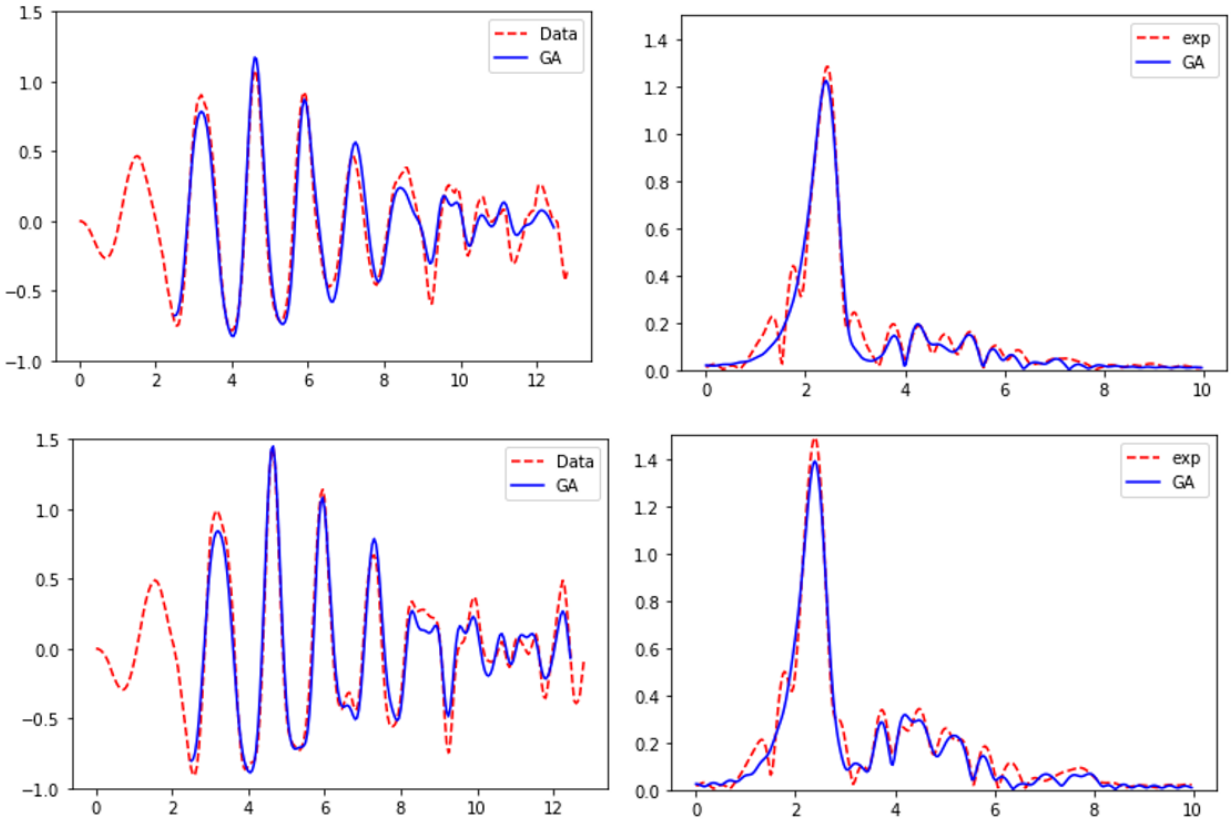

Figure C-11. Results obtained with a genetic algorithm for HfAl3 irradiated in INL's ATR. The top row represents a unannealed sample while the bottom presents an annealed sample.

Key Publications

Terry, J., M.L. Lau, J. Sun, C. Xu, B. Hendricks, J. Kise, M. Lnu, S. Bagade, S. Shah, P. Makhijani, A. Karantha, T. Boltz, M. Oellien, M. Adas, S. Argamon, M. Long, D.P. Guillen, "Analysis of extended X-ray absorption fine structure (EXAFS) data using artificial intelligence techniques," *Applied Surface Science*, vol. 547, 2021. https://doi.org/10.1016/j.apsusc.2021.149059

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Laboratory Directed Research and Development

C.6. Development of Structural Elements in MOOSE

Report Participants

Albert Casagranda[1], Benjamin Spencer[1]

1 Idaho National Laboratory

Scientific Achievement

This project developed new capabilities in MOOSE for beam and shell elements and lumped mass models. This work targeted two specific problems of interest to the nuclear industry, the seismic analysis of nuclear power plant structures and modeling the distortion of fuel assemblies. These simulations are computationally expensive and required the use of HPC resources to complete in a reasonable time. The BISON code was used to perform a simulation of a full fuel assembly that coupled fuel performance and assembly distortion. This model predicted the assembly behavior under various applied power gradients and frictional conditions between the fuel rods and spacer grids in the assembly.

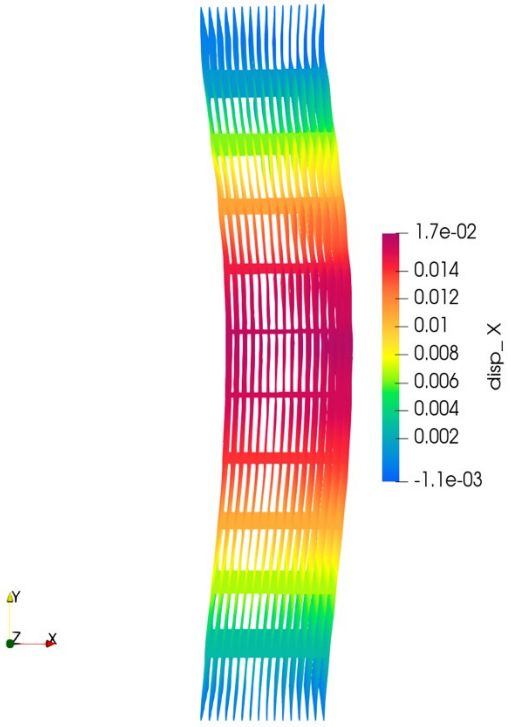


Figure C-12. 16×16 fuel assembly distortion results (displacements and axial direction scaled for clarity).

Significance

Using the beam elements and the mechanism for the strain transfer from a 2D model to a beam model developed in this project, the bowing of a PWR fuel assembly as a result of spatially asymmetric power profiles was analyzed. This model uses a beam representation of the 3D fuel assembly (see Figure C-12). Past studies on this topic have focused on the mechanical deformation of the fuel assembly with a simplistic modeling of the fuel rod elongation, which is the major factor driving the fuel assembly bowing. This study uses sophisticated BISON fuel performance models of the individual fuel rods to capture all the intrinsic mechanisms that cause the elongation of the fuel rod or guide tube and transfer the cladding elongation to the beam models of the fuel elements in the 3D fuel assembly model. This study shows that both the magnitude as well the shape of fuel assembly bowing changes significantly with

variations in the spatial power profile and the fuel rod–spacer grid contact conditions. The distortion due to this effect could have serious consequences for the safe shutdown of the reactor during operation (i.e., an incomplete control rod insertion) and also the removal of fuel assemblies during normal outages for refueling the reactor.

Key Publications

- Veeraraghavan, S., Coleman, J., "Effect of non-vertically propagating earthquake waves and nonlinear soil-structure interaction on nuclear facility response", 25th International Conference in Structural Mechanics in Reactor Technology, Charlotte, NC, August 4-9, 2019. (INL/CON-18-51251)
- Veeraraghavan, S., Casagranda, A., Spencer, B., "Modeling fuel assembly distortion in light water reactors using Bison", TopFuel 2019 conference, Seattle, WA, September 22-26, 2019. (INL/CON-19-52771)

Sponsor/Program

Laboratory Directed Research and Development

C.7. Factors Affecting the Vacancy Formation Energy in Fe70Ni10Cr20 Random Concentrated Alloy

Report Participants

Anus Manzoor[1], Yongfeng Zhang[2,3], Dilpuneet S. Aidhy[1]

1 University of Wyoming

2 University of Wisconsin-Madison

3 Idaho National Laboratory

Scientific Achievement

This study aims to understand the role of various factors, such as the first and second nearest neighbor chemistry, structural arrangements of nearest neighbors, vacancy volume, atomic relaxation, and magnetic moments of first nearest neighbors, on the vacancy formation energy in random Fe70Ni10Cr20 austenitic stainless steel. This work is aimed at developing a generic understanding of defect energetics in concentrated alloys, including high entropy alloys.

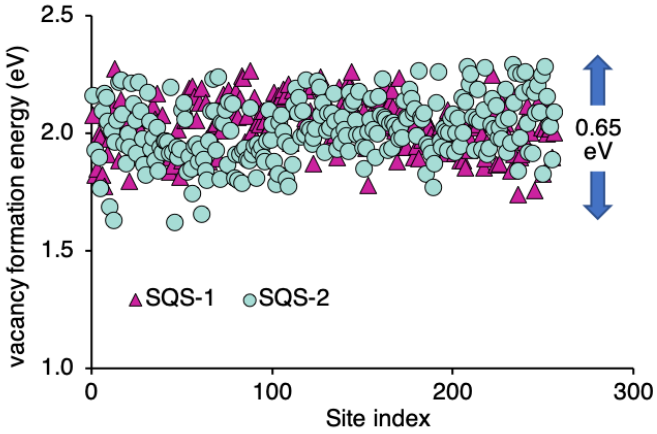


Figure C-13. Vacancy formation energy of every atomic site in two SQS structures containing 256 atoms. The maximum variation in the vacancy formation of 0.65 eV is observed in one of the SQS structure.

Significance

DFT calculations are performed on two different special quasirandom (SQS) structures of Fe70Ni10Cr20 to explain the large variation of vacancy formation energy observed in different atomic environments in a given alloy composition. This works 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 a given alloy. Surprisingly, the large variation is primarily due to the arrangement of first nearest neighbors (i.e., despite 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

Manzoor A., Zhang Y., Aidhy D.S. 2020. “Factors affecting the vacancy formation energy in Fe70Ni10Cr20 random concentrated alloy.” Submitted to the Acta Materialia journal, under review.

Sponsor/Program

Laboratory Directed Research and Development

C.8. Local Mechanics for MARMOT Phase-Field Module

Report Participants

Lucas Robinson[1], Larry Aagesen[2]

1 Purdue University

2 Idaho National Laboratory

Scientific Achievement

Thermal and externally applied stresses play an important role in the microstructural evolution of spark plasma sintered materials, including nuclear fuels. Characterizing the mechanical, electrical, and thermal conditions under which desirable densification occurs in a computationally efficient way is an important step in informing experimental efforts to improve and optimize the fuel sintering process.

Significance

Identified and patched a bug in the MARMOT distribution allowing for the incorporation of new physics in the phase-field module. The calculation of the off-diagonal Jacobian precluded the use of mechanical energetic contributions when using the phase-field module. The purpose of this report is to renew Lucas' account so that he can submit his changes to the MARMOT code base and validate the code against an analytical thermal eigenstrain model from the literature. After validation, local plasticity will be introduced into the model.

Incorporating Plasticity into Phase Field

Free energy functional:

$$\Omega = \int_V (\omega_{mw} + \omega_{grad} + \omega_{chem} + \omega_e) dV$$

For single particle (grain) in void phase:

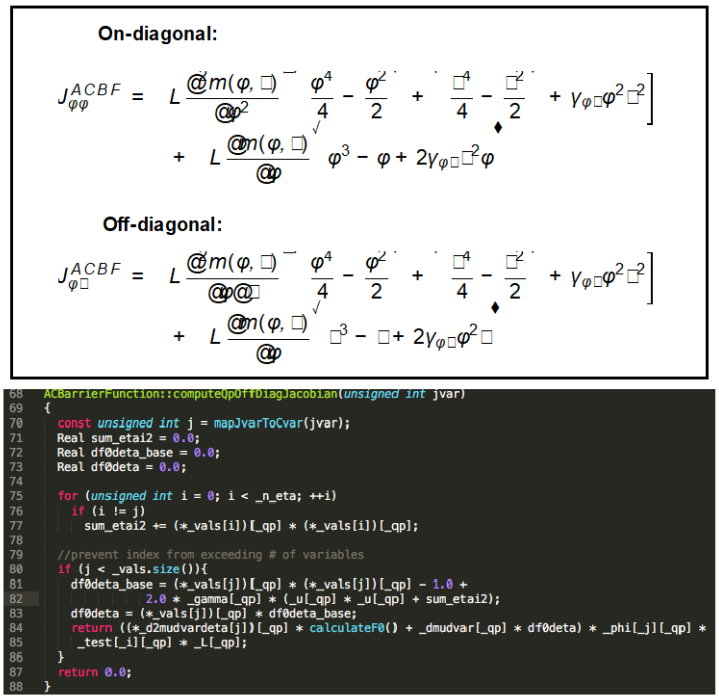
$$\Omega = \int_V \left(m(\phi,\eta)\left[\left(\frac{\phi^4}{4} - \frac{\phi^2}{2}\right) + \left(\frac{\eta^4}{4} - \frac{\eta^2}{2}\right) + \frac{\gamma_{\phi\eta}}{2}\phi^2\eta^2 + \frac{1}{4}\right] + \frac{\kappa}{2}|\nabla\phi|^2 + \frac{\kappa}{2}|\nabla\eta|^2 + h_\phi\omega_\phi + h_\eta\omega_\eta + \frac{1}{2}\left(C^\eta_{ijkl}h_\eta(\eta) + C^\phi_{ijkl}h_\phi(\phi)\right)\epsilon_{ij}\epsilon_{kl}\right) dV$$

Allen-Cahn:

$$\frac{\partial\phi}{\partial t} = -L\frac{\delta\Omega}{\delta\phi}$$

$$= -L\left[m(\phi,\eta)\left(\phi^3 - \phi + \gamma_{\phi\eta}2\eta^2\phi\right) + \frac{\partial m(\phi,\eta)}{\partial\phi}\left[\left(\frac{\phi^4}{4} - \frac{\phi^2}{2}\right) + \left(\frac{\eta^4}{4} - \frac{\eta^2}{2}\right) + \gamma_{\phi\eta}\phi^2\eta^2\right] - \kappa\nabla^2\phi + \frac{\partial h_\phi}{\partial\phi}\omega_\phi + \frac{1}{2}C^\phi_{ijkl}\frac{\partial h_\phi}{\partial\phi}\epsilon_{ij}\epsilon_{kl}\right]$$

Figure C-14. A slide outlining the free energy formulation—including an elastic energy contribution—and Allen-Cahn evolution equation for a nonconserved order parameter representing the particle phase (η) suspended in a vacuum phase (ϕ).




```
ACBarrierFunction::computeQpOffDiagJacobian(unsigned int jvar)
{
  const unsigned int j = mapJvarToCvar(jvar);
  Real sum_etai2 = 0.0;
  Real df0deta_base = 0.0;
  Real df0deta = 0.0;

  for (unsigned int i = 0; i < _n_eta; ++i)
    if (i != j)
      sum_etai2 += (*_vals[i])[_qp] * (*_vals[i])[_qp];

  //prevent index from exceeding # of variables
  if (j < _vals.size()){
    df0deta_base = (*_vals[j])[_qp] * (*_vals[j])[_qp] - 1.0 +
                   2.0 * _gamma[_qp] * (_u[_qp] * _u[_qp] + sum_etai2);
    df0deta = (*_vals[j])[_qp] * df0deta_base;
    return ((*_d2mudvardeta[j])[_qp] * calculateF0() + _dmudvar[_qp] * df0deta) * _phi[_j][_qp] *
     _test[_i][_qp] * _L[_qp];
  }
  return 0.0;
}
```

Figure C-15. On- and off-diagonal Jacobian elements of the Allen-Cahn equation (top) and the proposed indexing change implemented in the code (bottom) that allows for the addition of other nonlinear variables.

Key Publications

Publication(s) are expected studying the impact of thermal expansion and applied stresses on particle morphology and densification.

Sponsor/Program

Laboratory Directed Research and Development

C.9. Modeling and Simulation for Fuel Cycle Separations

Report Participants

Valmor de Almeida[1], Kevin Lyon[2], Taha Azzaoui[1]

1 University of Massachusetts Lowell

2 Idaho National Laboratory

Scientific Achievement

Flowsheet-level models do not account for explicilty coupled models of water, acid, and radiolysis. The present work is aimed at developing an extensive flowsheet simulation capability using models for solvent extraction employed in cross-cutting applications in nuclear separations, safeguards, materials protection, special materials for national security and nonproliferation, critical materials, mining, and metallurgy applications. Our approach takes into account the participating aqueous, organic, and vapor phases and the homogeneous and heterogeneous chemical reactions, coupled with the radiolysis and hydrolysis of the aqueous and organic phases.

Significance

An important enabling component of the current research is the computational framework developed to allow for the dynamic coupling of multiple stages of solvent extraction. This parallel development, named Cortix (https://cortix.org), facilitates the time-coupling of multiple contacting stages or multiple contacting banks of typical solvent extraction equipment.

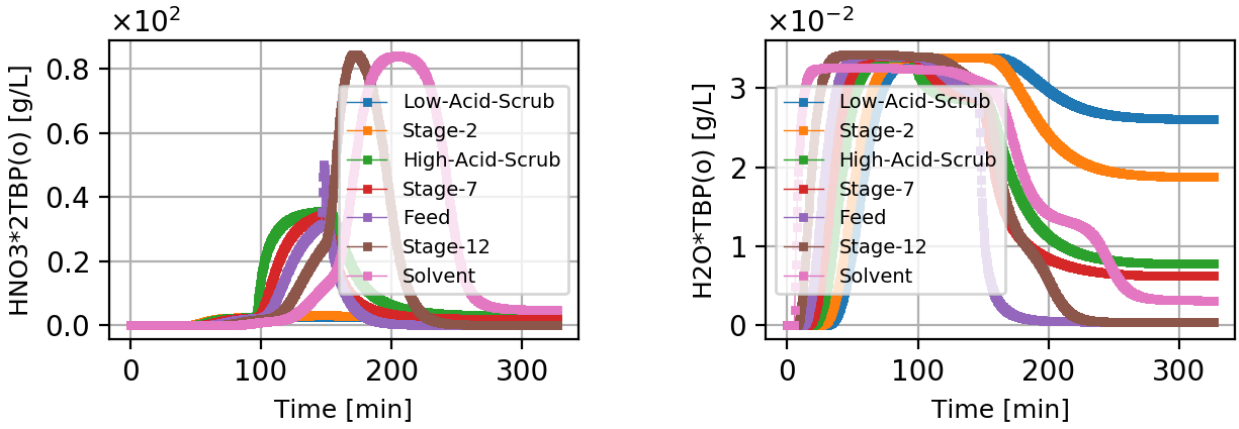


Figure C-16. Simulation of the extraction of nitric acid and water in a mixture of tributylphosphate and n-dodecane for various stages in a contactor bank.

Key Publications

- Azzaoui, T., Lyon, K. L, de Almeida, V. F. (2019) “Design and Implementation of a Flowsheet Solvent Extraction Simulator,” *Transactions of the American Nuclear Society*, vol. 120, pp. 106–9.
- de Almeida, V. F., Azzaoui, T., and Lyon, K. L. (2019) “Solvent Extraction Flowsheet-Level Modeling and Simulation with Radiolysis,” Global 2019 Proceedings, pp 386–9.
- Talk presented by an undergraduate student: Design and Implementation of a Flowsheet Solvent Extraction Simulator; Taha Azzaoui, Kevin Lyon, and Valmor F. de Almeida, ANS Annual Meeting, 11 June 2019 Minneapolis, MN, Session: University Research in Fuel Cycle and Waste Management II, https://www.ans.org/meetings/file/view-901/.

- Talk presented: Solvent Extraction Flowsheet-Level Modeling and Simulation with Radiolysis; Valmor F. de Almeida, Taha Azzaoui, and Kevin Lyon, Global 2019 International Fuel Cycle Conference, 24 Sep 2019, Seattle, WA.
- Talk presented: Solvent Extraction Flowsheet-Level Modeling and Simulation with Radiolysis, Valmor F. de Almeida, Taha Azzaoui, Kevin L. Lyon, AIChE Annual Meeting, 13 November 2019, Orlando, FL, (https://aiche.confex.com/aiche/2019/meetingapp.cgi/Paper/577507).
- Talk presented: Liquid-Liquid Micromixing by Combined Centrifugal and Shearing Forces: Modeling and Simulation with Front Tracking, Valmor F. de Almeida, Hyunkyung Lim, James Glimm, and Xiaolin Li, 7th European Seminar in Computing, GPU/HPC for Industrial Applications MS (https://www.esco2020.femhub.com/minisymposia/), 10 June 2020, Online, Pilsen, Czech Republic.

Sponsor/Program

Laboratory Directed Research and Development

Fuel Cycle Research and Development

C.10. Modeling and Simulation of TREAT with Thermal Graphite Model Validation

Report Participants

Gavin Ridley[1], Logan Harbour[2], Derek Gaston[2], Mark DeHart[2], Kord Smith[2], Guillaume Giudicelli[1]

1 Massachusetts Institute of Technology

2 Idaho National Laboratory

Scientific Achievement

High-fidelity neutron transport transient simulations with multiphysics feedback were successfully led for the TREAT reactor with a newly developed reactor physics code called MOCkingbird. This entailed creating novel computational algorithms for massively parallel ray-tracing, mesh partitioning, mesh adaptivity, mesh generation, and sparse parallel communication.

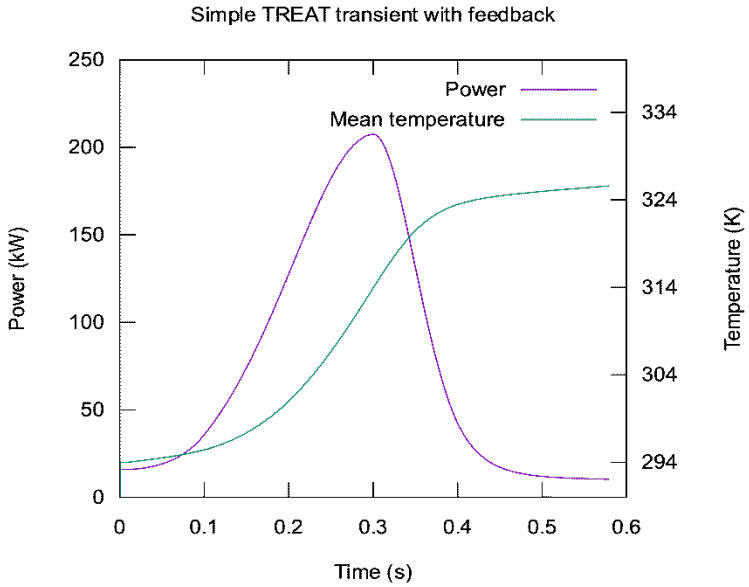


Figure C-17. TREAT can be pulsed by removing the control rods from the core. The doppler effect, a natural feedback mechanism increasing neutron absorption with the temperature, controls the power surge.

Significance

Over the last few years INL has successfully restarted TREAT Facility. A large component of future operations in TREAT depends on reliable modeling and simulation. TREAT represents a challenging modeling and simulation problem. It is inherently transient; has interelement air gaps, providing long streaming paths for neutrons; has strong thermal feedback by design; and has an uncommon geometry, compared to operating LWRs. All of these factors combine to require a specialized multiphysics-capable reactor analysis tool combined with a science-based approach for verification, validation, and nuclear data generation. This project leveraged unique characteristics of the newly developed MOOSE-based reactor analysis tool, MOCkingbird, for the high-fidelity simulation of the radiation transport of the TREAT reactor.

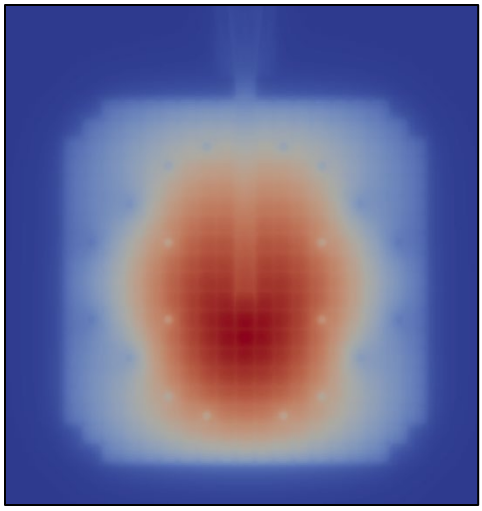


Figure C-18. TREAT M8Cal configuration fast flux with a transient rod bank in. Streaming effects can be seen through the hodoscope channel, which current diffusion-based TREAT simulators cannot predict.

This new neutron transport capability will continue to be developed by the NEAMS program. In addition, the effects of this project will be felt across the modeling and simulation landscape of INL, DOE, and the larger scientific community utilizing MOOSE, as the new general massively parallel ray-tracing capabilities developed offer wide-ranging new opportunities outside of nuclear reactor physics. The cutting edge, foundational algorithms developed here will power a whole new generation of computational science, helping INL, DOE, and the United States to continue to lead the world in multiphysics simulation.

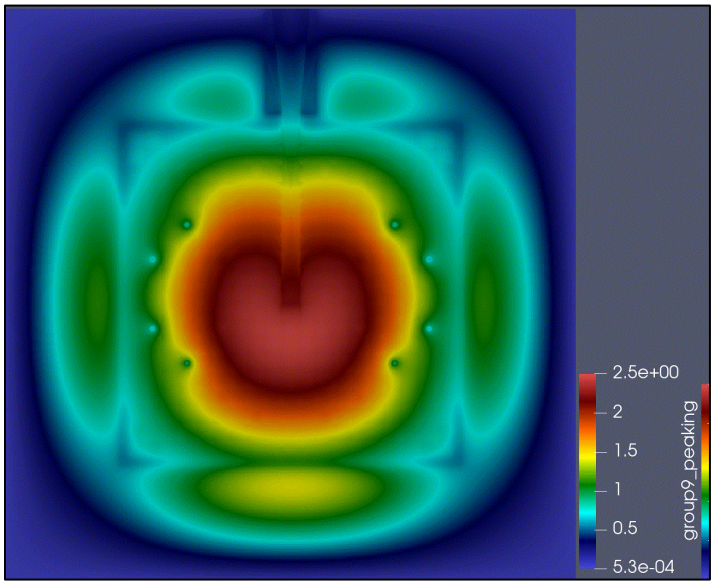


Figure C-19. Evolution of the thermal flux (normalized at every state-point) during a TREAT rod ejection transient. Initially, the flux peaks in the reflector and the center of the core, with dips at the absorbing control rods. The flux distribution shifts dramatically throughout the transient, which can only be captured with highly accurate time integration schemes.

Key Publications

"Novel Transient Capabilities of MOCkingbird, an Unstructured Mesh 3D MOC Neutron Transport Code," in progress.

Sponsor/Program

Laboratory Directed Research and Development

C.11. Modeling the Coevolution of Pores and Grains from Electron Backscatter Diffraction Experiments Using MOOSE and MARMOT Frameworks

Report Participants

Bradley Fromm[1], Cody Permann[2], David Field[1]

1 Washington State University

2 Idaho National Laboratory

Scientific Achievement

Combining computational modeling with advanced material characterization techniques is a critical step to future success in developing new reactor materials. The objective of this research is to enhance the MOOSE and MARMOT frameworks to enable the computational modeling and visualization of porous datasets obtained from electron backscatter diffraction (EBSD) experiments. Because phase field models utilize a diffuse interface, it is difficult to distinguish the boundaries of the pores and grains. A new integration scheme was developed and integrated into MOOSE that resolves this segmentation issue and improves the visualization of the evolving microstructure. The phase field method is also memory intensive, making it challenging to simulate large meshes. This issue was resolved by incorporating the new integration scheme with the GrainTracker algorithm in MOOSE. Additionally, enhancements to LibMesh and MOOSE were made to enable the parallel appending of output files during the restart process.

Figure C-20 shows an image quality map of a surrogate UO_2 microstructure obtained by EBSD. A phase field simulation was performed using INL's Lemhi HPC system. Figure C-21 shows the results of the simulation that utilized the MOOSE and MARMOT frameworks. The reconstructed microstructure consisted of 711 grains represented by 1.9 million elements with 32.2 million total degrees of freedom. Utilizing 20,000 processors over 50 nodes on Lemhi, 32 hours of simulated annealing at 2273 K were performed over 2,169 time steps in 62.7 hours of total wall time.

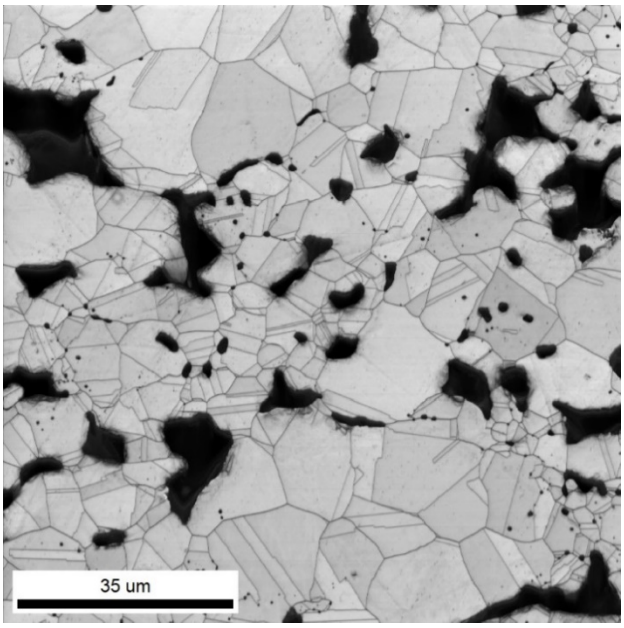


Figure C-20. Image quality map of a surrogate UO_2 microstructure consisting of 711 grains and a porosity of 17.5% that was obtained through EBSD experiments.

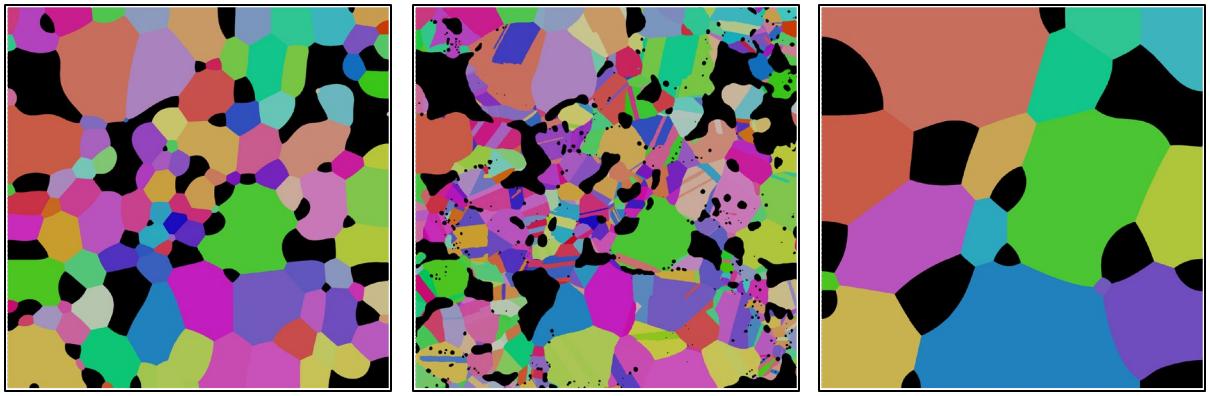


Figure C-21. Results of a phase field simulation illustrating the coevolution of the grains and pores during simulated annealing at 2273 K; left image represents the initial condition of 711 grains; middle image consists of 110 grains after 1 hour of simulated annealing; and the right image contains the 14 remaining grains and 13 large pores after 32 hours of grain evolution.

Scientific Achievement

The migration of voids and pores within reactor materials can be better represented by using an integration scheme where the value of each variable at every quadrature points is numerically integrated and summed over the element. The variable with the largest value is then assigned as the dominate feature of the element. This solves the issue with grain boundary segmentation and improves the visualization of the evolving pores and grains. We addressed memory challenges by utilizing the new integration scheme within the GrainTracker algorithm of MOOSE. This enabled all 711 grains to be represented with only eight order parameters, using 90 times less memory usage. Updates to both LibMesh and MOOSE were made to enable Nemesis file appending during restarts. Additionally, a new divergence tolerance from PETSc and a custom power-law based time stepper reduced the number of time steps required to evolve the microstructure. An interesting finding is that the ratio of wall time to anneal time was approximately two. This is notable due to the time and cost associated with performing real experiments in a test reactor.

Key Publications

- Fromm, B.S., Permann, C.J., Field, D.P. (2020). “Modeling the Coevolution of Pores and Grains from Electron Backscatter Experiments Using the MOOSE and MARMOT Frameworks,” in progress.
- Fromm, B.S. (2020. “Phase Field Based Microstructure Reconstruction of Reactor Materials,” (Doctoral dissertation, Washington State University, Pullman, Washington), in progress.

Sponsor/Program

Laboratory Directed Research and Development

Nuclear Energy Enabling Technologies

C.12. Moving Beyond DPA: A New Approach for Rapidly Quantifying Radiation Damage

Report Participants

Charles Hirst[1]

1 Massachusetts Institute of Technology

Scientific Achievement

This research will conduct a long timescale annealing of multi-PKA damage cascades to simulate differential scanning calorimetry.

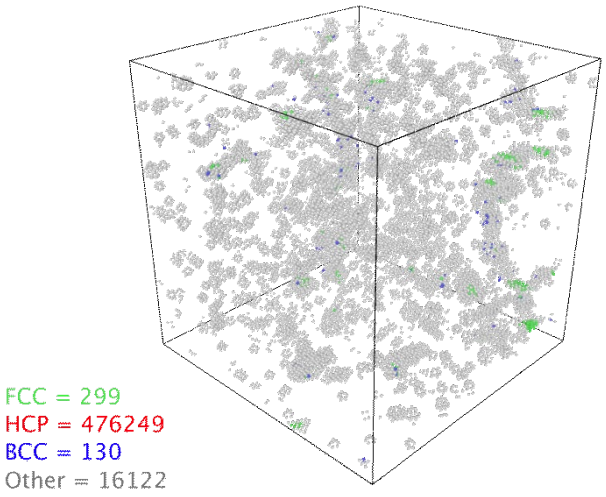


Figure C-22. Supercell of Ti subject to 8000 PKA cascades to be annealed.

Significance

This study successfully simulated the heating of Al over 2μs = 1E9 timesteps. Future research will plan to anneal Ti simulations to complement the differential scanning calorimetry experiments of neutron-irradiated Ti.

Key Publications

- 149th Minerals, Metals and Materials Society (TMS), February 2020. “Direct measurement of radiation damage through the energy stored in defects.”
- 4th Mettler Toledo Flash DSC Conference, November 2019. “Developing a method to measure radiation damage in metals using calorimetry.”
- 1st Materials in Nuclear Energy Systems (MiNES). October 2019. “Developing a method to quantify radiation damage using stored energy: simulations and experiments.”

Sponsor/Program

Laboratory Directed Research and Development

C.13. Theoretical Calculations-Driven Electrocatalysts Development for CO_2 Transformation

Report Participants

Meng Li[1], Bin Hua[1], Lucun Wang[1], Dong Ding[1]

1 Idaho National Laboratory

Scientific Achievement

The transformation of CO_2 molecules into valuable products is of increasing interest due to the negative impact of anthropogenic CO_2 emissions on global warming. The CO_2-to-methanol hydrogenation is an economically profitable method of carbon fixation, but it lacks the efficient and selective catalysts to be adopted for widespread industrialization. The rational design of materials, interfaces, and morphology is vital to reforming the time-consuming trial-and-error experimental efforts. We developed a theoretical calculations-driven electrocatalysts development framework for the efficient investigation of highly active materials for CO_2 transformation in an advanced electrochemical membrane reactor. We performed density functional theory calculations for materials screening using VASP. We also investigated CO_2 reaction pathways and interactions between CO_2 molecules and the catalysts' surfaces to reveal mechanisms in this system.

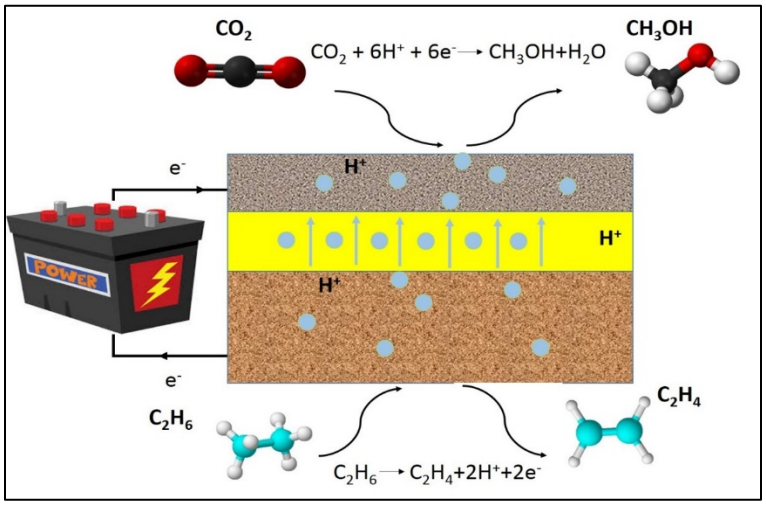


Figure C-23. An illustration showing the CO_2 transformation process in an advanced EMR.

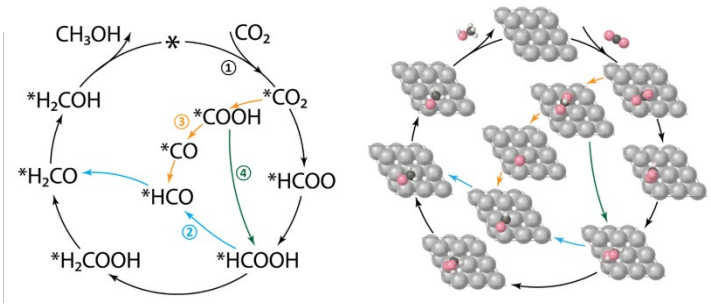


Figure C-24. Investigation of possible reaction pathways of CO_2 transferring into methanol on a catalyst surface.

Significance

We performed a comprehensive study on the electrocatalyst development for CO_2 transformation in an electrochemical membrane reactor. We established density functional theory benchmarking and identified catalysts with improved activity. The investigation on the charge density difference between catalysts' surfaces and CO_2 adsorbates indicates that an enhanced electrons redistribution was achieved by doping metals, which activates the absorbates for following the hydrogenation reactions. This work provides a better understanding of the effects of tuning the catalyst's surface by doping metals, opening the path for the design of more active catalysts for CO_2 transformation reactions. Several provisional patents have been filed based on the results from this project. This work will ultimately facilitate the discovery and development of electrocatalysts for CO_2 transformation, serving as guidance to experiments and theoreticians alike.

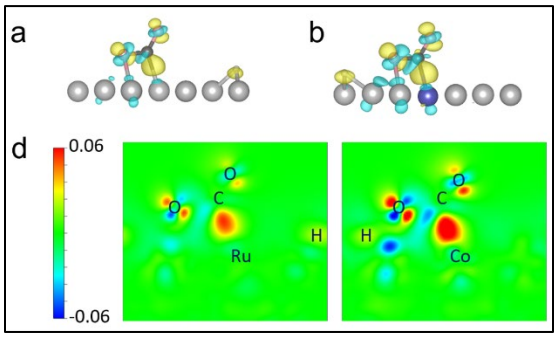


Figure C-25. Tunable interactions between CO_2 molecules and the catalyst surface illustrated by the charge density difference.

Key Publications

- Li, M., Hua, B., Wang, L.-C., Sugar, J. D., Wu, W., Ding, Y. Ding, D., "Switching of metal-oxygen hybridization for selective CO2 electro hydrogenation under mild temperature and pressure," *Nature Catalysis*, in progress.
- Li, M., Hua, B., Wang, L.-C., Zhou, Z., Stowers, K. J. Ding, D., "Discovery of single-atom alloy catalysts for CO2-to-methanol reaction by density functional theory calculations," *Catalysis Today*, in press. https://doi.org/10.1016/j.cattod.2020.04.059.

Sponsor/Program

Laboratory Directed Research and Development

Appendix D

IDAHO UNIVERSITY CONSORTIUM

Table of Contents

D.1. Computational Modeling of Terrestrial and Extraterrestrial Volcanic Eruption Plumes with Temperature-Dependent Heat Capacity

Report Participants

Meghan Fisher[1]

1 Idaho State University

Scientific Achievement

Heat capacity is not temperature independent and can vary greatly over large temperature ranges. Explosive volcanic (forced) plumes are examples of anisothermal systems; temperatures range from 900 K to 1200+ K (several hundred degrees warmer than the ambient atmosphere) at the source and can fall to below 250 K (175 K in extraterrestrial atmospheres) in upper regions. While a high temperature (>300 K) heat capacity can be modeled using a polynomial, the low temperature (<300 K) heat capacity is modeled using either a series of fitted Einstein and Debye equations, which can only be computed using numerical methods, or a set of temperature tabulated values. For each of the 35 most common volcanic minerals and glasses, 5,210 different closed form, rational polynomial equations that combine both high and low temperature heat capacities were fitted using a Python's minimization. Akaike information criterion was used to pick the best model for each material. Calculation of heat capacity is up to 45x faster than previous methods.

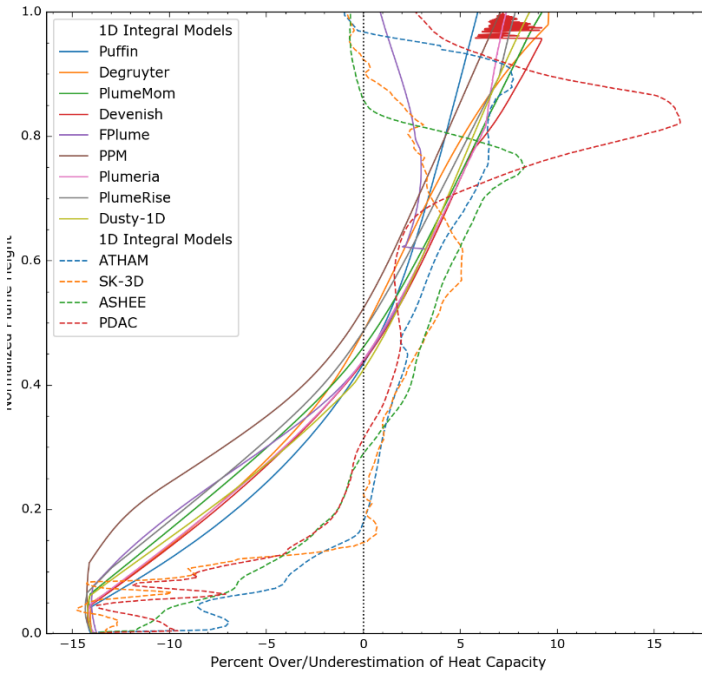


Figure D-1. Percent error in bulk plume heat capacity from modeled 1991 eruption of Mt. Pinatubo for nine different 1D models and four 3D models.

All previous volcanic plume models (both 1D steady-state integral models and 3D unsteady Navier-Stokes simulators) treat the heat capacity of all plume components (ash, volcanic gases, and entrained air) as constant, resulting in both over- and underestimation of the plume's thermal energy budget and thus hotter and colder plume temperatures. This can lead to an artificial plume collapse and stability as well as inflated overall plume height and mass eruption rates. The effects of inaccurate heat capacity calculations are exacerbated in CO_2 dominated atmospheres like Mars; the heat capacity of nitrogen and oxygen vary by less than 15%, whereas CO_2 can vary by more than 50% through the plume temperatures. It is theorized that volcanic eruptions may have been a greenhouse gas source on early Mars that allowed for planetary warming (and thus liquid water) if the eruptions were sufficiently large enough and penetrated the stratosphere.

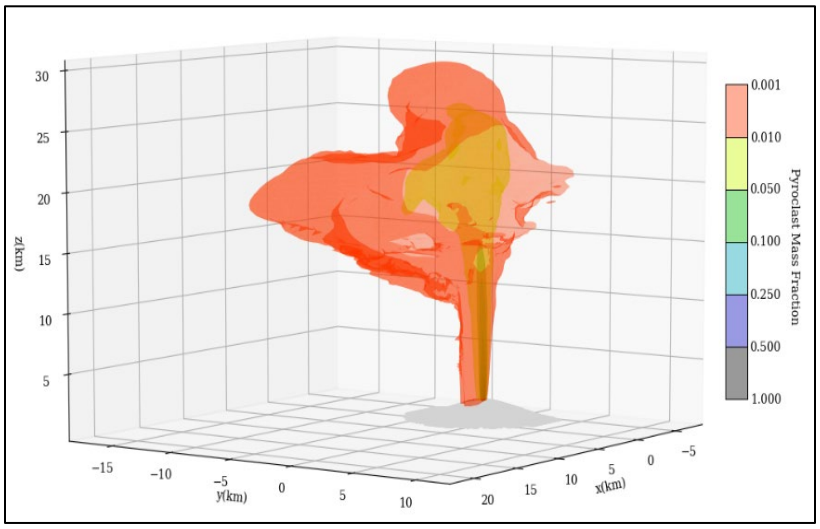


Figure D-2. Isosurfaces of erupted material from a time-averaged stable snapshot of a simulated volcanic eruption on early Mars.

A new 1D plume model was developed (Thermal Equilibrium Model for Plumes) and an existing 3D Navier-Stokes model (Active Tracer High Resolution Atmospheric Model) was extended to incorporate temperature-dependent heat capacity and allow for nonterrestrial atmospheric thermodynamics. Simulations for the 1991 Pinatubo and 2010 Shinmoe-dake eruptions were performed for both new models in order to compare the results to previous studies. Using the 1D and 3D martian models, eruptions on early Mars were computed for a suite of different mass eruption rates and different hypothesized early Martian atmospheres, using both constant and variable heat capacity.

Significance

This is the first study to recognize that the effects of the temperature-dependent heat capacity on volcanic eruption dynamics cannot be ignored; preliminary results indicate that it can better help parameterizing entrainment for highly anisothermal, non-Buossinesq forced plumes. The Martian Active Tracer High Resolution Atmospheric Model module is the first nonterrestrial Navier-Stokes plume model, providing the first visualization of early Martian volcanic eruptions. It also allows for a better constraining of early Martian plume height and size as well as the viability of proposed minor components of the early Martian atmosphere. Preliminary results indicate that the terrestrial parametrization of entrainment does not fully apply to CO_2 dominated atmospheres. Additionally, there is evidence that Jezero Crater, the landing site for the Mars Perseverance Rover, may be a pyroclastic fall deposit. If this is the case, the constraining of early Martian plume height and eruption size will be key for identifying potential volcanic source locations.

Key Publications

- Fisher, M.A., Nawotniak, S.K. (2020a). "Role of temperature-dependent heat capacity in eruption column dynamics." Manuscript in preparation.
- Fisher, M.A., Nawotniak, S.K. (2020b). "Effects of entrainment, thermodynamic parameterization, and atmospheric composition on early Martian volcanic plume height." Manuscript in preparation.

Software Releases

- Specheat—a C++ library with Python/Fortran bindings to calculate the temperature dependent heat capacity and heat flux of volcanic minerals and glasses (part of Fisher & Nawotniak [2020a])
- TEMP (Thermal Equilibrium Model for Plumes)—a Python library for a 1D steady-state buoyant plume model with a temperature-dependent heat capacity (part of Fisher & Nawotniak [2020a])

Sponsor/Program

Idaho University Consortium

D.2. First-Principles Studies of Atomic Layer Deposition for MoS2

Report Participants

Matthew Lawson[1], Lan Li[1]

1 Boise State University

Scientific Achievement

Our project uses DFT to uncover the nucleation mechanisms during the atomic layer deposition (ALD) of MoS2. The ALD process is difficult to study in situ due to the nanoscale features and interactions. Specifically, we couple our DFT calculations with experimental measurements performed at Boise State University to understand how to deposit 2D MoS2. On the HPC cluster, we use VASP.

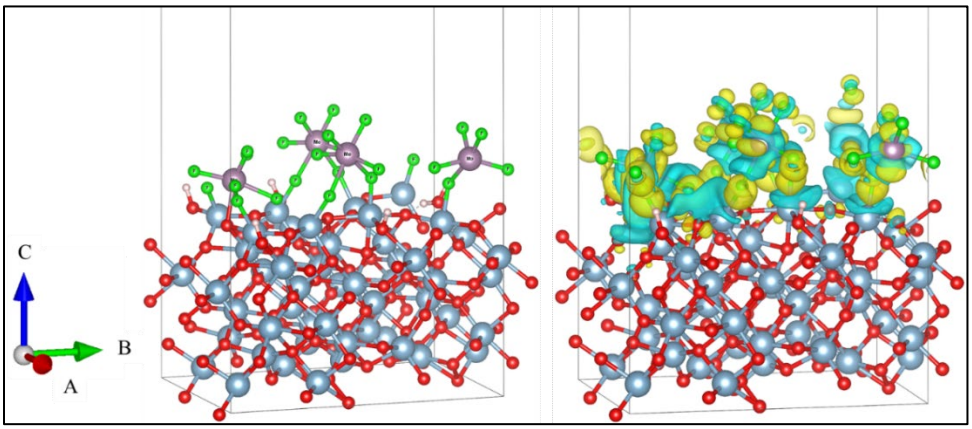


Figure D-3. Electron density difference calculations of MoF6 on hydroxylated alumina. Blue and yellow isosurfaces indicate a gain or loss of electrons, respectively.

Significance

Recently we have uncovered the importance of hydroxyl groups on metal oxides and how hydroxyl groups are important for the ALD of MoS2. DFT calculations reveal an increase in electron density above hydroxylated surfaces, and this helps promote the deposition of MoF6. Without hydroxyl groups, physisorption occurs with the MoF6 precursor, while the prescence of hydroxyl groups promotes chemisorption. Further studies have indicated that the concentration of hydroxyl groups plays a roll during ALD. We have found that hydroxyl groups attack surface bonds on alumina, which promotes the formation of highly ionic AlF3. This highly ionic AlF3 was also found in our experimental measurements, confirming our DFT calculations.

Key Publications

- M. Lawson, E. Graugnard, and L. Li, “First-principles studies of MoF6 absorption on hydroxylated and non-hydroxylated metal oxide surfaces and implications for atomic layer deposition of MoS2”, *Applied Surface Science*, Under review (2020)
- M. Lawson, J. Soares, S. Martin, E. Graugnard, and L. Li, (2020) “Hydroxyl concentration effects on ALD-grown MoS2”, in progress.

Sponsor/Program

Boise State University Graduate Assistance Line

D.3. Implementing and Assessing an Alchemical Method for Calculating Protein-Protein Binding Free Energy

Report Participants

Dharmeshkumar Patel[1], Jagdish Suresh Patel[1], F Marty Ytreberg[1]

1 University of Idaho

Scientific Achievement

Protein-protein binding is fundamental to most biological processes. It is important to be able to use computation to accurately estimate the change in protein-protein binding free energy due to mutations in order to answer biological questions that would be experimentally challenging, laborious or time consuming. Although nonrigorous free energy methods are faster, rigorous alchemical molecular dynamics-based methods are considerably more accurate and are becoming more feasible with the advancement of computer hardware and molecular simulation software. Even with sufficient computational resources, there are still major challenges to using alchemical free-energy methods for protein-protein complexes, such as generating hybrid structures and topologies, maintaining a neutral net charge of the system when there is a charge-changing mutation, and setting up the simulation. In the current study, we have used the pmx package to generate hybrid structures and topologies and a double-system/single-box approach to maintain the net charge of the system. To test the approach, we predicted relative binding affinities for two protein-protein complexes (1BRS and 3HFM) using a non-equilibrium alchemical method based on the Crooks fluctuation theorem and compared the results with experimental values.

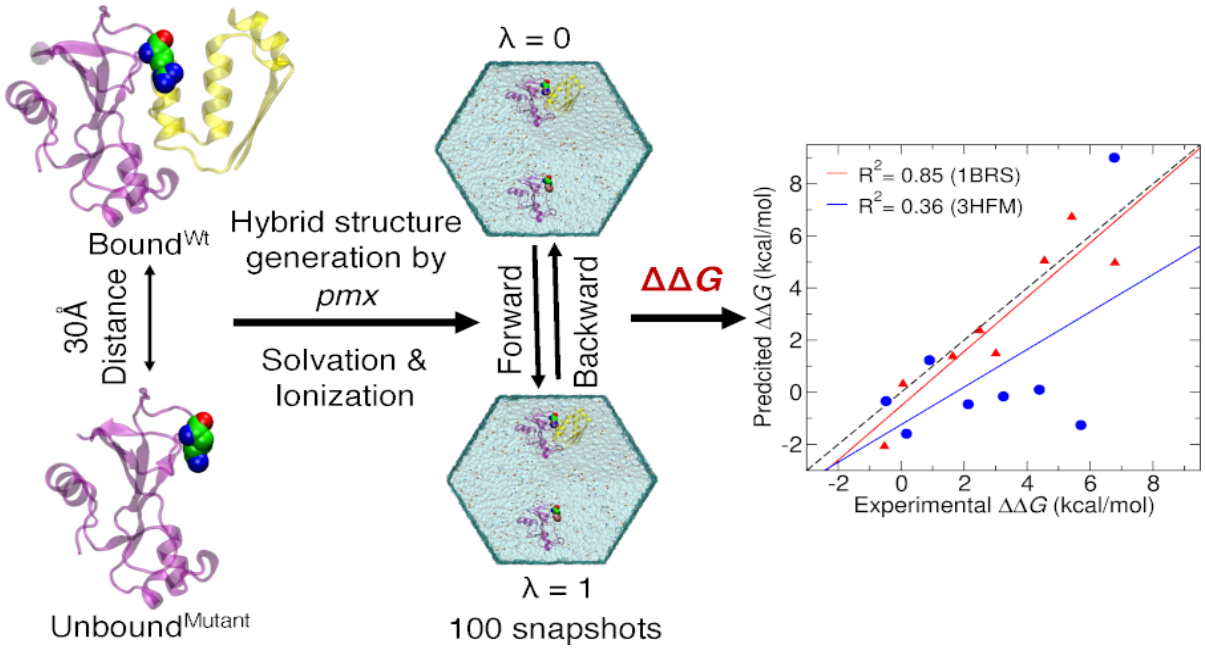


Figure D-4. Flow chart of calculating ΔΔG using pmx with double-system/single-box simulation setup. The correlation is shown between predicted and experimental ΔΔG values for 1BRS (red) and 3HFM (blue) systems. The dashed black line shows perfect correlation.

Significance

Here, we tested the performance of using pmx with a double-system/single-box approach in a systematic manner using two protein-protein complexes of different size with a wide range of experimental ΔΔG values. For each system, we selected eight mutations from different sites with a broad range of experimental ΔΔG values. We estimated ΔΔG values using pmx hybrid topologies with a double-system/single-box approach and the non-equilibrium CGI method. Predicted ΔΔG values were compared with experimental values. A higher correlation was found for the smaller protein-protein complex compared to the larger, more complex, antigen-antibody system. Our results suggest that there is still room for improvement in rigorous binding free energy methods, especially for large, complex protein-protein systems. The method correctly identified stabilizing from destabilizing mutations for a small protein-protein complex but was not as successful with the larger, more challenging antibody complex. In addition, the correlation between predicted and experimental relative binding affinities was high for smaller complex and low for the other larger complex. Future work could involve using the alchemical double-system/single-box method but with the coarse-grained protein models. Based on results from our previous study, this may significantly reduce computational cost and still retain a similar accuracy. However, coarse-grained hybrid topologies of the proteins have not yet been developed. Another approach to reducing computational cost could be the use of a dual-resolution water model where water around the protein is atomistic and the rest of the water molecules coarse grained.

Key Publications

- Patel, D., Patel, J. S., Ytreberg, F.M. 2020. "Implementing and assessing an alchemical method for calculating protein-protein binding free energy" bioRxiv 2020. https://doi.org/10.1101/2020.10.02.324442
- Patel, D., Patel, J. S., Ytreberg, F.M. 2019. "Testing and Improving Alchemical Methods for Protein-Protein Binding Affinity Calculation" *Biophysical Journal,* vol. 118, no.3, p.142a. https://doi.org/10.1016/j.bpj.2019.11.898
- Patel, D., Patel, J. S., Ytreberg, F.M. 2020. "Implementing and assessing an alchemical method for calculating protein-protein binding free energy," JCTC (under major revisions).

Sponsor/Program

Idaho University Consortium

D.4. Modeling the Dispersal of Volcanic Ash on Mars

Report Participants

Tyler Paladino[1], Shannon Kobs Nawotniak[1]

1 Idaho State University

Scientific Achievement

In this project, we seek to model the deposition of volcanic ash on a planet-wide scale on Mars. We seek to find correlations between ash deposition and current-day hydrated regolith that blankets the Martian surface. To accomplish this, we use two pieces of software, one that simulates an explosive eruption plume in a rudimentary atmosphere (The Mars Active Tracer High Resolution Atmospheric Model [MATHAM]) and another that simulates the motion of an entire atmosphere as well as the many physical processes happening therein (the Laboratoire de Météorologie Dynamique General Circulation Model [LMD GCM]). The MATHAM and LMD GCM solve many higher order differential equations in 3D space over time and, as such, benefit from being run over many CPU cores. This project is in its infancy; as such, we have only begun to implement the two models and couple them together smoothly.

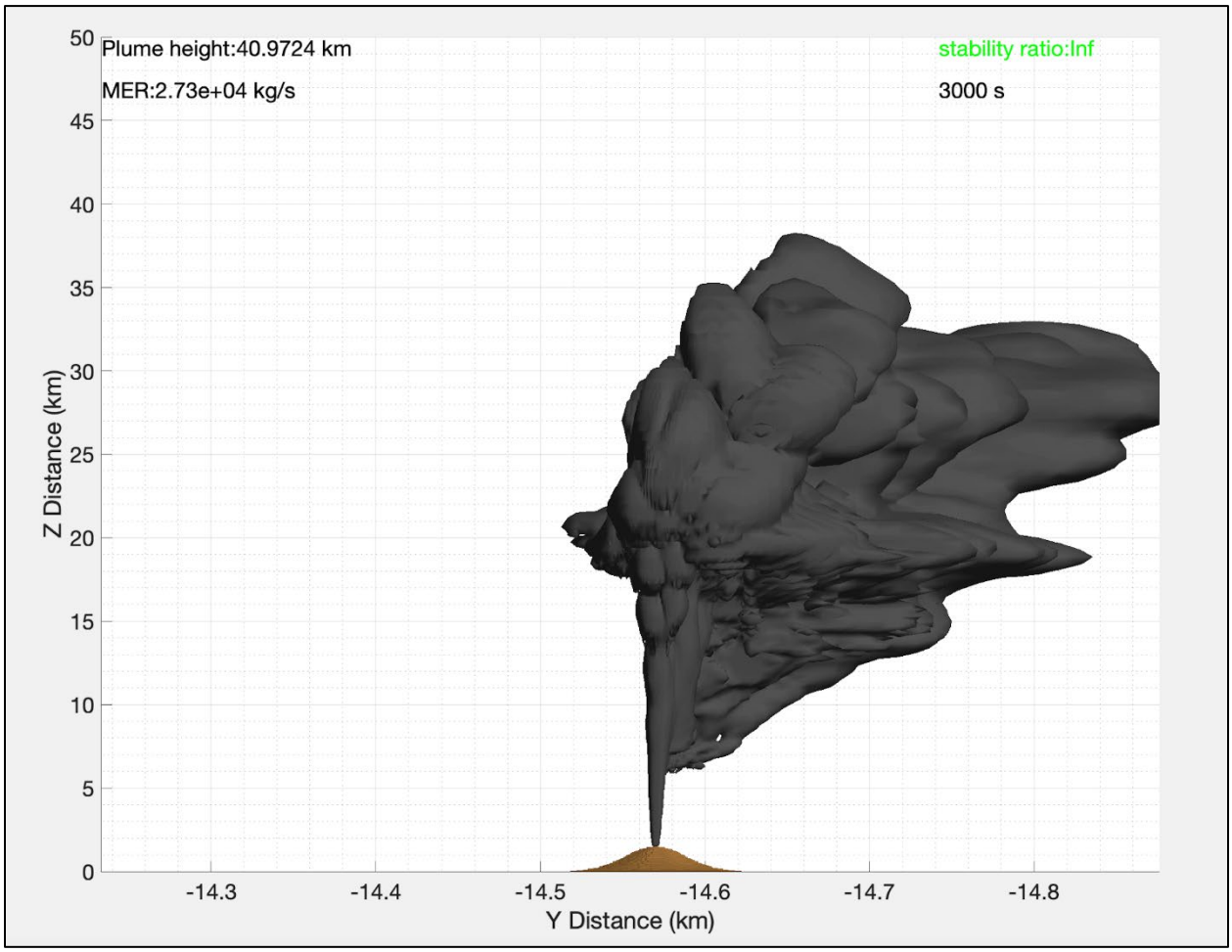


Figure D-5. A snapshot of MATHAM output visualized in MATLAB. This figure shows a stable plume at a mass eruption rate (i.e., eruption strength) of 2.73×104 kg/s. The plume is also being modified by a wind moving from left to right.

Significance

This work will help uncover a mystery of Mars, namely, what creates the observed patterns of regolith hydration on Mars? As of now, no one hypothesis has been able to explain the patterns we see in the upper 10's of cms of regolith. If areas of high hydration are formed by explosive volcanic eruptions (which are capable of depositing much more than 10's of cms of ash), it may be worthwhile to explore these areas as key in situ resource utilization zones for future manned martian missions. To date, we have installed and run test simulations for both models, performed sensitivity analyses on MATHAM simulations, and begun to convert some code associated with volcanism in the LMD GCM software from serial to parallel.

Key Publications

No publications yet as this project is in its infancy, though do we plan on publishing.

Sponsor/Program

National Aeronautics and Space Administration Mars Data Analysis Program

Idaho University Consortium

D.5. Multiscale Parallel Algorithms for Simulation of the Evolutionary Development and the Geographic Spread of the Coronavirus Disease at the Country, State, and Local Level

Report Participants

Dr. Yury Gryazin[1], Dr. Daniel Korytowski[1], Yun Teck Lee[1], Ron Gonzales[1]

1 Idaho State University

Scientific Achievement

The fast development of the COVID-19 disease poses serious challenges for local governments and hospitals with respect to the allocation of the resources, rapid response programs, and education of the population. Our main considerations are the identification of the most vulnerable regions as well as estimating the propagation speed of the disease and the recovery time of the regions. In our project, we are planning to address all three by using a multilevel simulation approach to the geographic spread of COVID-19. This research will focus on Idaho's rapid response program but can be adapted to any local and national prediction simulation of a similar emergency situation.

The proposed multilevel simulation is computationally intense. To make it feasible, a series of new fast parallel algorithms must be developed and implemented. The main algorithmic focus of the project will be on the development of parallel algorithms for the time integration, direct parallel graph system solvers, and the efficient implementation of the diffusion process simulator on a local level. Dr. Yury Gryazin, Mr. Ronald Gonzales, and Mr. Yun Teck Lee will focus on the first two tasks. Dr. Daniel Korytowski will be responsible for the third and the overall validation of the mathematical epidemic models under consideration. We will use deep neural network algorithms to implement the calibration of the proposed epidemic models. This study will investigate the stability of the underlying mathematical problems and developed numerical methods.

Significance

The current state of the project is in the first level of the simulation. MATLAB native functions are being used to estimate the parameters for multiple modified SEIR models. The next stage will require the use of high-performance computing. This will allow for more accurate estimations and the expansion to multilevel simulations.

Key Publications

Gryazin, Y., Gonzales, R. F., Lee, Y. T., "Scalable Algorithms for High-Order Approximations on Compact Stencils." ArXiv abs/1912.03565 (2019)

Sponsor/Program

Idaho University Consortium

D.6. Quantifying Wind-Driven Collapse Scenarios of Volcanic Plumes

Report Participants

Tyler Paladino[1], Shannon Kobs Nawotniak[1]

1 Idaho State University

Scientific Achievement

In this project, we seek to better understand the relationship between wind and explosive eruption plume stability. Stability in eruption plumes is defined by whether or not the plume is positively buoyant and rises into the atmosphere or if the plume is negatively buoyant and collapses into one or more ground-hugging pyroclastic density currents, the latter of which are far more dangerous. To understand the wind-stability relationship, we use the Active Tracer High Resolution Atmospheric Model (ATHAM), which simulates a plume from fragmentation to deposition while also allowing us to place plumes into wind fields of any profile or strength we desire. By running many simulations with different eruption strengths and wind speeds, we can develop an understanding of how wind affects plume stability.

Significance

This work will help first responders as well as disaster response groups with evacuation plans by increasing our understanding of how wind affects eruption plumes, which has been understudied. By characterizing a general scheme of eruption strengths and wind speeds, we can provide experts with the information they need accurately and quickly. We have run simulations at five different eruption rates, with wind speeds varying from 0 to 50 m/s in 5 m/s increments. We have covered very weak (1×104 kg/s) eruptions as well as very strong eruptions (1×1010 kg/s). As of right now, we are filling in gaps within these two endmembers to characterize intermediate eruption strengths, which tend to be more common than very large or very small eruptions.

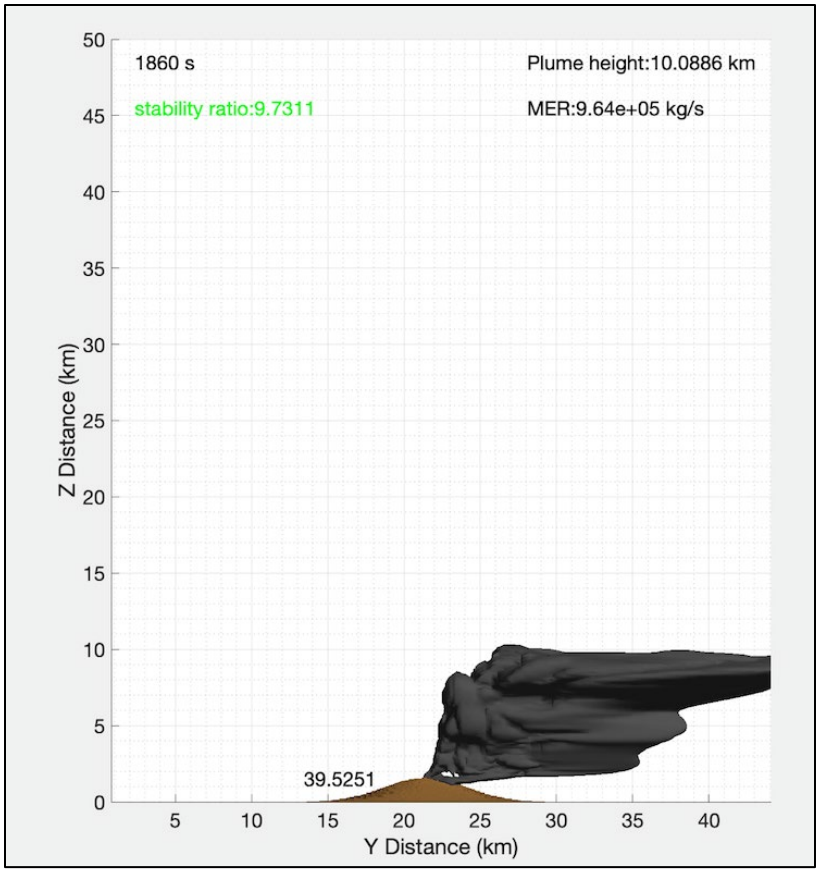


Figure D-6. A snapshot of an ATHAM simulation visualized in MATLAB. This figure shows a bent plume in a 30 m/s wind field. The eruption strength here is 9.64×105 kg/s. This plume remains stable but is approaching instability as wind continues to bend it downwind.

Key Publications

Paladino, T., Nicholson, B.C., Kobs-Nawotniak, S. E., (2019, December). "Quantifying Wind Driven Collapse Scenarios of Explosive Volcanic Eruption Plumes" [Poster Session]. American Geophysical Union Conference, San Francisco, CA, USA.
https://ui.adsabs.harvard.edu/abs/2019AGUFM.V23G0289P/abstract

Sponsor/Program

Idaho University Consortium

Appendix E

RENEWABLE ENERGY

Table of Contents

E.1. A Nonlinear Hysteretic Contact Model for DEM Modeling Considering Strain-Hardening Effect

Report Participants

Feiyang Chen[1,2], Yidong Xia[1]

1 Idaho National Laboratory

2 Clemson University

Scientific Achievement

This work has developed a prototype of specialized discrete element modeling (DEM) particle contact model specifically for capturing the strain-hardening behavior between biomass particles under compression. Most of the DEM packages provide a simple hysteretic linear contact force-displacement model. This model is usually sufficient to represent the stiff collision between hard particles, such as rocks, sands, and pharmaceutical pellets. However, to represent the contact between biomass particles, such as milled loblolly pine, we have found that this simple contact model is not very suitable. Thus, we have developed a prototype of hysteretic nonlinear contact force-displacement model, with its schematic illustrated in the following figures. The strain-hardening effect is conceptualized by assuming a history-dependent stiffness of particle that shall grow by increased stress asserted on the particle. This model is designed to save the complete history of particle stiffness in computer memory to account for the possible scenarios of particle separation and recontact. Unlike the simple hysteretic model, in which the reloading is along the previous unloading path, this strain-hardening stiffness model makes the reloading stress-strain curve evolve in a separate path. This model even considers the case of partial unloading and reloading along a different path, which is essential to represent the bulk mechanical characteristics of loblolly pine particles.

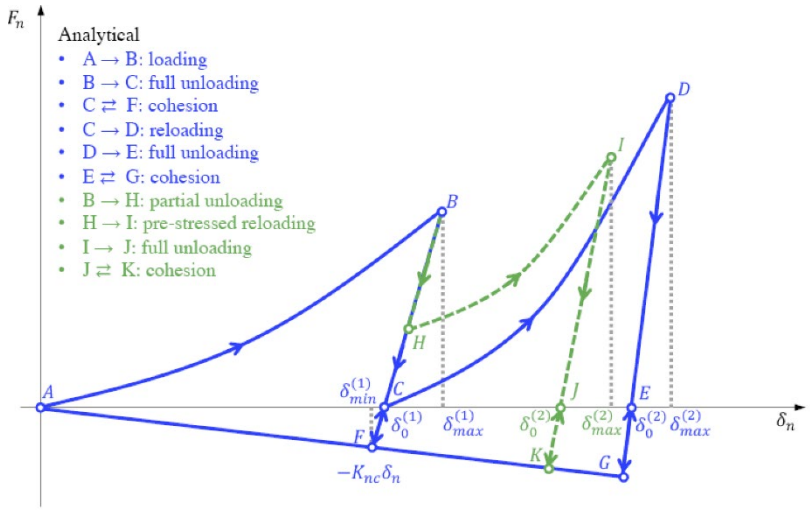


Figure E-1. Schematic of nonlinear hysteretic contact force-displacement model.

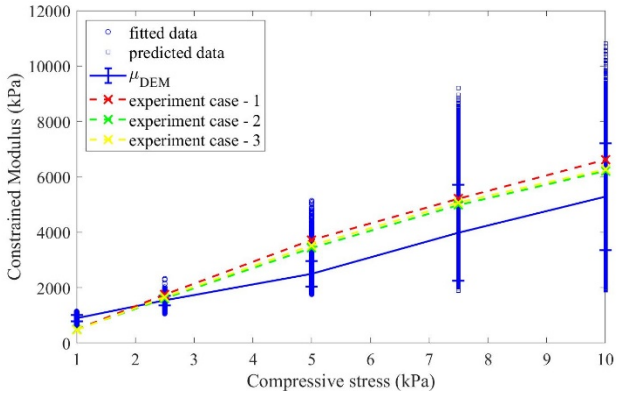


Figure E-2. Comparison of constrained modulus between experimental results and DEM results.

Significance

The formulation that describes the contact model between loblolly pine particles is conceptualized based on the experimental data of an axial cyclic loading-unloading test conducted at INL (Subtask 3.5). This new DEM contact model has been implemented in the open-source LIGGGHTS-INL DEM package. The calibration of the parameters in the new model requires parametric studies that may take massive simulations. Using INL's Sawtooth supercomputer (ranked 40th in the world on the TOP500 list as of June 2020), we have made it possible to easily run over 100,000 test simulations (each simulation used 48 CPU cores for a few hours) to determine the optimal set of model parameters and meet the requirement of material mechanical behavior of loblolly pines with the experimental stress-strain histories. We developed specified criteria for the DEM model calibration by requiring the DEM simulated stress-strain curves to match experimental data with the limited error in the bulk strain under the third, fourth, and fifth peak loading stresses, and with a fixed error in the constrained modulus during the linear strain recovery period during the third, fourth, and fifth unloading. The linear strain recovery period refers to the range of bulk strain that starts from the beginning of unloading and ends when the instantaneous constrained modulus is below the specified error range of the value at the beginning of unloading.

Key Publications

- Chen, F., Xia, Y., Chen, Q., and Guo, Y. (2020). "A hysteretic nonlinear elastoplastic contact model for discrete element modeling of milled woody biomass." AICHE 2020, San Francisco, USA. (Abstract accepted).
- Xia, Y., Chen, F., Klinger, J., Chen, Q. (2020). "A nonlinear hysteretic contact model for the discrete element modeling of strain hardening of woody biomass," in progress.

Sponsor/Program

Department of Energy Office of Energy Efficiency and Renewable Energy

Bioenergy Technologies Office and the Feedstock-Conversion Interface Consortium

E.2. Finite-Discrete Element Simulation for Complex Fracturing Under Hydraulic Stimulation

Report Participants

Jiaoyan Li[1], Robert Podgorney[2], Aleta Finnila[3]

1 University of Buffalo

2 Idaho National Laboratory

3 Golder Associates Inc.

Scientific Achievement

Simulating the hydraulic fracturing process is quite difficult due to the need to model the complex fracture growth on existing natural fractures as well as the generation and growth of new fractures. The combined finite-discrete element method was selected for this effort, with the choice being made to start with 2D modeling due to the complexity and size of meshing both the intact rock matrix and discrete fractures. The discrete crack elements (as shown in Figure E-3) enable the easy study of complex fracturing induced by the hydraulic stimulation. Finite-discrete element method simulations were performed on the Irazu platform.

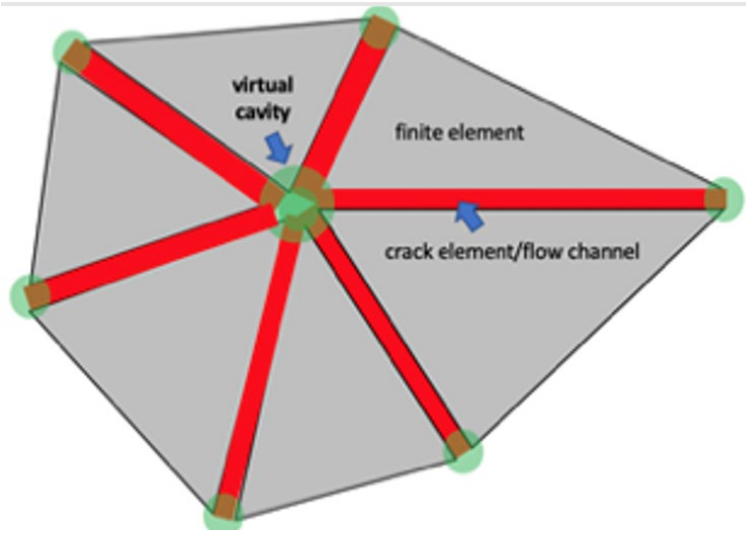


Figure E-3. Sample portion of the 2D mesh consisting of three-node triangular elements and four-node interface elements as crack elements to form a flow channel network.

Significance

The stimulation simulation was performed under the boundary condition of in-situ mechanical stress. Based upon the equilibrium state under in-situ mechanical boundary conditions, the hydraulic stimulation was imposed on the injection point with a prescribed constant fluid rate. The injection point was set to the end of the open hole section, which was located at the center of the simulation domain. The fluid pressure was chosen as an indicator to identify the fracture pattern, considering that the fluid pressure could be increased only when the flow channel was formed. The pressure distribution is shown in Figure E-3. As shown in Figure E-3, the stimulation extent can be estimated from the circle with the measured radius around the injection point. The analysis of pressure change and fracture extend will provide guidance on the injection plan for the Frontier Observatory for Research in Geothermal Energy site, with physical parameters set up accordingly.

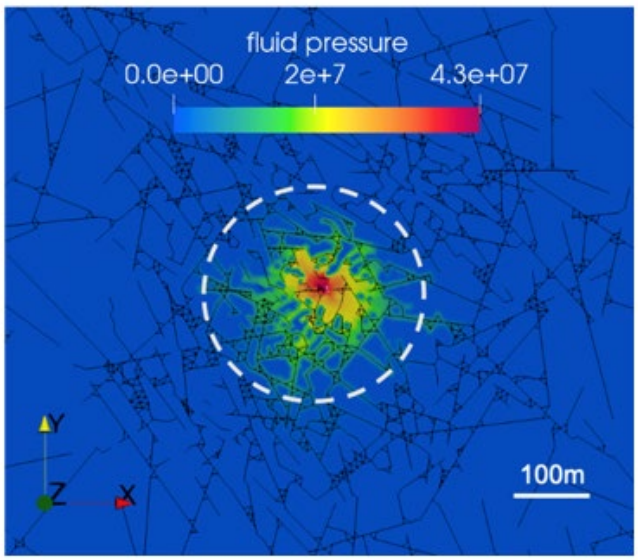


Figure E-4. A close-up view of the hydraulically fractured vertical 2D slice aligned with the proposed new injection well. The intersecting facture traces (colored lines) mediate fluid pressure near the injection point.

Key Publications

Finnila, A.B, Li, J., Podgorney, R.K., "Finite-Discrete Element Method hydraulic stimulation of the FORGE geothermal reservoir," in progress.

Sponsor/Program

Frontier Observatory for Research in Geothermal Energy

E.3. Flow Characterization of Compressible Biomass Particles Using Coupled Eulerian-Lagrangian Analysis with Advanced Continuum Models

Report Participants

Wencheng Jin[1]

1 Idaho National Laboratory

Scientific Achievement

The poor flowability of compressible biomass particles poses severe handling challenges in all processes of biorefineries, which results in poor energy-yielding in conversion. In this project, the computational modeling of biomass flow is leveraged to develop first-principles-based design tools that enable a continuous, steady, trouble-free bulk flow transport through the processing train to reactor throat. With the finite element computational package Abaqus, multiscale flow simulations from lab-scale ring shear tests to pilot-scale hopper flow tests were performed using the coupled Eulerian-Lagrangian method. Modeling results are compared to experimental measurements to evaluate the capabilities of advanced constitutive models and to inform the formulation of a new model. A parametric study with the new model has been carried out to optimize the design and operation of the biomass handling equipment and to engineer the biomass feedstock.

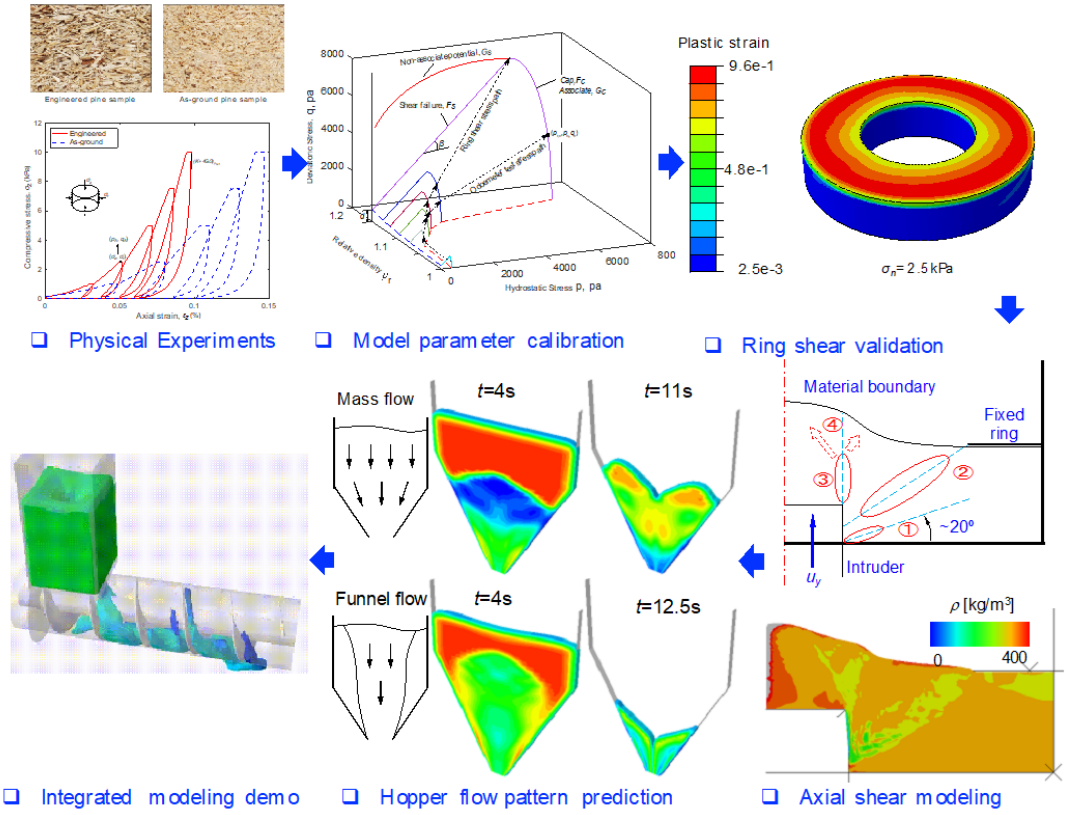


Figure E-5. Demonstration of the established workflow to model biomass granular flow through constitutive material parameter calibration, ring and axial shear validation, and hopper and auger applications.

Significance

This work has shown that the traditional characterization methods suffer from either an incomplete stress state measurement (ring shear tests) or limited strain range to achieve a steady or critical state (triaxial shear tests) for biomass materials with a high compressibility and high shear resistance. The stress state of ground pine chips can be characterized using a combination of relatively simple laboratory tests and numerical simulations. This work also demonstrates that the advanced finite element method (i.e., coupled Eulerian-Lagrangian) with the new hypoplastic model is a valid tool to predict the flow behavior at both the quasistatic and the dense flow regimes for ground loblolly pine. With this tool, simulation at an industrial scale can be done to identify the critical material attributes that control material flow. A sensitivity analysis using the tool will be able to decipher and resolve material handling upsets in biorefineries and other energy industries that utilize forest products.

Key Publications

- Jin, W., Stickel, J. J., Xia, Y., Klinger, J. (2020). "A Review of Computational Models for the Flow of Milled Biomass Part II: Continuum-Mechanics Models." *ACS Sustainable Chem. Eng*., vol. 8, no.16, pp. 6157-6172. https://doi.org/10.1021/acssuschemeng.0c00412
- Jin, W., Klinger, J., Westover, T., and Huang, H. (2020). "A density dependent Drucker-Prager/Cap model for ring shear simulation of ground loblolly pine." *Powder Technology*, 368, 45-58. https://doi.org/10.1016/j.powtec.2020.04.038
- Lu, Y., Jin, W., Klinger, J., Westover, T., and Dai, S. (2021). "Flow characterization of compressible biomass particles using multiscale experiments and a hypoplastic model." *Powder Technology*, vol. 383, p. 396-409, https://doi.org/10.1016/j.powtec.2021.01.027

Sponsor/Program

Department of Energy, Bioenergy Technology Office

Feedstock Conversion Interface Consortium

E.4. FORGE: Running Simulations for Multifractured EGS

Report Participants

Pranay Asai[1]

1 University of Utah

Scientific Achievement

To validate how fluid flow distribution happens in a multifractured enhanced geothermal system EGS. The study requires a computational resource to run the heat and fluid flow using the Falcon system.

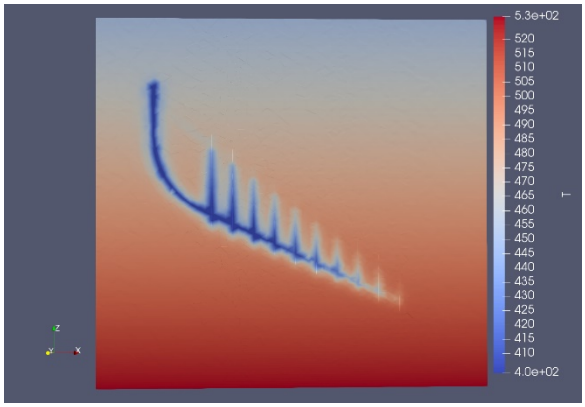


Figure E-6. Fluid distribution in EGS with 10 fractures.

Significance

The project includes studying the fluid flow distribution in a multifractured enhanced geothermal system. This would allow researchers to create an efficient enhanced geothermal system that would allow researchers to harness the energy from the entire reservoir. The work is still in progress. So far, a basic model has been created, and we are slowly working on adding intricacies and making the model more robust.

Key Publications

None.

Sponsor/Program

Frontier Observatory for Research in Geothermal Energy

Appendix F

OTHER

Table of Contents

F.1. An Atomistic Study of Defect Energetics and Diffusion with Respect to Composition and Temperature in γU and γU-Mo Alloys

Report Participants

Gyuchul Park[1], Benjamin Beeler[2], Maria A. Okuniewski[3]

1 Purdue University

2 North Carolina State University

3 Purdue University

Scientific Achievement

The point defect formation energies in γU and γU-xMo (x= 7, 10, 12 wt.%) alloys were calculated between 400 K and 1200 K using molecular dynamics simulations. Using the point defect energetics, self-diffusion coefficients in U-xMo alloys are also calculated at the equivalent temperature ranges.

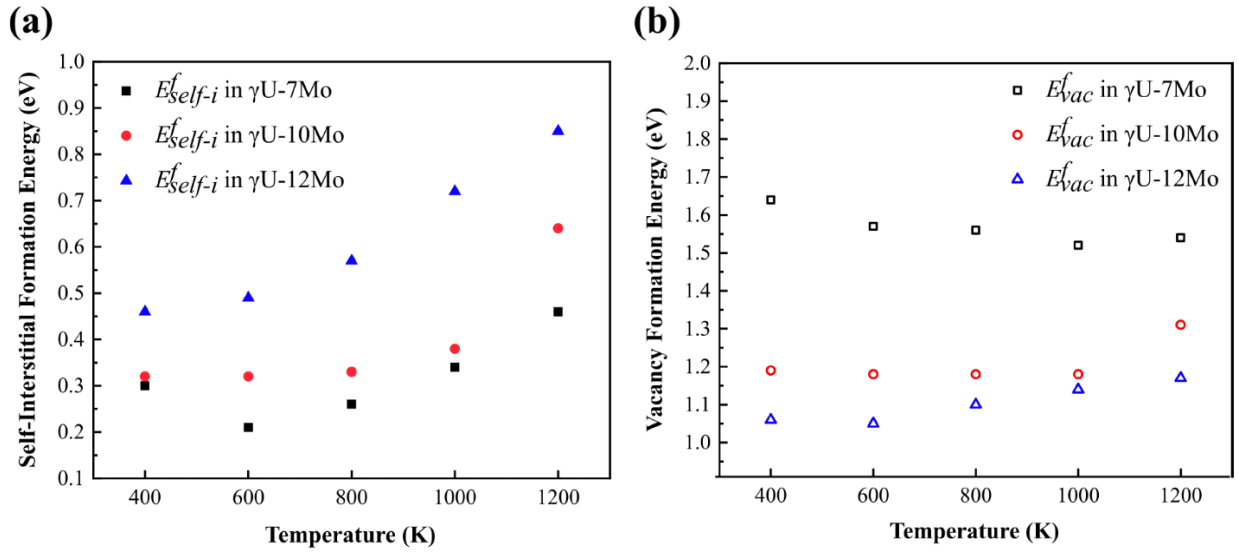


Figure F-1. (a) Vacancy formation energy and (b) self-interstitial formation energy in γU-xMo as a function of temperature.

Significance

In both γU and γU-xMo (x= 7, 10, 12 wt.%) alloys, the vacancy formation energy was greater than the self-interstitial formation energy between 400 K and 1200 K. This implies that diffusion will primarily occur through interstitials rather than vacancies. In γU-xMo, as the Mo concentration increased, the vacancy formation energy increased, whereas the self-interstitial formation energy decreased between 400 K and 1200 K. Subsequently, as the Mo concentration increased, the self-diffusion coefficients decreased, and the diffusion activation energies increased, which qualitatively agreed with previous experimental results. Point defect formation energies and self-diffusion coefficients in the γU-xMo alloys obtained in this work can be used as input parameters in both microscale and mesoscale nuclear fuel modeling codes.

Key Publications

Park, G., Beeler, B., Okuniewski, M. (2020). "An atomistic study of defect energetics and diffusion with respect to composition and temperature in γU and γU-Mo alloys," *Journal of Nuclear Materials*, submitted, in progress.

Sponsor/Program

U.S. High Performance Research Reactor Conversion program of the National Nuclear Security Administration's Office of Material Management and Minimization

F.2. Fuel Pellet Microstructural Fracture Modeling

Report Participants

Janne Heikinheimo[1], Jussi Peltonen[1], Tom Andersson[1], Huan Liu[2], Diogo Ribeiro Costa[2]

1 VTT Technical Research Centre of Finland Ltd

2 KTH Royal Institute of Technology, Sweden

Scientific Achievement

This project studies nuclear fuel microstructural modeling and its implications to the macroscopic models. The activity connects the KTH Royal Institute of Technology's (KTH's) expertise in atomistic scale calculations and VTT Technical Research Centre of Finland's (VTT's) expertise in macro- and mesoscale modeling. VTT studies the applicability of different models on cracking behavior and consequences to macroscopic modeling applying MARMOT, Abaqus, BISON, and FINIX codes. KTH studies atomistic scale fracture parameters and related calculations for different kinds of fuels. VTT and KTH will discuss the possible connection of the atomistic model parameters to microscopic scale fracture modeling. The project started in 2020 and in the first year, modeling will focus on UO2.

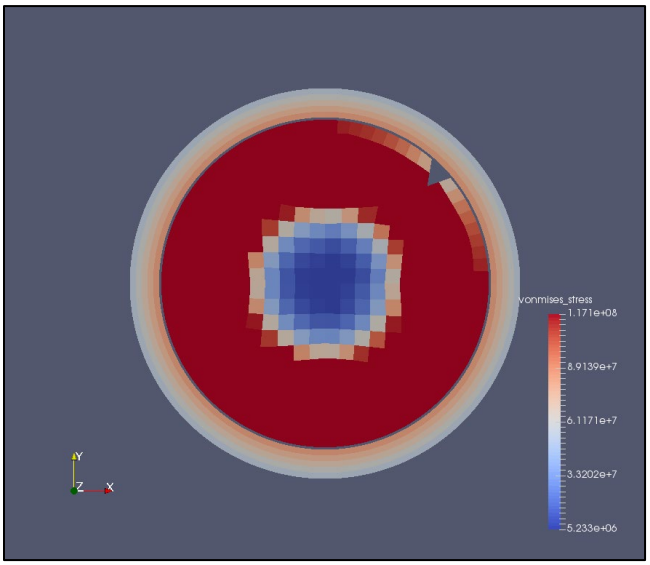


Figure F-2. 2D Von Mises stress in a low-burnup UO2 fuel, where a pellet has a macroscopic crack in it.

Significance

The work is in progress, and some of the midterm results will be published in January 31, 2021 in a public report.

Key Publications

Publications in process. We had planned participations in the NuMat2020 and MMM10 conferences to present and discuss initial results, but these were canceled due to the coronavirus pandemic.

Sponsor/Program

Finnish Nuclear Safety Programs SAFIR2022 and KYT2022 and the Nordic NKS Program

F.3. Modeling Solvated-Electron Penetration Depth and Aqueous Chemistry at the Plasma-Water Interface

Report Participants

Shane Keniley[1], Davide Curreli[1]

1 University of Illinois at Urbana-Champaign

Scientific Achievement

Plasmas directly interacting with liquid water will inject electrons directly into the liquid phase, which drives a unique set of non-equilibrium electrochemical reactions leading to the production and destruction of reactive oxygen species. The objectives of this work are to further develop the model of the dynamically coupled plasma-water interface currently employed in the MOOSE-based plasma transport model, Zapdos, and use it to study solvated-electron reactions in the near-surface water. A multispecies model employing over 200 reactions and 30 individual plasma and aqueous species was developed and used to model solvated-electron-driven chemical reaction pathways. Results show a qualitative agreement with experimental results; solvated-electron penetration depth decreases with an increasing electron current density, and the near-surface pH is increased to above 10 due to the production of OH anions in the liquid.

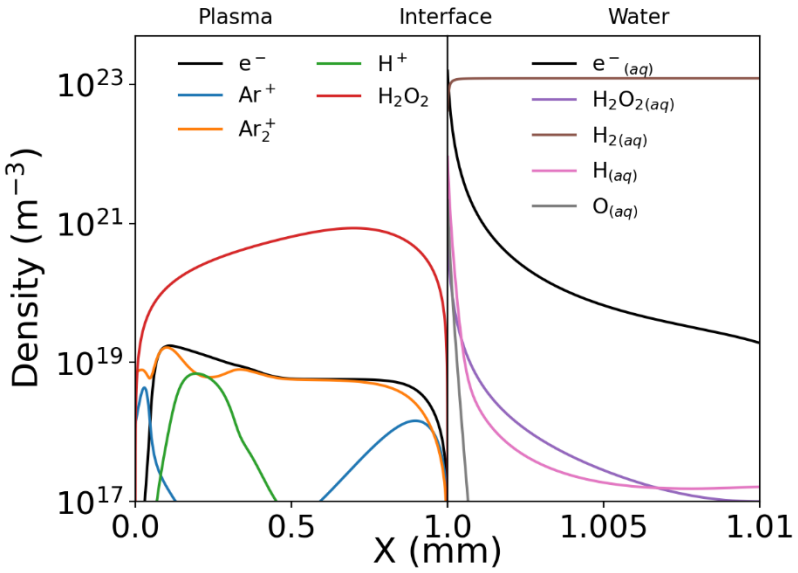


Figure F-3. Example of the dynamically coupled plasma-water interface. Left half shows the gas phase species, and the right half shows electron species. Electrons and selected neutral species directly penetrate the liquid phase and become solvated.

Significance

Plasma-water systems are highly studied due to their ability to produce reactive species capable of disinfecting surfaces (including wounds on human tissue) and treating toxic metals in industrial wastewater. Despite this interest, there remains no consensus on the effect solvated electrons injected into the water from the plasma have on the generation of reactive species. Whether reactive species are produced in the gas phase and transported into the water through solvation processes or produced directly in the liquid phase through aqueous chemistry also remains an open question. The non-equilibrium chemical reactions that are induced by the plasma treatment of water are highly nonlinear and operate on

spatial scales ranging from microns near the plasma-water interface to centimeteres far from the interface, and solvated electrons injected into the liquid operate on even smaller spatial scales ranging of 10–100 nanometers with lifetimes of tens of nanoseconds. Computational modeling enables the observation of spatially and temporally resolved concentrations of individual species in both gas and liquid phases. This work is focused on quantifying the effect solvated electrons have on the production of reactive species in plasma-treated water. This project provides a tool for modeling the tightly coupled plasma-water interactions, and the model is capable of studying solvated electrons in the liquid phase. Understanding the behavior of solvated electrons, observing how they affect the chemical makeup of the treated water, and determining the main gaseous and aqueous rection mechanisms responsible for the production of reactive oxygen species will allow experimental plasma-water treatment systems to be tailored to the generation of specific species.

Key Publications

- S. Keniley, D. Curreli. 2020. “Modeling solvated electron penetration depth and aqueous chemistry in the humid air plasma-water interface.” APS Gaseous Electrons Conference 2020 San Diego, CA. http://meetings.aps.org/Meeting/GEC20/Session/YF3.4
- S. Keniley, D. Curreli. 2020. “Modeling solvated electron penetration depth and aqueous chemistry at the plasma-water interface,” Plasma Sources Science and Technology, in progress.
- C. DeChant, Y. Xiao, C. Icenhour, S. Keniley, A. Lindsay, D. Curreli, S. Shannon. “Validations for Improvements of the Open Source Plasma Code, Zapdos.” APS Gaseous Electrons Conference 2020 San Diego, CA. http://meetings.aps.org/Meeting/GEC20/Session/QW2.3

Sponsor/Program

Other.

Appendix G

ENVIRONMENTAL MANAGEMENT

Table of Contents

G.1. Modeling Aluminum-Clad Spent Nuclear Fuel Stored in DOE Standard Canisters

Report Participants

Alexander Abboud[1]

1 Idaho National Laboratory

Scientific Achievement

This program assessed one alternative to the H-canyon processing of the Savannah River Site spent nuclear fuel, through packaging dried fuel in the road-ready DOE standard canister. A computational fluid dynamics model was built to assess the extend storage trends for the thermal profiles of the storage canisters over a 50-year period, this model was built with Star-CCM+. MCNP results of the storage configurations were also used to assess dose rates over this 50-year period of storage. The storage configurations studied were for a hypothetical MTR box spent fuel, the MURR spent fuel, and the High-Flux Isotope Reactor (HFIR) spent fuel. These storage configurations represent bounding scenarios for the decay heat and aluminum oxide surface area for aluminum-clad spent fuel at SRS. The resulting scenarios showed that the spent fuel surface temperatures are not expected to reach above 100°C during the storage time, and an examination of the storage configurations found that the surface area to volume ratio does not exceed that of similarly package ATR spent fuel.

Figure G-1. CAD geometry for a HFIR outer element stacked 3-high in a 24-inch diameter DOE standard canister.

Significance

The results in this work will provide inputs into the radiolytic chemical reaction modeling of the aluminum oxide layer coupled with the free volume of gas within the canister for hydrogen generation rates during extended storage scenarios. Due to the calculated dose rates for these storage configurations, combined with the low temperatures and lower aluminum surface area to free volume ratio, it is expected that the ATR fuel stored in DOE standard canisters will be the bounding scenario for all aluminum-clad spent fuel stored at DOE sites with regards to hydrogen generation.

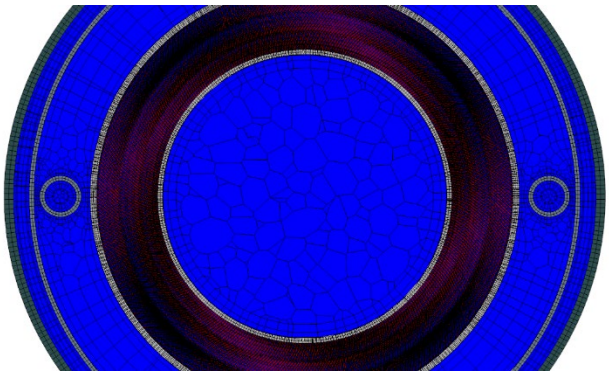


Figure G-2. Fully resolved mesh for the HFIR CFD model, blue shows free volume of air, red shows the fuel plates, light grey shows the aluminum, and dark grey shows the stainless-steel canister and inner bucket.

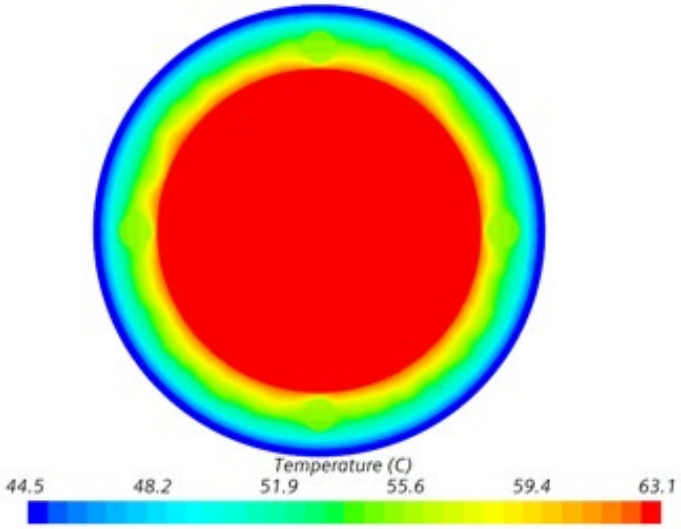


Figure G-3. A horizontal slice temperature profile for the nominal case of an HFIR outer fuel element storage.

Key Publications

Abboud, A. W. (2020). “Modeling of SRS Aluminum-clad Spent Nuclear Fuel in Standard DOE Sealed Canisters,” (INL/EXT-20-57893-Rev000). Idaho National Laboratory (INL), Idaho Falls, ID (United States). https://doi.org/10.2172/1644680

Sponsor/Program

Department of Energy, Office of Environmental Management

G.2. Modeling of Waste Glass Vitrification

Report Participants

Alexander Abboud[1], Donna Guillen[1]

1 Idaho National Laboratory

Scientific Achievement

The computational modeling and simulation being performed at INL supports the vitrification of legacy tank waste at the Waste Treatment and Immobilization Plant. INL is providing insight into the processes occurring within the high level and low activity waste melters. Our support includes the heat transfer and computational fluid dynamics modeling of glass melters at various scales using a resolved two-phase flow and conjugate heat transfer. Processes occurring in the melters are represented using a volume-of-fluid model to resolve the bubbling and Joule heating in the glass melt pool below the cold cap layer. Thermal radiation from the 1150ºC melt pool provides heating to the plenum region. Computational predictions were shown to match experimental glass and plenum temperatures within the uncertainty of the measurements. In addition, the dependence of the plenum temperatures on the batch layer (referred to as a cold cap) coverage and emissivity was also predicted by the model, showing the largest dependence on the cold cap coverage. Further investigation used a simplified model with only the plenum space modeled via a steady-state approximation. This simplified model was run for 1000 randomized cold cap coverage topologies consisting of regions of batch coverage and vent holes. A convolutional neural network (CNN) was built to infer the cold cap coverage from a sparse set of temperatures provided by the CFD model. Preliminary testing of this CNN showed an 89% predictive accuracy for the cold cap coverage. Since cold cap coverage is important to optimize batch melt rate, this capability holds promise for providing nonvisual feedback to inform process control during the vitrification campaign.

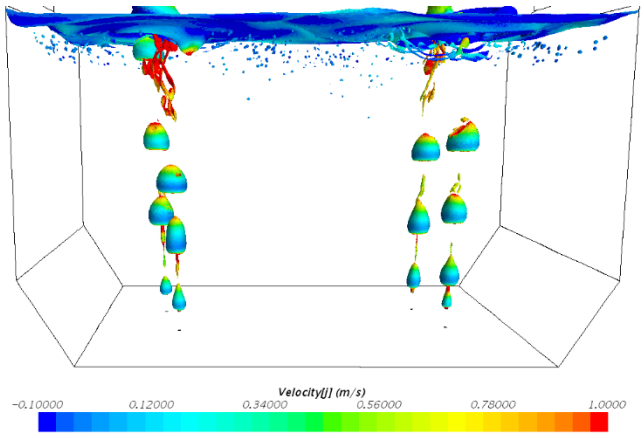


Figure G-4. Fully resolved bubbling within the glass melt pool.

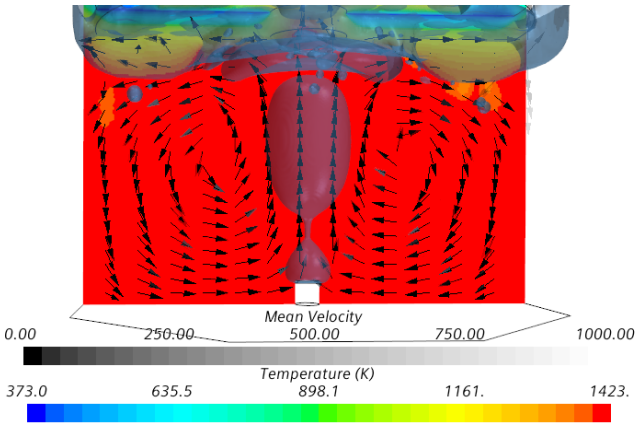


Figure G-5. Simulation results for melt pool and cavity layer under the cold cap showing velocity vectors overlaid on the temperature and gas volume fraction.

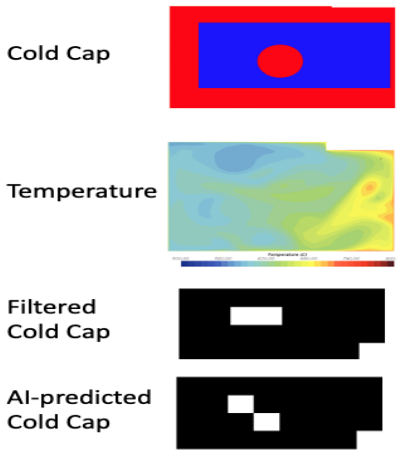


Figure G-6. Cold cap topology and temperature field from the CFD simulation with the filtered CNN prediction showing AI-predicted coverage and vent hole location.

Significance

Validated models can be used to inform melter operations at the plant. Additionally, models have been developed for small test melters designed to evaluate the efficacy of the off-gas systems. Eventual modeling of the full-scale WTP melter may help improve the understanding of the batch-to-melt process when the actual nuclear waste vitrification campaign begins at Hanford. The CNN deep learning method has the potential to provide a nonvisual indicator for cold cap coverage that can be used for operational process control.

Key Publications

- A.W. Abboud, D.P. Guillen, R. Pokorny, (2020), "Effect of cold cap coverage and emissivity on the plenum temperature in a pilot-scale waste vitrification melter," *International Journal of Applied Glass Science*, vol. 11, no. 2, pp. 357-368. https://doi.org/10.1111/ijag.15031
- A.W. Abboud, D.P. Guillen, R. Pokorny, "Convolutional Neural Network Model for the Prediction of Plenum Temperature in a Waste Glass Melter," ASME 2020 Power Conference, August 2-6, 2020. https://doi.org/10.1115/POWER2020-16993

- A.W. Abboud, D.P. Guillen, P. Hrma, A.A. Kruger, J. Klouzek, and R. Pokorny, (2020), “Heat Transfer from Glass Melt to Cold Cap: Computational Fluid Dynamics Study of Cavities Beneath Cold Cap,” *International Journal of Glass Science*, in press. https://doi.org/10.1111/ijag.158"63
- D.P. Guillen, A.W. Abboud, P. Hrma, A.A. Kruger, J. Klouzek, and R. Pokorny, “Computational Fluid Dynamics Study of Cavities Beneath Cold Cap Layer in Waste Glass Melter,” GLASS MEETING 2020 on Web with Advances in Fusion and Processing of Glass (AFPG), December 7 to 10, and 16-18, 2020.
- Guillen, D.P., A.W. Abboud, M. Hall, W.C. Eaton, A. Kruger, R. Pokorny, “Computationally Aided Design of a Small-Scale Waste-Glass Melter” WM Symposia, Phoenix, AZ, March 8-12, 2020. https://www.osti.gov/servlets/purl/1673741
- W.C. Eaton, M.A. Hall, A.W. Abboud, D.P. Guillen, D.R. Dixon, C.D. Lukins, C.M. Stewart, A.A. Kruger, “Melter Optimized for Fast Turnover, Steady State Testing," WM Symposia, Phoenix, AZ, March 8-12, 2020.

Sponsor/Program

Department of Energy, Office of River Protection

Appendix H

INL OPERATIONS

Table of Contents

H.1. North Radiography Station Neutron Beamline Precollimator at the Neutron Radiography Reactor

Report Participants

William Chuirazzi[1], Aaron Craft[1], Andrew Smolinski[1], Kyrone Riley[1]

1 Idaho National Laboratory

Scientific Achievement

The North Radiography Station (NRS), located at the Neutron Radiography Reactor (NRAD), consists of a neutron beamline that is used for neutron imaging and scattering experiments. This project aims to install a beamline collimator to better focus the neutrons in the beam and the reduce dose rates and activation in surrounding equipment and areas. The HPC resources were used to run the Monte Carlo N-Particle simulation software to design a collimator that produces a desirable calculated impact on the neutron beam. The HPC resources were necessary to quickly run simulations that provided enough accuracy to justify modifications to a nuclear facility. This model was also used to characterize the existing neutron energy spectrum of the NRS beamline.

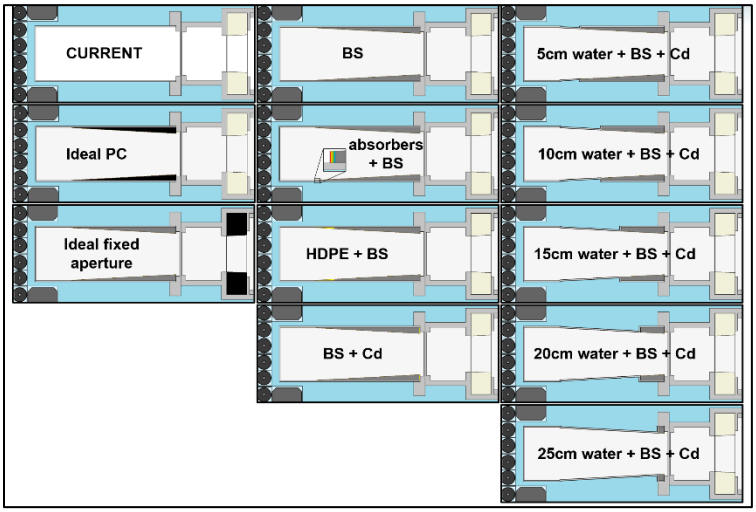


Figure H-1. Diagram of collimators geometries simulated with MCNP.

Significance

This project is still in progress, although preliminary design results have been generated through HPC. Design results show a mere 2.6% decrease in the neutron flux at the NRS imaging plane and a >20% decrease in gamma-ray dose. The precollimator also reduces the neutron flux by ~60% and the gamma-ray dose by ~42% in some areas along the beamline, helping to reduce the shielding necessary along the beamline. This project will benefit experiments at NRAD as the quality of data from neutron beamline experiments will improve because of the reduced noise. NRAD operations will also benefit from the reduced radiation dose to workers and reduced neutron activation to surrounding equipment.

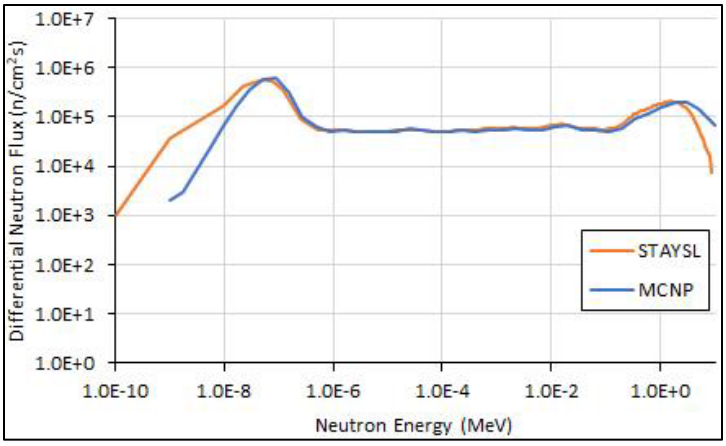


Figure H-2. Measured (orange) and simulated (blue) neutron spectrum at the NRS image plane.

Key Publications

- Chuirazzi, W. C. (2020). "Combinatorial Optimization of Scintillator Screens for Digital Neutron Imaging," Columbus, OH: The Ohio State University. PhD. Dissertation.
- An internal Engineering Calculations and Analysis report is currently under revision. The calculations from HPC will be used in this report to justify the modifications to the NRAD reactor facility.

Sponsor/Program

Materials and Fuels Complex

H.2. CFD Modeling of the HENRI Facility

Report Participants

Cole Leingang1, Dr. Guillamue Mignot1, Cody Race2

1 Oregon State University

2 Idaho National Laboratory

Scientific Achievement

The access to HPC resources was used to run STAR-CCM+ in order to simulate the Helium-3 Negative Reactivity Insertion (HENRI) Facility and study its pressure, temperature, and density time-evolution. The purpose was to test the fast pressurization of a cartridge that would be installed in place of a fuel assembly in the TREAT nuclear reactor facility at INL. The ultimate goal of the HENRI system is to reduce the full width at half maximum of the power pulse generated in the TREAT facility from its current 100 ms to values ranging from 25 to 75 ms The CFD simulations run and work done allowed for a current best-estimate representation of HENRI when it is placed inside the TREAT facility.

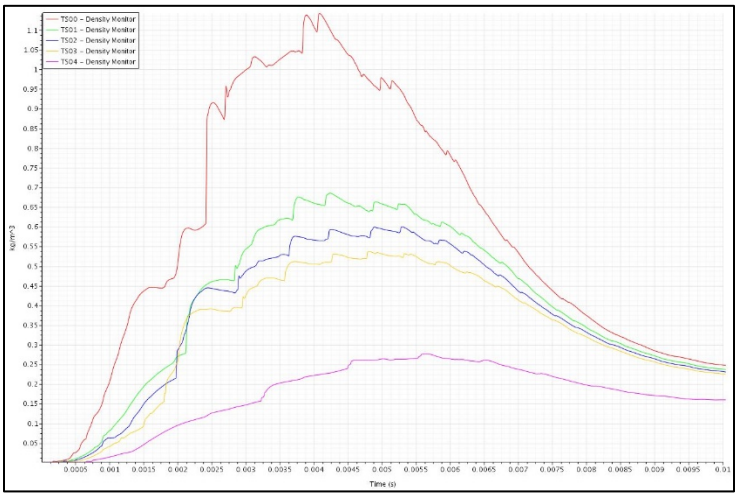


Figure H-3. Density evolution of He-3 in HENRI.

Significance

Key-findings were the study of the density evolution, which was provided to INL staff in order to better facilitate the design and study of the Helium-3 neutron capture reaction effect on the HENRI cartridge operation. This detailed study of density evolution and capture reaction effect further facilities the ongoing design work. Future work will involve the Serpent 2 code.

Key Publications

C. Leingang, G.P. Mignot. “STAR CCM+ Simulation of the Helium-3 Neutron Capture Reaction Effect on the Helium-3 Negative Reactivity Insertion (HENRI) Cartridge Operation”. Submitted to the 2020 ANS Winter Meeting, November 16-19, 2020. https://ans.org/pubs/transactions/a_49062

Sponsor/Program

Idaho National Laboratory

Appendix I

OFFICE OF SCIENCE

Table of Contents

I.1. GEM3 Genes by Environment–Mapping Adaptive Capacity

Report Participants

Donna Delparte[1], Youngwoo Cho[1]

1 Idaho State University

Scientific Achievement

We processed an unmanned aircraft thermal, multispectral, and optical imagery to map thermal refugia and riparian habitat in desert stream systems for Redband Trout.

Figure I-1. UAV data collection at Big Jacks Creek, Idaho.

Significance

This project combines expertise across gneomics, biology, and mapping to examine the Redband Trout response to thermal stressors in desert stream systems. Processing UAV data is time consuming and resource intensive—the GPU HPC capability at INL has accelerated our UAV image processing step in preparation for an advanced analysis.

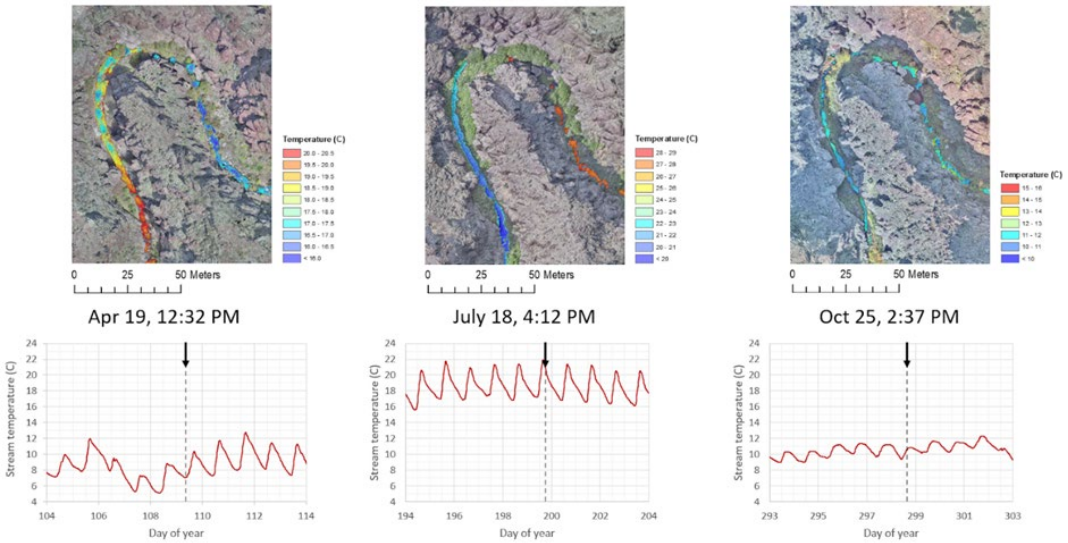


Figure I-2. Thermal gradients in Little Jacks Creek, Idaho over summer 2019.

Key Publications

In progress.

Sponsor/Program

Idaho EPSCoR (https://www.idahogem3.org/)

I.2. Multiscale Modeling of Nitrogen Adsorption Using Zeolites

Report Participants

Donna Guillen[1], Miu Lun Lau[2]

1 Idaho National Laboratory

2 Boise State University

Scientific Achievement

The researchers are developing a comprehensive multiscale model of nitrogen adsorption using various zeolites in a pressure swing adsorption unit. The zeolites will be processed using advanced manufacturing techniques with various binders and additives to produce a topology that provides an improved adsorption efficiency. The adsorption process will be evaluated using breakthrough curves at various pressures, temperatures, and flow rates. Computational models are constructed at various length scales using DG-OSPREY implemented using the MOOSE framework at the continuum scale, with input parameters supplied from the open source molecular dynamics software LAMMPS.

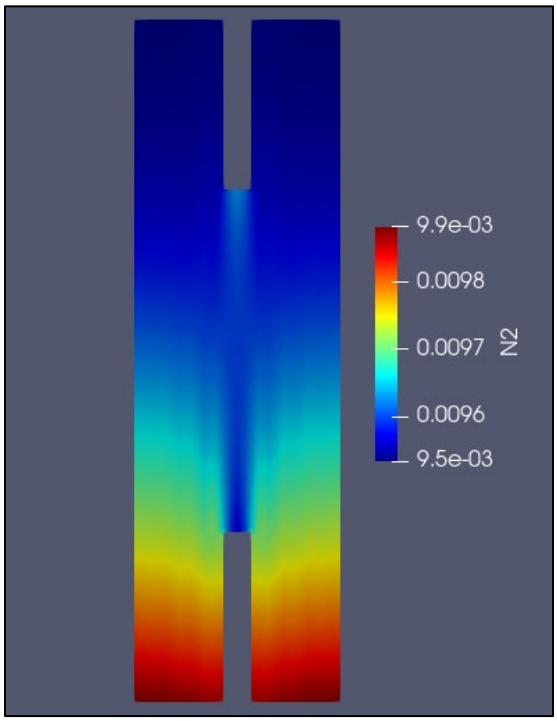


Figure I-3. Adsorption result for Zeolite 13X using DG-OSPREY.

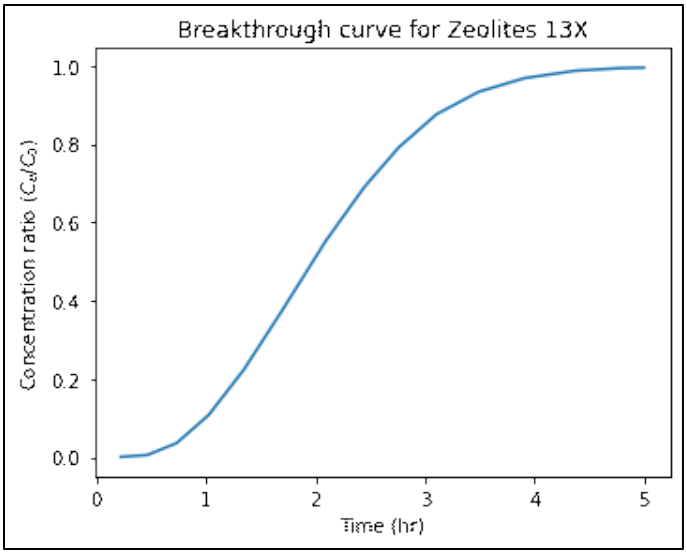


Figure I-4. The corresponding breakthrough curve.

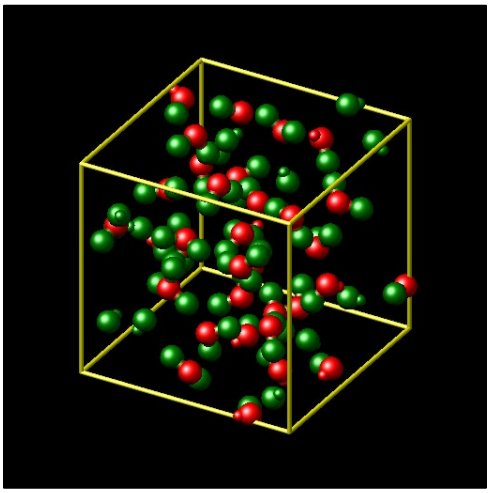


Figure I-5. Preliminary model of nitrogen adsorption in a zeolite structure using a grand canonical Monte Carlo simulation predicted using LAMMPS.

Significance

The ability to evaluate the adsorption efficiency for a given material is crucial in many types of engineering and medical applications. Nitrogen adsorption, for example, is used mainly in the medical field to generate enriched oxygen. An improvement can be made by studying the relationship of zeolite adsorption under various conditions, geometries, and additives, in addition to the processing conditions from additive manufacturing.

Key Publications

None.

Sponsor/Program

Department of Energy, Office of Science

Appendix J

ADVANCED RESEARCH PROJECTS AGENCY–ENERGY

Table of Contents

J.1. Development of a Nearly Autonomous Management and Control System for Advanced Reactors

Report Participants

Taeseung Lee[1]

1 Argonne National Laboratory

Scientific Achievement

The project seeks to establish a technical basis for, and preliminary development of, a nearly autonomous management and control (NAMAC) system in advanced reactors. The numerical demonstration of NAMAC and GOTHIC plant model shows that NAMAC can successfully diagnose the plant state and recommend action that stabilizes the plant state. Currently, the databases for Q4 issue space with more refined samples are being generated at Falcon using a RAVEN-GOTHIC coupled simulation.

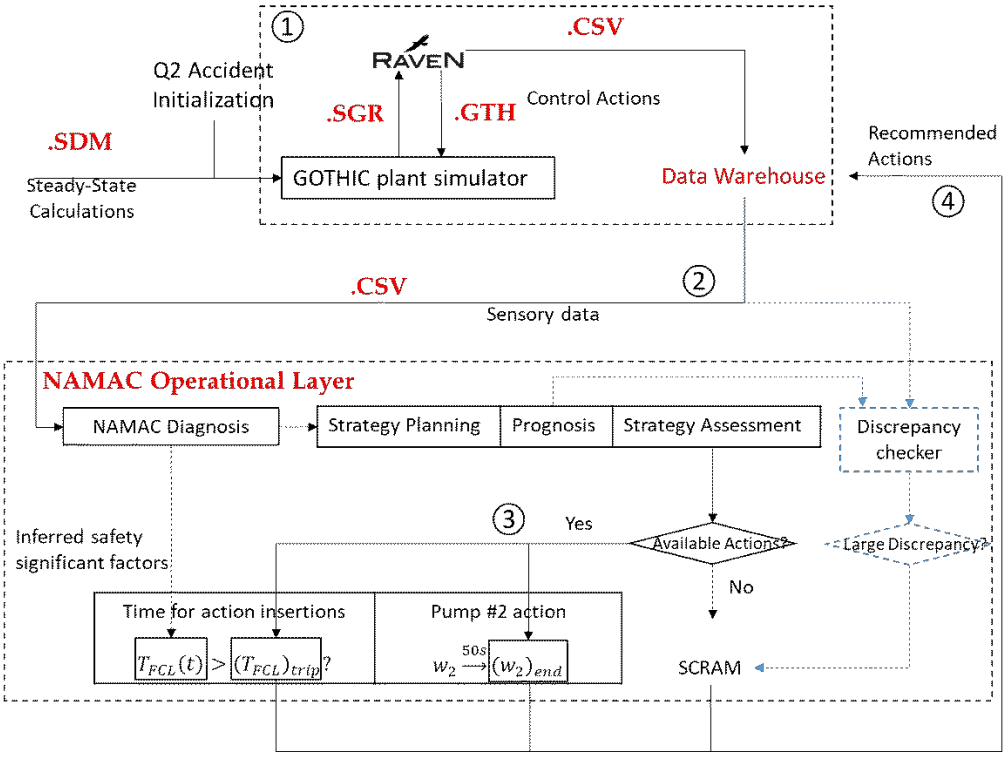


Figure J-1. Schematic of a NAMAC demonstration through the decoupled system.

Significance

The NAMAC system is intended to provide recommendations to operators during all modes of plant operation except shutdown operations, ranging from normal operation to accident management. These recommendations are to be derived within a modern, AI guided system, making use of the continuous extensive monitoring of plant status, knowledge of current component status, and plant parameter trends; the system will continuously predict the near-term evolution of the plant state and recommend a course of action to plant personnel. The NAMAC system utilizes simulation-informed, data/knowledge-driven, AI-guided, plant-data-assimilated real-time operating procedures and accident management guidelines to effectively support the operator in risk-informed management.

Key Publications

Q4 Quarterly Report

Sponsor/Program

Advanced Research Projects Agency-Energy