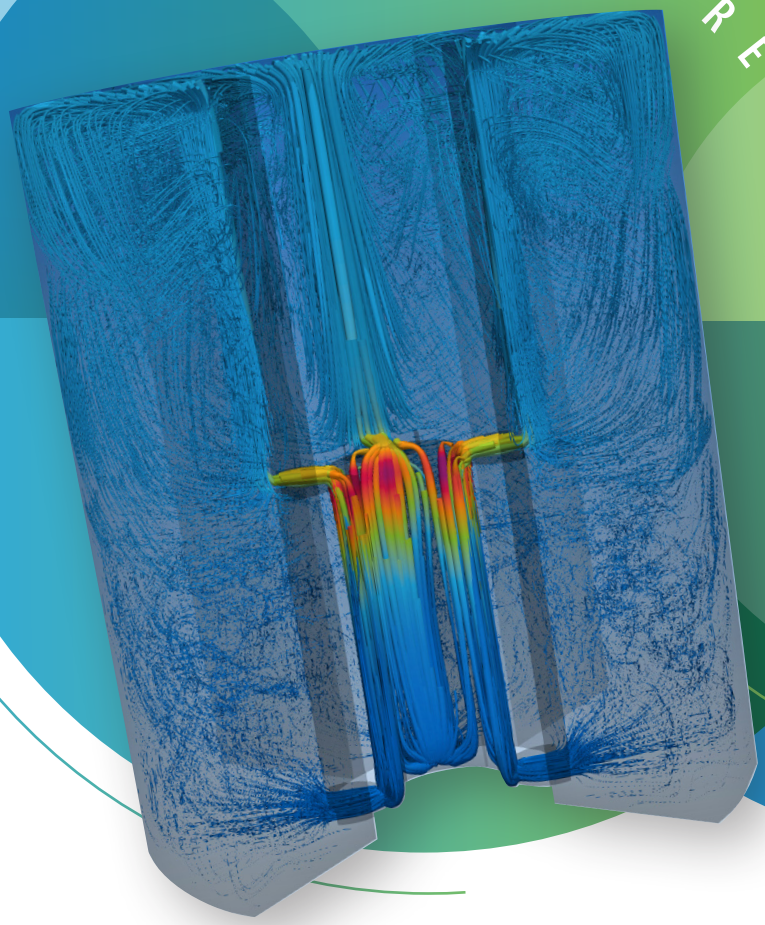
NUCLEAR SCIENCE USER FACILITIES

High Performance Computing

ANNUAL REPORT

2023



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FY-23 HPC Annual Report Cover Page Design
The figure shows streamlines of air around a spent fuel cask. There is also a helium circulation inside of the cask due to heat coming from spent nuclear fuel.

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Nuclear Science User Facilities High Performance Computing

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Nuclear Science User Facilities High Performance Computing

FY 2023 Annual Report

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 fiscal year (FY) 2023, INL HPC systems Sawtooth, Lemhi, and Hoodoo supported 3,732,911 computational jobs from 1,320 users, totaling 939 million core-hours. Of this total usage, 86% directly supported nuclear energy research and development. The remaining core-hours supported education efforts, security, operations, and energy storage research. Some salient examples of the impact of the HPC systems during FY-23 include enabling the modeling and simulation in support of the Microreactor Applications Research Validation and EvaLuation microreactor 90% final design notable outcome and supporting analysis on the Advanced Test Reactor butterfly valve.

During FY-23, INL HPC capabilities were utilized by a diverse set of 1,320 computing and applied researchers. The majority came from national laboratories (806) with university users making up the second largest group of users (264) and industry partners making up the third largest group of users (250). In addition, INL also supported 12 users from nuclear regulatory agencies, demonstrating our commitment to foster relationships between research and regulatory personnel.

INL HPC capabilities were instrumental enablers for a wide range of research and engineering activities in FY-23, with summaries of a number of these activities presented as user-provided project reports (see Appendices A–H). A large portion of HPC use was geared towards nuclear energy, with numerous computational studies on important topics relevant in nuclear energy. 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.

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CONTENTS

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ACRONYMS

6-DOF	six degree of freedom
AI	Artificial Intelligence
AIMD	Ab-initio Molecular Dynamics
AFC	Advanced Fuels Campaign
AFM	antiferromagnetic
Ag	Silver
AGU	American Geophysical Union
AKMC	Atomic Kinetic Monte Carlo
Al	aluminum
ALCC	ASCR Leadership Computing Challenge
AM	additive manufacturing
AMO	Advanced Manufacturing Office
AMS	American Meteorological Society
ANL	Argonne National Laboratory
AOO	Anticipated operational occurrences
AOR	angle of repose
ARDP	Advanced Reactor Demonstration Program
ARMOR	Advanced Remote Monitoring for Operations Readiness
ARPA-E	Advanced Research Projects Agency - Energy
ASC	Advanced Scientific Computing
ASR	alkali-silica reaction
ATF	Accident Tolerant Fuel
ATR	Advanced Test Reactor
ATRC	Advanced Test Reactor Critical
BART	Bidirectional Auto-Regressive Transformers
BATR	Broad Application of Test Reactor
BCC	body-centered-cubic
BEPU	Best Estimate Plus Uncertainty
BERT	Bidirectional Encoder Representations from Transformers
BES	Basic Energy Sciences
BETO	Bioenergy Technologies Office
BH	basin-hopping
BlueCRAB	Comprehensive Reactor Analysis Bundle
BSU	Boise State University
Bu	burnup
BWR	Boiling-Water Reactor
C3	Collaborative Computing Center
CAES	Center for Advanced Energy Studies
CAP	corrective action programs
CASL	Consortium for Advanced Simulation of Light Water Reactors
CATS	Catalytic After Treatment System

CBIR	Content Based Image Retrieval
CBS	concrete biological shield
CCB	cellular ceramic breeders
CCPC	Consortium for Computational Physics and Chemistry
CEF	Compound Energy Formalism
CEN	Collaboratory for Epitaxy of Nanomaterials
CEX	charged exchange
CIC	core internals changeout
CILC	Crud Induced Localized Corrosion
CIPS	Crud Induced Power Shift
CFD	Computational Fluid Dynamics
CHF	critical heat flux
CLOF	Complete Loss of Flow
CMCDT	Common Monte Carlo Design Tool
CMFDT	coarse-mesh finite difference
CNN	Convolutional Neural Network
CNT	carbon nanotubes
COG	Code Oversight Group
CPU	central processing unit
Cr	Chromium
CSAP	Core Safety Assurance Package
CSRO	chemical short-range order
CU	Copper
DBA	design-basis accidents
DBTT	ductile-brittle transition
DCA	design certification application
DEEP	Deep Metric Learning
DeepONets	deep operator networks
Deff	diffusion coefficient
DEM	Discrete Element Modeling
DET	Dynamic Event Tree
DFO	Forensics Operations Ground Collection Task Force
DFT	density functional theory
DFTB	density-functional tight-binding
DFT	Density Functional Theory
DG	discontinuous Galerkin
DGM	Dissolved Gas Model
DL	Deep Learning
DNB	Departure from Nucleate Boiling
DNN	deep neural network
DNS	Direct Numerical Simulations
DOE	Department of Energy
DOE-NE	Department of Energy Office of Nuclear Energy
DPD	Dissipative Particle Dynamics
DRL	deep reinforcement learning

EBR-II	Experimental Breeder Reactor II
EDU	Electrical Demonstration Unit
EERE	Office of Energy Efficiency and Renewable Energy
EFRC	Energy Frontier Research Center
ELTA-CL	Extended Length Test Assembly-Cartridge Lead
EM	Office of Environmental Management
EOL	end of life
EPRI	Electric Power Research Institute
EPSCoR	Established Program to Stimulate Competitive Research
EPP	effective plate power
EPtP	effective point power
ERCOT	Electric Reliability Council of Texas
ET	element test
EURAD	European Joint Programme on Radioactive Waste Management
EVND	Ex-Vessel Neutron Dosimetry
EXAFS	Extended X-ray Absorption Fine Structure
FE	Finite Element
FEM	finite element method
FCIC	Feedstock Conversion and Interface Consortium
FCT	fuel centerline temperature
FFRD	Fuel, Fragmentation, Relocation, and Dispersal
FFTF	Fast Flux Test Facility
FG	Fission Gas
FGR	Fission Gas Release
FGR	forced gas recirculation
FHR	high-temperature reactors
FIRST	Fluid Interface Reactions, Structures and Transport
FM	ferromagnetic
FMR	Fast Modular Reactor
FOA	Funding Opportunity Announcements
FORGE	Frontier Observatory for Research in Geothermal Energy
FNN	feedforward neural network
FNO	Fourier Neural Operator
FPoli-AAP	FPoli Agile Application Platform
FPoliDON	test data management
FPoliDOX	document management
FPoliSIM	simulation management
FT	Fischer-Tropsch
FV	Finite Volume
GA	Genetic Algorithm
GA-EMS	General Atomics-Electromagnetic Systems
GAIN	Gateway for Accelerated Innovation in Nuclear
GB	grain boundaries
GBS	Gas Bubble Superlattices

GPU	graphics processing unit
GRA	generation risk assessment
GRMHD	general relativistic magnetohydrodynamic
GSA	General Spectrum Analyzer
HB	High Burnup
HBS	high-burnup structures
HBu	high burnup
HEA	high entropy alloys
HENRI	Helium-3 Negative Reactivity Insertion
HERA	High burnup Experiments for Reactivity initiated Accident
HERON	Holistic Energy Resource Optimization Network
HEU	highly enriched uranium
HEX	Heat Exchanger
HFEF	Hot Fuel Examination Facility
HFIR	High-Flux Isotope Reactor
HFP	hot full power
Hi2Lo	high to low fidelity
HP	heat pipe
HPC	High-Performance Computing
HPP	Half Plate Power
HRSTEM	high-resolution scanning transmission electron microscopy
HTGR	High-Temperature Gas Reactor
HTR	High Temperature Reactor
HZP	hot zero power
IAEA	International Atomic Energy Agency
ICERR	International Center of Excellence based on Research Reactors
IED	irradiation-enhanced densification
INL	Idaho National Laboratory
IoT	Internet of Things
IRP	Integrated Research Projects
IRPhEP	International Reactor Physics Experiment Evaluation Project
IRUG	International RELAP5 User Group
ISP	Specific Impulse
ISU	Idaho State University
ITER	International Thermonuclear Experimental Reactor
IUC	Idaho University Consortium
KMC	Kinetic Monte Carlo
KTH	Kungliga Tekniska högskolan (Royal Institute of Technology)
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator
LANL	Los Alamos National Laboratory
LaRomance	Los Alamos Reduced Order Models for Advanced Nonlinear Constitutive Equations
LBE	lead-bismuth eutecti

LDC	La-doped ceria
LDRD	Laboratory Directed Research and Development
LES	large eddy simulations
LEU	low enriched uranium
LHGR	instantaneous linear heat generation rate
LIGGGHTS	LAMMPS Improved for General Granular and Granular Heat Transfer Simulations
LOCA	loss-of-coolant-accident
LOWE	Low-enriched
LPCIS	Lobe Power Calculating and Indication System
LPRM	Local Power Range Monitoring
LR	locked rotor
LSTM	long short-term memory
LSW	Lifshitz-Slyozov-Wagner
LWR	Light-Water Reactor
LWRS	Light Water Reactor Sustainability
M&S	Modeling and simulation
MATHAM	Mars Active Tracer High-Resolution Atmospheric Model
MBE	Molecular Beam Epitaxy
MC	Monte Carlo
MCNP	Monte Carlo N-Particle
MCO	Moisture Carryover
MD	molecular dynamics
MDMC	Molecular Dynamics/ Monte Carlo
MELCOR	Methods for Estimation of Leakages and Consequences of Release
MFC	Materials and Fuels Complex
mHNGD	Hydride Nucleation-Growth-Dissolution
MITR	Massachusetts Institute of Technology Reactor
MIRACLE	Machine Intelligence for Review and Analysis of Condition Logs and Entries
ML	Machine Learning
MOC	method of characteristics
MOAA	MCNP ORIGEN Activation Automation
MOOSE	Multiphysics Object-Oriented Simulation Environment
MMM/M3	Materials Management and Minimization
MPC	model predictive control
MPCMIV	multiphysics pellet-cladding mechanical interaction validation
MPE	Multi Principal Elemental
MQM	modified quasichemical
MSBR	Molten Salt Breeder Reactor
MSD	mean square displacement
MSFC	Marshall Space Flight Center
MSFR	Molten Salt Fast Reactor

MSLB	Main Steam Line Break
MSR	Molten Salt Reactor
MSTDB	Molten Salt Thermodynamic Database
MTHM	metric tons of heavy metal
MURR	University of Missouri Research Reactor
NASA	National Aeronautics and Space Administration
NBSR	National Bureau of Standards Reactor
NC	noncondensable
NCERC	National Criticality Experiment Research Center
NCG	non-condensable gases
NCL	natural circulation loops
NCRC	Nuclear Computational Resource Center
NCSU	North Carolina State University
NE	Nuclear Energy
NEA	Nuclear Energy Agency
NEAMS	Nuclear Energy Advanced Modeling and Simulation
NEGF	nonequilibrium Green's functions
NEUP	Nuclear Energy University Program
NF	nanofiber
NI	Nickel
NIH-NIGMS	National Institute of General Medical Sciences
NILO	Nonlinearly Implicit Low-Order
NLP	Natural language processing
NNIP	neural network interatomic potential
NNL	Naval Nuclear Laboratory
NNSA	National Nuclear Security Administration
NPP	nuclear power plants
NPV	net present value
NR	numerical relativity
NRAD	Neutron Radiography Reactor
NRC	Nuclear Regulatory Commission
NRIC	National Reactor Innovation Center
NRS	North Radiography Station
NSF	National Science Foundation
NSUF	Nuclear Science User Facilities
NTP	nuclear thermal propulsion
NTR	Nuclear Thermal Rocket
NURETH	Nuclear Reactor Thermal Hydraulics
NVT	Nose-Hoover thermostat
OECD	Organisation for Economic Co-operation and Development
OKMC	object kinetic Monte Carlo
ORNL	Oak Ridge National Laboratory
OS	Office of Science
O-SERTTA	The Oregon State University Static Environment Rodlet Transient Test Apparatus

OTHT-HX	Oval Twisted Tube Helical Coiled Heat Exchanger
PAW	projector augmented wave
PBR	Pebble-Bed Reactor
PC&O	Process Control and Optimization
PDF	pair distribution functions
PF	phase-field
PHM	prognostic health management
PIE	post-irradiation examination
PINNs	physics-informed neural networks
PKE	Point Kinetics Equation
PPD	Peak Power Density
PSA	Pressure Swing Adsorption
PUMA	Physics Unified Modeling and Analysis
PWR	pressurized water reactor
RC	reinforced concrete
R&D	Research and Development
RANS	Reynolds-averaged Navier-Stokes
RAVEN	Risk Analysis Virtual Environment
RCCS	Reactor Cavity Cooling System
RE	Reactor Engineering
RELAP5	Reactor Excursion and Leak Analysis Program
RF	radio frequency
RF	random forest
RIA	reactivity initiated accidents
RIS	Radiation-Induced Segregation
RISA	Risk Informed System Analysis
RISE	Risk-Informed System Engineering
RMSEn	normalized Root Mean Square Error
RNN	recurrent neural network
ROMS	reduced order models
S2Cl2	Sulfur monochloride
SA	sensitivity analysis
SAPHIRE	Systems Analysis Programs for Hands-on Integrated Reliability Evaluations
SAR	Safety Analysis Report
SBE	Saftey-Basis Events
SDC	Spectral Deferred Correction
SFC	Spent Fuel Characterization
SFE	stacking fault energy
SGRB	short gamma-ray burst
SHAP	Shapley Additive Explanations
SiC	silicon carbide
SMART	Scalable Massively Asynchronous Ray Tracing
SMR	small modular reactors
SNAP	Systems for Nuclear Auxiliary Power

SNF	spent nuclear fuel
SNP	Space nuclear propulsion
SOCl2	thionyl chloride
SQ	Sqauaraine
SQS	Special Quasi-Random
STGB	symmetric tilt grain boundaries
STIC	Strategic Thermal Irradiation Capability
TAPE	Transient Analysis PackagE
TBS	test blanket system
TCR	Transformational Challenge Reactor
TE	thermoelectric
TEM	transmission electron microscopy
TES	Thermal Energy Storage
TETI	Thermal Energy Transport under Irradiation
TD-DFT	time-dependent density functional theory
T/H	thermal-hydraulic
ThO2	thorium dioxide
TIGER	Text Interface Graphical Exodus Reader
TIP	Traversing In-core Probe
TLU	Texas Lutheran University
TMAP8	Tritium Migration Analysis Program
TPMS	Triple Periodic minimal surfaces
TREAT	Transient Reactor Test
TRISO	TRi-structural ISOtropic
UO2	Uranium Dioxide
UN	uranium mononitride
UQ	uncertainty quantification
USHPRR	United States High Performance Research Reactor
UTAB	Uncertain TABular
VASP	Vienna ab initio Simulation Package
VBMC	Variational Bayesian Monte Carlo
vdW	van der Waals
VERA	Virtual Environment for Reactor Analysis
VERT	Versatuke Economic Risk Tool
VHF	Van Hove correlation function
VHTGR	Very High Temperature Gas-cooled Reactor
VIF	variance inflation factor
VMD	Visual Molecular Dynamics
VPSC	visco-plastic self-consistent
VRE	Variable Renewable Energy
VUG	VERA User Group
VTB	Virtual Test Bed
VTR	Versatile Test Reactor
VTT	Valtion Teknillinen Tutkimuskeskus (Technical Research Centre [of Finland])

VVUQ	Verification, validation and uncertainty quantification
V&V	verification and validation
WCLL	water-cooled lithium lead
WRF	Weather Research and Forecasting
WTP	Waste Treatment and Immobilization Plant
XPS	X-ray Photoelectron Spectroscopy
XRD	X-ray Diffraction
Zry	Zirconium Alloy

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, artificial intelligence hardware, 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 developments in scientific computing, INL continues to look for new and innovative ways to expand our computational research capabilities through:

- Investing in scientific computing capacity
- Developing and validating innovative modeling tools
- Supporting data science gateways
- Supporting innovative software container strategies
- Expanding expertise in machine learning, artificial intelligence, advanced visualization, and large-scale data processing and analytics.

Fiscal Year (FY) 2023 saw a significant expansion into data curation and distribution strategies, external training support, and significant expansions in machine learning and visualization capabilities. HPC delivered 939 million core hours and 3,732,911 computational jobs from 1,320 users with 86% of those jobs directly supporting nuclear energy research. HPC also supported four external trainings that relied on HPC resources.

User-supplied HPC summaries are included as appendices to this report. These summaries are submitted as part of the 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 using 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 FY-23 are listed below and discussed in Sections 2.1–2.7:

- Delivered 20 million more core hours in FY-23 than in FY-22
- Supported multiple external trainings and expanded support for future trainings
- Deployed a large language model Chat Bot for answering HPC support questions
- Developed the Nuclear Research Data System (NRDS) portal for supporting NSUF data management
- Expanded the visualization support system from four nodes to 13 nodes
- Significantly expanded storage capabilities
- Published a container strategy widely adopted for HPC software deployments.

2.1. Delivered 20 million more core hours than in FY-23

Without any significant expansion in computing resources, INL HPC delivered 939 million core hours in FY-23. This is an increase of 20 million core hours over what was delivered in FY-22. This was accomplished by reducing system downtime, improving scheduling efficiency, and reducing the threshold to HPC usage for new users. For example, in FY-22 there were 12 planned outages whereas only seven were needed in FY-23.

2.2. Supported multiple external trainings

Availability and access to training on Nuclear Energy Advanced Modeling and Simulation (NEAMS) code is instrumental to continued adoption and refinement of capabilities. In FY-23, INL HPC staff, in collaboration with the Nuclear Computational Resource Center (NCRC) staff, supported four external training sessions and workshops that required HPC access to provide hands on exercises using NEAMS codes for attendees. HPC staff created a HPC account for each attendee, setup the OnDemand app, and scheduled a reservation to meet the requirements for each training. HPC staff were made available throughout the training sessions to assist with HPC-related questions from meeting organizers and attendees. Training opportunities, such as those supported by the HPC team in FY-23, promote the development of national computational science expertise.

2.3. Deployed a large language model Chat Bot for HPC support

In September 2023, the INL HPC team integrated Chat Bot, an innovative addition to the Open OnDemand Science Gateway, which has significantly enhanced user experience and streamlined the process of accessing HPC resources. The Chat Bot caters to users seeking on-the-spot assistance and guidance, offering a user-friendly interface for query resolution and HPC-related inquiries. This artificial intelligence (AI) driven tool has been utilized by 129 individuals, who have sent 222 messages before October 1, 2023, demonstrating its popularity and effectiveness within our user community. Key benefits include 24/7 support and a simplified approach to technical support. With the Chat Bot, users can easily address questions and resolve challenges. This further reinforces our commitment to providing a seamless HPC experience.

2.4. Developed the Nuclear Research Data System site for supporting NSUF data management

In 2022, NE-5 Alice Caponiti challenged HPC to create a way that would allow data to be stored and publicly viewed and HPC answered. This challenge was to help NSUF comply with DOE's requirement to have all scientific data be public past a predetermined embargo date. The Nuclear Research Data Systems (NRDS) site was made public in December 2023 to achieve this. It is a public science data gateway that will allow scientific data to be downloaded, previewed, and enhanced through AI all without logging in. Data is organized by NSUF projects, and metadata is collected to ensure that data is well documented. The NRDS system currently has GPUs that will allow for quick AI analysis requests. The data can be uploaded in either nonproprietary or proprietary formats but will be converted to a nonproprietary format for reusability.

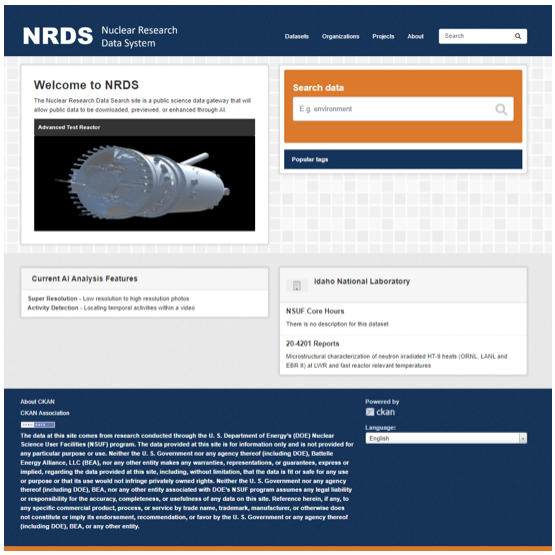

Figure 1: NRDS homepage—https://nrds.inl.gov/.

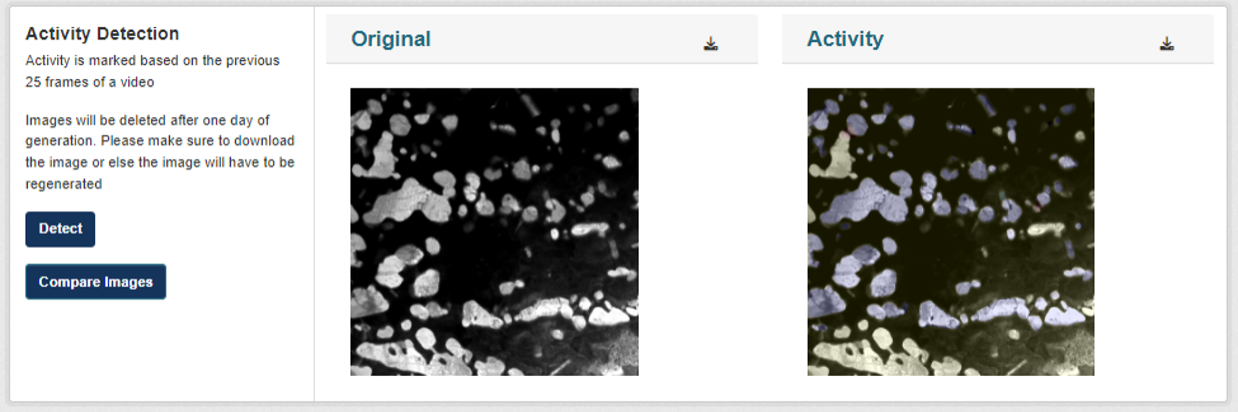

Figure 2: NRDS AI analysis feature that automatically segments feature in datasets.

2.5. Expanded the visualization support system

In FY-23, nine additional nodes were added to the HPC systems for visualization support. These nodes provide access to GPUs designed for visualization tasks as well as 10× as much memory as would typically be available on a standard Sawtooth compute node. These nodes support the increasing demand for visualization intensive applications, including ParaView, VisIt, and Barracuda.

2.6. Significantly expanded storage capabilities

HPC provides a high-speed scratch storage file system for researcher's code output. In FY-22, the current scratch file system was starting to become outdated, run low on storage space, and not be able to keep up with the current compute clusters. In December 2022, the INL HPC team expanded storage capabilities. The expansion provided up-to-date hardware, more capacity, and more bandwidth. The writable capacity went from 1 to 3 PB, increased the bandwidth from 12 to 91 GB/s, and added just over 1.3 million input/output operations per second.

2.7. Published a container strategy widely adopted for HPC software deployments

A comprehensive methodology for building software containers intended for portability on HPC systems was published by the HPC group and presented at the Practice and Experience in Advanced Research and Computing 2023 meeting. This methodology was adopted as the mechanism for container creation by the Multiphysics Object-Oriented Simulation Environment (MOOSE) group at Battelle Energy Alliance, LLC, and the Alegra software developers at Sandia National Laboratories. This work expedites the deployment of new supercomputers, helps ensure consistent results, and can be used to simplify distribution of INL software.

3. UTILIZATION

The Sawtooth, Lemhi, and Hoodoo systems combined delivered more than 939 million core hours of compute time in FY-23.

The average queue size is an important measure of demand for computational resources. The systems were all fully utilized. Oversubscription is a ratio of the average queue and computational demand relative to total system capacity. In FY-23, the average oversubscription of Sawtooth was 4.06, meaning the average number of requested cores in the queue at any given time during the year was 404,675. The average oversubscription of Lemhi was 27.77 (queue was 559,855 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 ensuring the most critical work runs first. Total utilization has increased by a factor of 10 over the past few years. Figure 3 shows the increase of HPC usage from April 2011 to September 2023.

4. USER INSTITUTIONS

The following pages present a summary of institutions utilizing INL's HPC resources in FY-23. As shown in Figure 4, INL HPC capabilities were utilized by 1,320 researchers during FY-23, with the majority coming from national laboratories (806) using 602.4 million core hours. University researchers and students, as a group, made up the second largest group of users (264) utilizing 245.5 million core hours, while industry partners also accounted for a substantial number of users (250) with 91.1 million core hours.

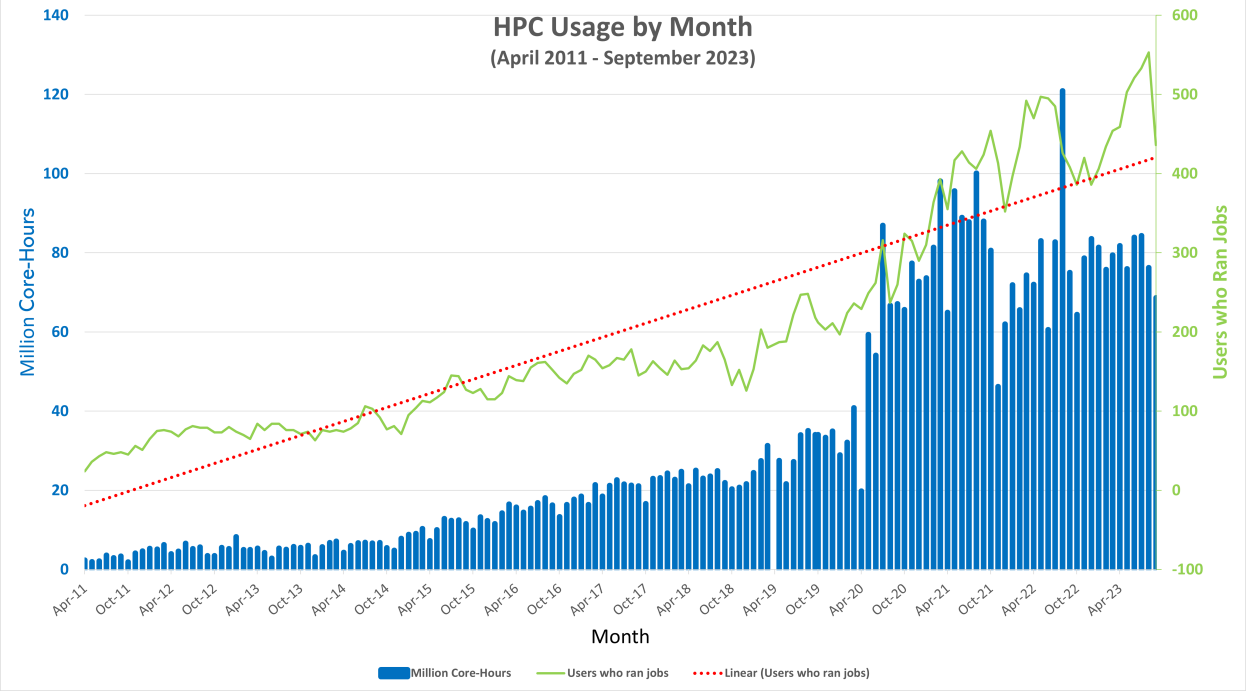

Figure 3: HPC utilization from April 2011 to September 2023.

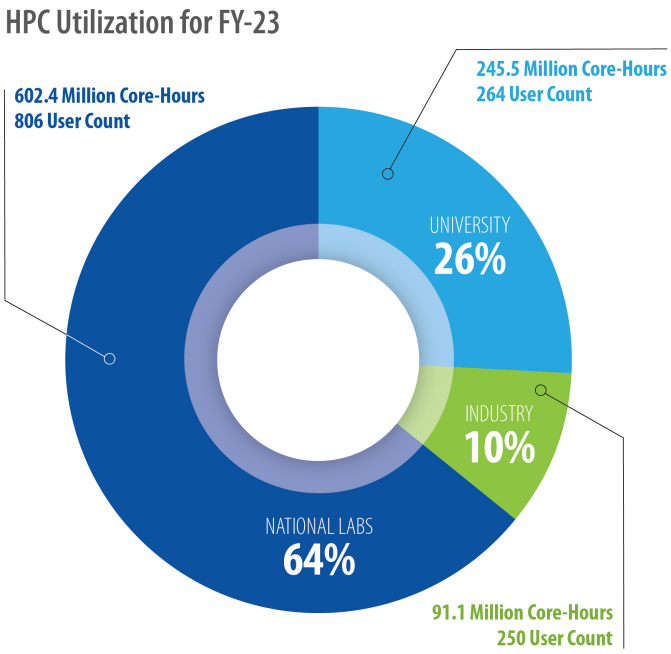

Figure 4: HPC utilization for FY-23. The percentages shown are the distribution of core-hours used by each user group type.

Table 1 lists the top 32 institutions with largest user count utilizing INL HPC systems as of September 30, 2023. The majority of users come from INL (405), followed by Naval Nuclear Laboratory (86). The remaining top 30 organizations include a mix of universities (169), industry partners (87), other national laboratories (66), and the Nuclear Regulatory Commission (12).

Institution	User Count	Million Core-Hours
Idaho National Laboratory	405	481.4
Naval Nuclear Laboratory	86	23.2
Argonne National Laboratory	32	22.2
MPR Associates	27	20.9
Oak Ridge National Laboratory	25	66.5
Westinghouse Electric Company	22	16.8
North Carolina State University	22	97.6
University of Tennessee Knoxville	16	11.0
Texas A&M University	14	12.2
Georgia Institute of Technology	14	2.6
Pennsylvania State University	13	2.6
Nuclear Regulatory Commission	12	19.0
University of Wisconsin-Madison	12	6.2
Idaho State University	10	5.2
Oregon State University	10	9.6
Massachusetts Institute of Technology	10	15.1
TerraPower	9	3.3
Los Alamos National Laboratory	9	6.0
University of Idaho	8	17.6
Rolls-Royce	8	0.0
University of Michigan	7	1.8
University of Illinois Urbana-Champaign	6	2.1
Boise State University	6	7.6
BWX Technologies, Inc	6	3.4
Radiant Industries Incorporated	5	1.8
FPoliSolutions LLC	5	0.0
Analytical Mechanics Associates	5	2.3
University of Florida	5	18.4
Purdue University	4	1.0
The Ohio State University	4	0.0
University of Mississippi	4	11.3
Virginia Commonwealth University	4	9.8

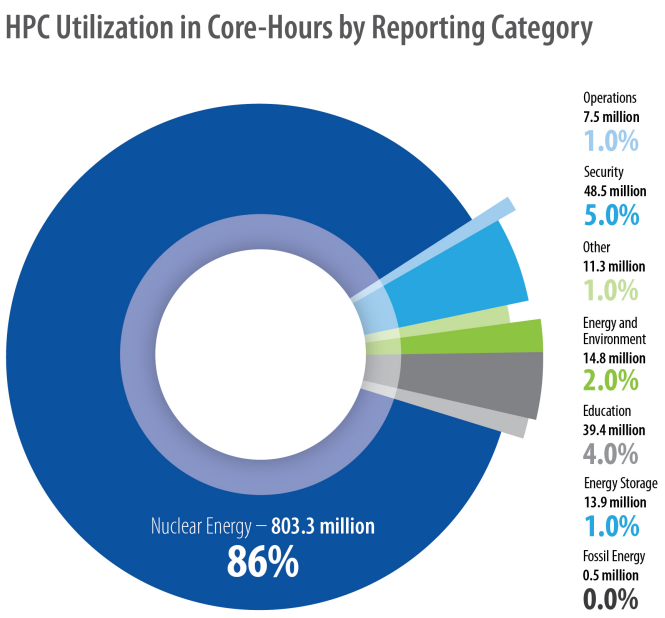

Figure 5: FY-23 HPC utilization in million core hours by reporting category.

Figure 5 shows compute utilization in million core hours for all project categories and systems from October 1, 2022, through September 30, 2023 for a total of 939 million core hours. The majority of utilization (86.4%) was from nuclear-energy-related projects.

The following appendices highlight a subset of projects completed in FY-23 by researchers using INL's HPC resources, grouped in specified project reporting categories for the research. All reports are provided by the users.

Publications that used INL HPC resources are required to include the following attribution to NSUF: "This research made use of Idaho National Laboratory's High Performance Computing systems located at the Collaborative Computing Center and 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 Education

Table of Contents

A.1 INL AI ML Summer 2023 Symposium (S23S)

Report Participants

Walker, Cody M[1]
1 Idaho National Laboratory

Scientific Achievement

This symposium was a follow-up from the courses conducted during 2022 where participants had the opportunity to understand and apply concepts related to artificial intelligence (AI) and machine learning (ML). Over the course of seven 1.5 hour sessions, we explored a variety of current topics within the AI/ML community. This exploration focused on applications but also investigated the theory behind these topics and provided a framework for demonstrating the concepts.

Significance

The goal of S23S was to impart knowledge and raise awareness of AI/ML possibilities for technical applications at Idaho National Laboratory (INL).

Key Publications

Symposium presentation to INL employees and students.

Sponsor/Program

INL

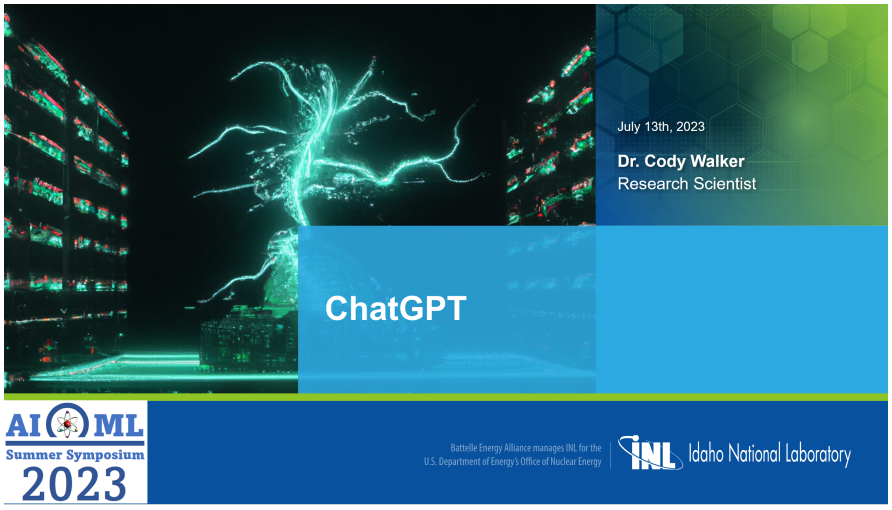

Figure 1: ChatGPT was one of several cutting-edge topics covered during the symposium.

Appendix B Nuclear Energy

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B.1 Release of a High-Temperature Engineering Test Reactor Steady-State Multiphysics Model to the Virtual Test Bed

Report Participants

Swanson, Kylee R[1], Guidicelli, Guillaume [1]
1 Idaho National Laboratory

Scientific Achievement

The release of a High Temperature Engineering Test Reactor (HTTR) steady-state multiphysics model to the Virtual Test Bed utilized Multiphysics Object-Oriented Simulation Environment (MOOSE), BISON, Griffin, and RELAP7. Our paper is a summary of the model and results generated using previously listed software.

Significance

The HTTR proved to be a viable test reactor model. The model, even with its modeling approximations, accurately simulates the behavior of the measured fission power and the average moderator and fuel temperatures in agreement with the original Japan Atomic Energy Agency model. The multiplication factor of this model was calculated as 1.0123, which is satisfactory as the uncertainties in the graphite composition are very high. The HTTR is a great addition to the collection of advanced test reactors available on the Virtual Test Bed.

Key Publications

V. M. LABOUR, M. A. E. BERG LINDELL, J. OR- TENSI, G. STRYDOM, and P. BALESTRA, FY22 Status Report on the ART-GCR CMVB and CNWG International Collaborations, Tech. rep., Idaho National Laboratory (2022).

V. LABOUR, J. ORTENSI, N. MARTIN, P. BALESTRA, D. GASTON, Y. MIAO, and G. STRY- DOM, Improved Multiphysics Model of the High Temperature Engineering Test Reactor for the Simulation of Loss-of-Forced-Cooling Experiments, Annals of Nuclear Energy, 189, 109838 (2023).

V. LABOURE, J. ORTENSI, Y. WANG, S. SCHUNERT, F. GLEICHER, M. DEHART, and R. MARTINEAU, Multiphysics Steady-State Simulation of the High Tem- perature Test Reactor with MAMMOTH, BISON and RELAP-7, Tech. rep., Idaho National Laboratory (2019).

Sponsor/Program

Idaho National Laboratory (INL)

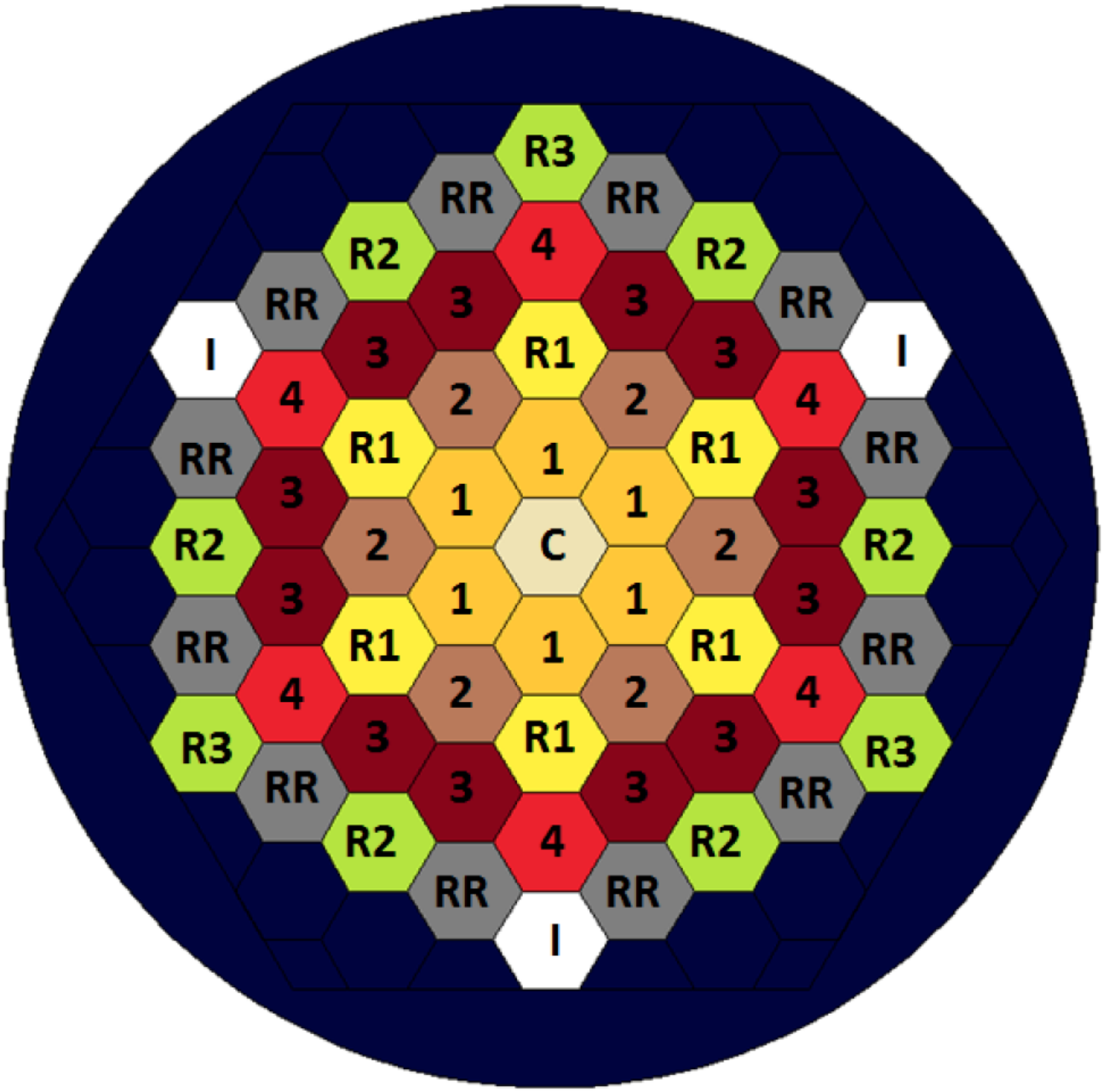


Figure 1: HTTR core layout with fuel (Columns 1-4), control rods (C, R1, R2, R3), replaceable reflectors (RR), and instrumentation (I).

B.2 HPC User Highlights—Department of Energy Packaging Demonstration (Road-Ready Demonstration)

Report Participants

Imholte, Daniel D[1]
1 Idaho National Laboratory

Scientific Achievement

The Department of Energy (DOE) Packaging Demonstration (a.k.a Road-Ready Demonstration) is a collaborative project between INL and Idaho Cleanup Project for packaging DOE-managed spent nuclear fuel (SNF) into road-ready dry storage. All DOE-managed SNF is currently in dry storage and is not suitable for transportation to an interim storage or disposal facility. It is important for INL and Idaho Cleanup Project to pursue road-ready dry storage for all of its SNF in a good faith attempt to meeting the 1995 Idaho Settlement Agreement.

The high-performance computing (HPC) was used in Calendar Year 2023 to perform drop testing simulations using Abaqus CAE. These drop tests were performed to determine the significance of proposed design changes to the DOE Standard Canister (DOESC), which is the primary containment for DOE-managed SNF. The DOESC was designed in 1998 and has been extensively modeled and tested under accident drop conditions. The drop testing simulations were also performed to compare previous predictions, made using Abaqus CAE 2018 and even earlier.

Significance

After several iterations, results consistent with 2018 simulations were observed.

Furthermore, drop tests indicated that proposed design changes to assist with SNF loading and DOESC closure should be investigated further. The design changes did not cause the originally predicted unacceptable increase in the plastic strains.

Key Publications

N/A

Sponsor/Program

INL

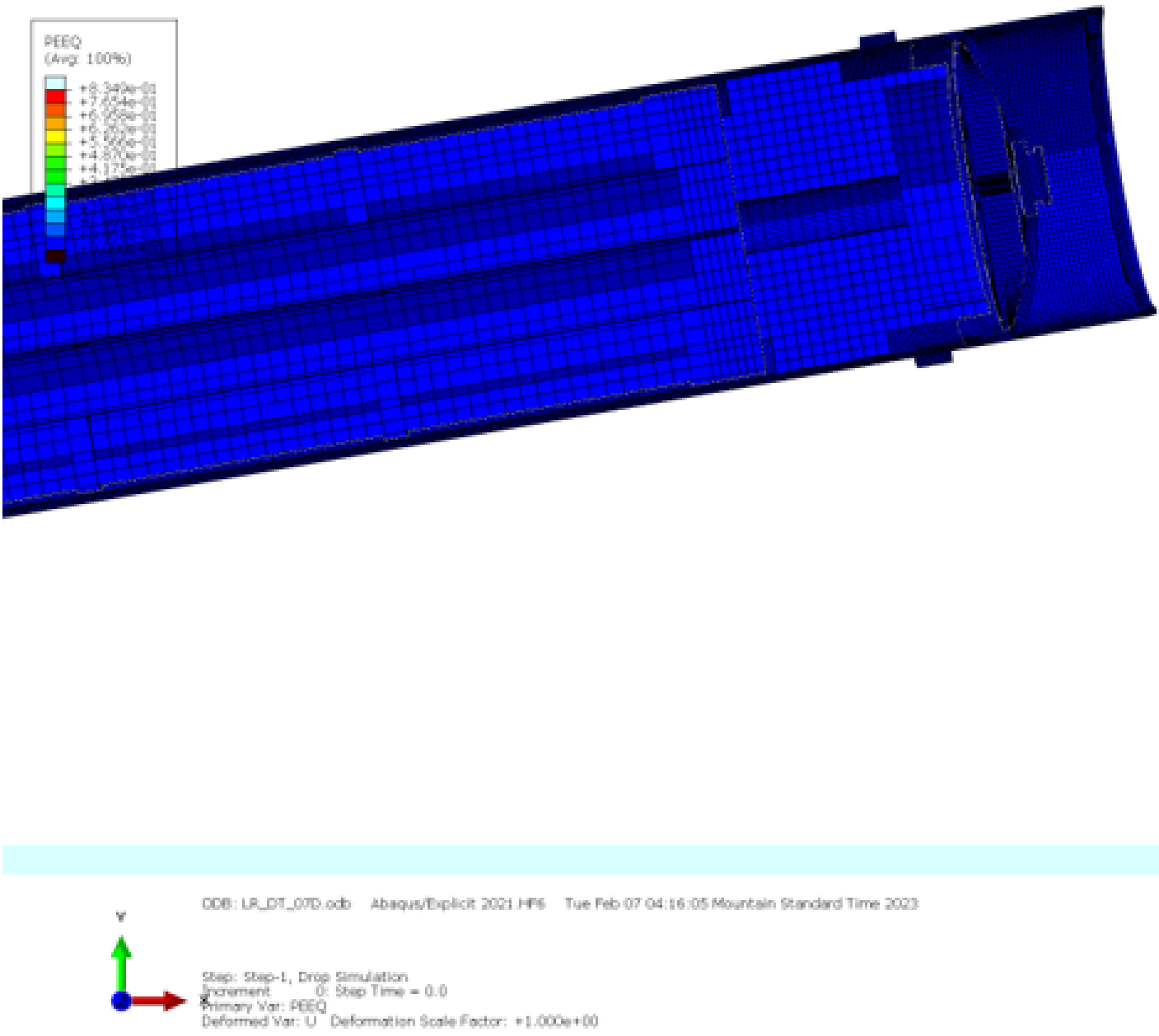


Figure 1: DOESC scoping drop simulation with lifting ring.

B.3 Density Functional Theory Investigation into the Optical Absorption Spectra of Radiation-Induced Transients in Iodine-Containing Molten Chloride Salts

Report Participants

Conrad, Jacy K[1], Horne, Gregory P[1]
1 Idaho National Laboratory

Scientific Achievement

Molten-salt reactors (MSRs) are thought to be a key component of the nuclear energy future because they are safe, cost-effective, and provide sustainable commercial electricity. However, very little is known of the radiation-induced chemistry in these systems as compared to the decades of knowledge for analogous water-cooled reactor technologies. Understanding the role of iodine, a high-yield fission product with potentially harmful biological effects, in MSRs is essential for deploying this technology. Therefore, this work used a combination of experimental and computational calculations to identify the radiation-induced transients using their optical absorbance spectra in systems of molten lithium chloride and potassium chloride (LiCl-KCl) eutectic salt with small amounts of I ions (d" 10 wt%). Geometry optimizations and frequency calculations were performed using density functional theory (DFT) methods for the potential transient halide compounds: Cl2", ICl", and I2" radical anions. Gaussian 16 software was used to run calculations for each species in the gas phase at the B3LYP/6-311++G(d,p) level of theory for the chlorine atom, and the Def2TZVP effective core potential basis set for the iodine atom. All optimized geometries were found to be minima on the potential energy surface using harmonic vibrational frequency analysis at the same level of theory. The minimum energy structures were analyzed using DFT to predict electronic absorption spectra using the same level of theory.

Significance

The DFT simulated optical absorbances for the transient halide radical cations in the gas phase agreed well with the experimental values determined in literature, thus allowing for the identification of an unknown product in this work: the ICl", radical. The transient products in these molten-salt systems have lifetimes on the order of tens of microseconds and therefore are not stable or easy to isolate experimentally. Using computational methods to identify these products was invaluable to the project. Identification of the transients in molten-salt systems under irradiation provides insights into the ultimate products that may be formed. In this case, the ICl" radical will likely react via disproportionation to yield ICl2, which provides a potential pathway for forming volatile interhalogen species, such as ICl. This information is key to developing models of molten-salt behavior under its extreme operating conditions at high temperatures and under irradiation.

Key Publications

Conrad, J.K., Iwamatsu, K., Woods, M.E., Gakhar, R., Layne, B., Cook, A.R., Horne, G.P. (2023) Impact of Iodide on the Speciation of Radiolytic Transients in Molten LiCl-KCl Eutectic Salt Mixtures. Physical Chemistry Chemical Physics, 25, 16009-16017.

Sponsor/Program

DOE Office of Science Basic Energy Sciences

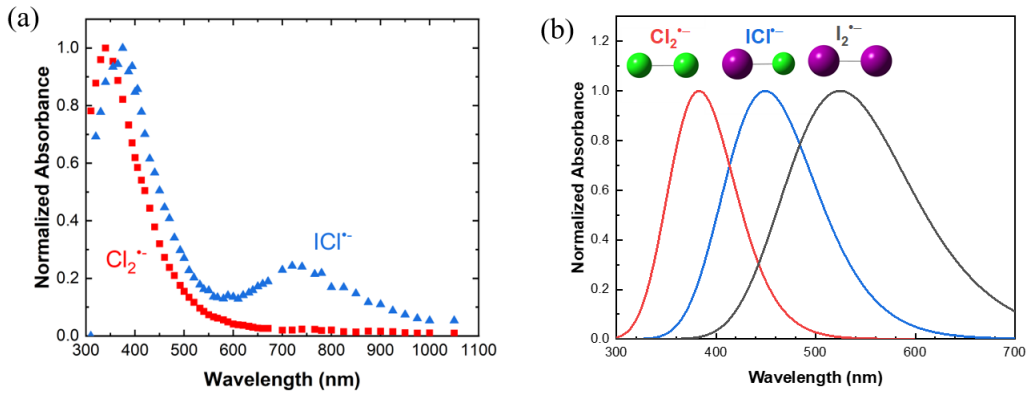


Figure 1: The optical absorption spectrum of the transient Cl2", and ICl", radical anions determined: (a) experimentally using picosecond electron pulsed radiolysis and (b) computationally via gas-phase DFT, as compared to I2", the other potential halide radical anion.

B.4 Development and Validation of Smoothed Particle Hydrodynamics-Based Oxide Reduction Model for Uranium Oxides

Report Participants

Kim, Jin-Woo [1], Yoo, Tae-Sic [2], Yoon, SuJong [2], Kim, Eung Soo [1]
1 Seoul National University
2 Idaho National Laboratory

Scientific Achievement

This work aimed to develop and validate a novel model based on smoothed particle hydrodynamics (SPH) to simulate the process of oxide reduction in used oxide nuclear fuel using molten LiCl. The model utilizes the open-source SPH code, SOPHIA, which was developed at Seoul National University. This development expands the existing one dimensional (1D) kinetic model into a multidimensional (2D/3D) multiphysics model, allowing for more realistic modeling and simulation of the oxide reduction process. It solves various associated multiphysics phenomena, such as chemical reactions, molecular diffusion and convection, fluid dynamics, and heat transfer. The GPU-based computation of the SOPHIA SPH code enables high-fidelity computational simulations, providing effective computing capabilities. The SPH simulation of the oxide reduction process was performed utilizing the GPUs of INL HPC clusters.

Significance

In this work, an SPH-based model of the oxide reduction process has been developed, and a numerical study has been conducted to investigate the effects of various numerical parameters on the SPH model. Additionally, the study examined the impact of design parameters, including basket thickness, oxide pellet size and shape, local bed compaction, physical property uncertainty, and molten-salt flow boundary conditions. Furthermore, a correlation was developed to estimate the oxide reduction time in a pelletized fuel by applying a superposition method to single pellet models with different sizes. This correlation proves valuable in reducing the intensive computing load required for simulating and analyzing the scaled-up process. The development of the SPH-based model provides comprehensive insights into the reduction process. It not only facilitates a simulation-based design of the oxide reduction process facility but also allows for process optimization.

Key Publications

Jin-Woo Kim, Tae-Sic Yoo, Eung Soo Kim, Su-Jong Yoon, Smoothed particle hydrodynamics modeling and analysis of oxide reduction process for uranium oxides, Chemical Engineering Science, Volume 261, 2022, 117974, ISSN 0009-2509, https://doi.org/10.1016/j.ces.2022.117974.

Jin-Woo Kim, Su-Jong Yoon, Tae-Sic Yoo, Eung Soo Kim, Modelling and analysis of salt-convection effect on oxide reduction process for uranium oxides using smoothed particle hydrodynamics, International Journal of Heat and Mass Transfer, Volume 206, 2023, 123965, ISSN 0017-9310, https://doi.org/10.1016/j.ijheatmasstransfer.2023.123965.

Sponsor/Program

INL

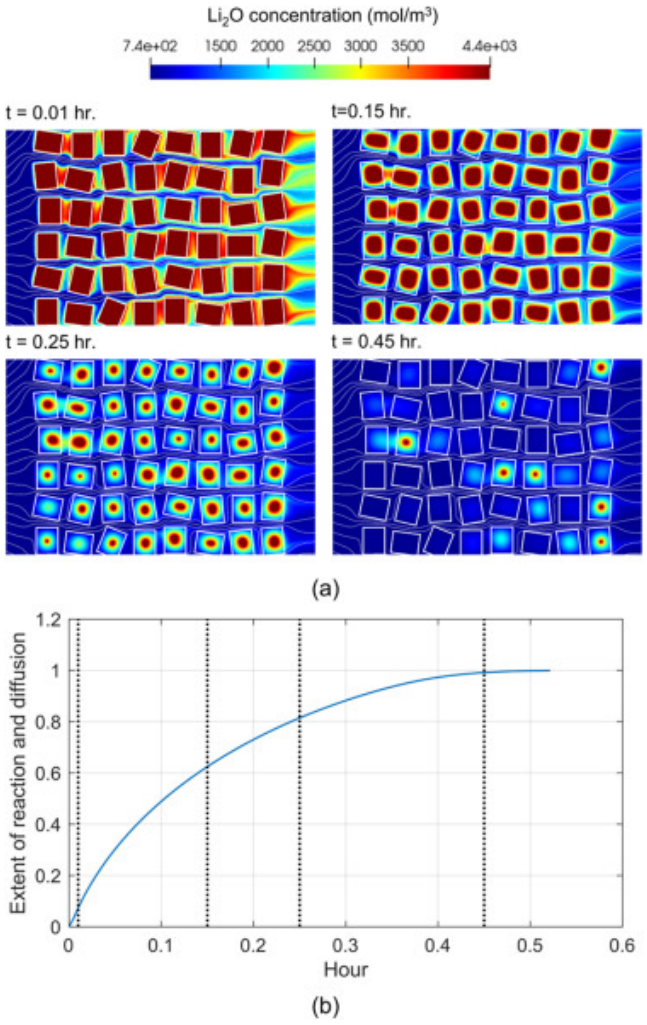


Figure 1: Oxide reduction process in the intermediate Peclet number (Pe=56, W=24mm): (a) concentration field of Li2O at several time instants and (b) extent of reaction and diffusion.

B.5 Development of Detector Response and Material Reaction Rates for Reactor Metrology and Nuclear Forensics

Report Participants

Holschuh Thomas, Vernon I[1]
1 Idaho National Laboratory

Scientific Achievement

For these projects, Monte Carlo N-Particle (MCNP) is used to perform high-fidelity evaluations of neutron energy spectra from various nuclear reactors, including the Transient Reactor Test (TREAT) Facility and the Advanced Test Reactor (ATR). The spectra are used to predict reaction and dose rates obtained from experimental materials irradiated in each reactor, and the predictions feed into shipping paperwork for INL and other national laboratories. Additionally, MCNP is used to predict detector response for DOE nuclear forensics by simulating gamma-ray energies from fission products to obtain a predictive model for various fissile materials.

Significance

The key outcomes of this work have been several programs and graphical user interfaces used by the various projects to obtain rapid predictions for activation material reaction rates (for reactors) and quantitative detector response gamma-ray spectra (for nuclear forensics). For forensics work, this benefits the sponsor by providing real-time predictions for training scenarios that can be changed for various parameters of interest.

Key Publications

"Impact of Flux Wire Selection on Neutron Spectrum Adjustment," In Progress "Modeling the Performance of High-Purity Germanium Detectors for Quantitative Gamma-Ray Spectrometry," In Progress

Sponsor/Program

INL

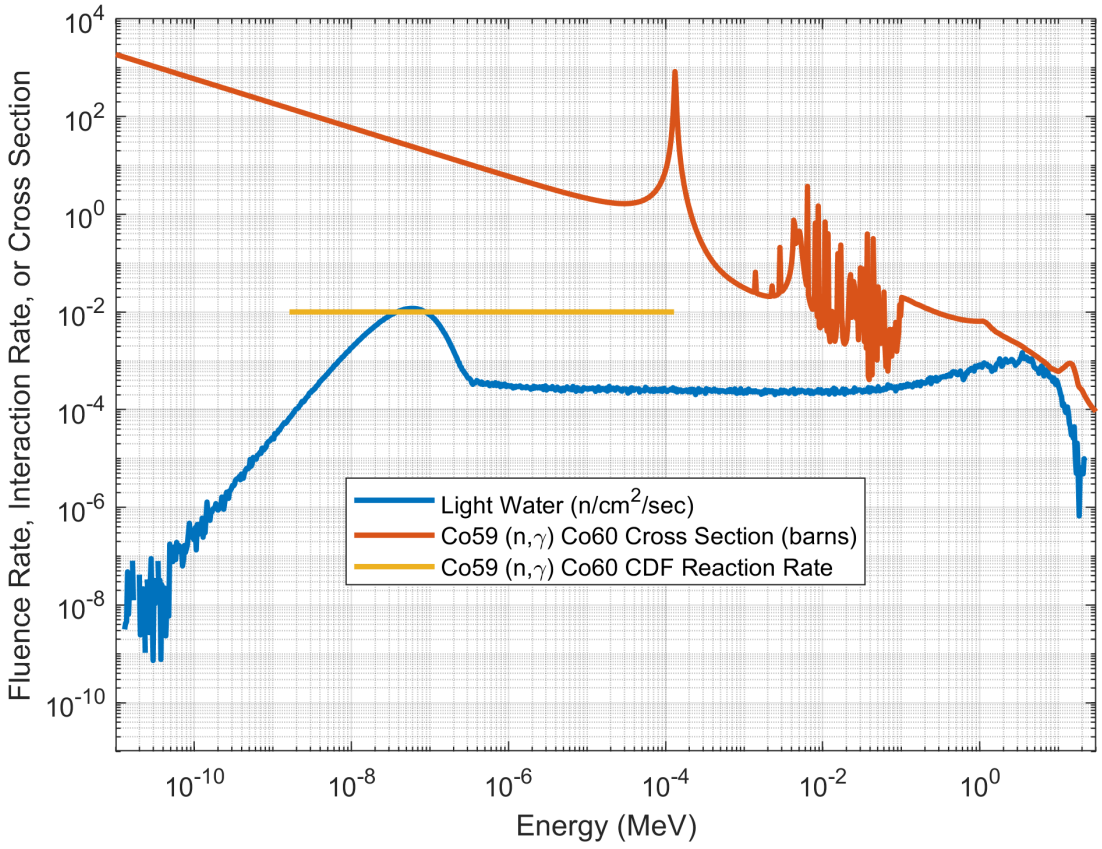


Figure 1: Co-59 thermal neutron absorption in a light-water spectra.

B.6 Computational Fluid Dynamics of Advanced Test Reactor Spent Fuel in New Canister Configurations

Report Participants

Abboud, Alexander W[1]
1 Idaho National Laboratory

Scientific Achievement

This project modeled ATR spent fuel in sealed DOESCs for eventual transport and disposition to assess the safety of the storage with regards to pressure buildup and flammability concerns. The Star-CCM+ software was used on the Sawtooth supercomputer to simulate the temperature and recirculation fields within the base canister configuration and two alternative densely packed configurations over a course of 200 years. The Cantera Python code was then used to model the radiolysis chemistry in the canisters based on the results of the temperature field to model potential buildup of pressure and hydrogen in the canister.

Significance

Road-ready and final disposition packaging configurations for ATR fuel currently specifies storage within helium-backfilled, sealed DOESCs. The aluminum cladding of the ATR fuel contains an oxyhydroxide layer of boehmite/bayerite that generates hydrogen when subjected to irradiation. Understanding the effect of this hydrogen buildup over time is important for long term storage considerations. Previous modeling efforts have built a coupled computational fluid dynamics (CFD) chemical model to simulate the temperature gas phase concentrations within the sealed DOESCs. These models have coupled the temperature conditions to both the gas phase radiolysis chemistry and the surface chemistry associated with the oxyhydroxide layer.

Continued experimental work has identified trends for aluminum surrogate samples with oxyhydroxide layers for tests done at higher dose rates. At low initial doses, a fast generation rate of hydrogen occurs that starts to roll over to a lower generation rate as the total dose applied in increased. A previous study created a small-scale chemical model that was built to replicate a mini-canister surrogate system at Savannah River National Laboratory as well as for the smaller capsule tests performed at INL. The previous iteration of the model utilized a step function for its G-values for the hydrogen generation over a 200 year period. This model updates the surface chemistry to account for theorized surface chemistry reactions allowing for oxygen to remain bounded to the oxyhydroxide layer. As additional experiments continue, the kinetic fits may be adjusted to adapt to new data.

Three canister configurations are modeled: the base 18 inch, 15 foot DOESC with 30 ATR fuel elements; an 18 inch, 10 foot DOESC with 32 ATR fuel elements; and a 24 inch, 10 foot DOESC with 40 ATR fuel elements. In previous reports, the primary sensitivities of the canister conditions were identified as the decay heat and dried conditions of the fuel. Only these parameters are studied. For the nominal case with dried fuel, the hydrogen generation is only about 2%, so it is even less than the flammability limit if it were exposed to oxygen. For the densely packed 18 inch case, the total hydrogen concentration is only around 4% with the nominal decay heat. For the densely packed 24 inch case, the total hydrogen concentration is only 2.5%, roughly 20% higher than the original packing design, and still under flammability conditions if exposed to oxygen.

Key Publications

Eidelpes, E., Jarrell, J. J., Lister, T. E., Horne, G. P., Parker-Quaife, E. H., Conrad, J. K., ... & Sindelar, R. L. (2023). Technical basis for extended dry storage of aluminum-clad spent nuclear fuel. Journal of Nuclear Materials, 577, 154299.

Abboud, A. W. (2022). Sensitivity study of coupled chemical-CFD simulations for analyzing aluminum-clad spent nuclear fuel storage in sealed canisters. Nuclear Engineering and Design, 390, 111691.

Abboud, A. W. (2023). Coupled chemical CFD modeling of unsealed dry storage of advanced test reactor spent fuel. Annals of Nuclear Energy, 183, 109646.

Abboud, A.W. (2023). Modeling DOE Standard Canister Configurations with Updated Surface Chemistry. INL-RPT-23-73230.

Sponsor/Program

DOE Office of Environmental Management

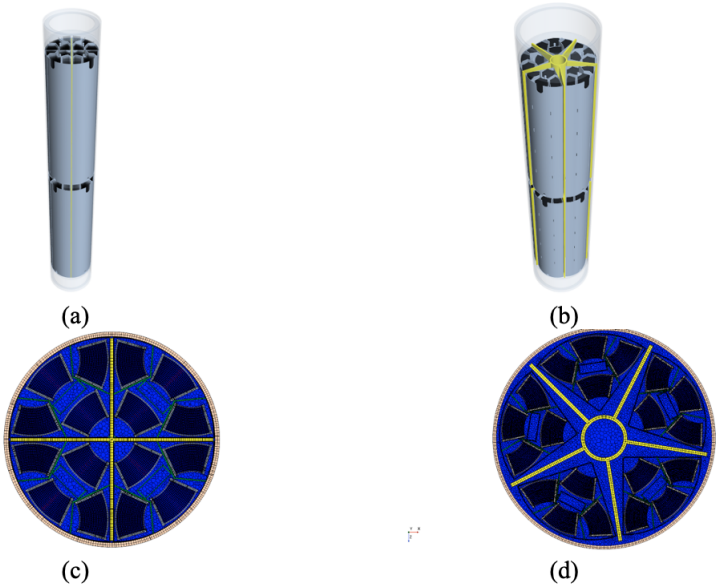


Figure 1: The geometry layout for (a) 18 inch diameter and (b) 24 inch diameter canisters, and the meshed geometry for (c) 18 inch diameter and (d) 24 inch diameter canisters.

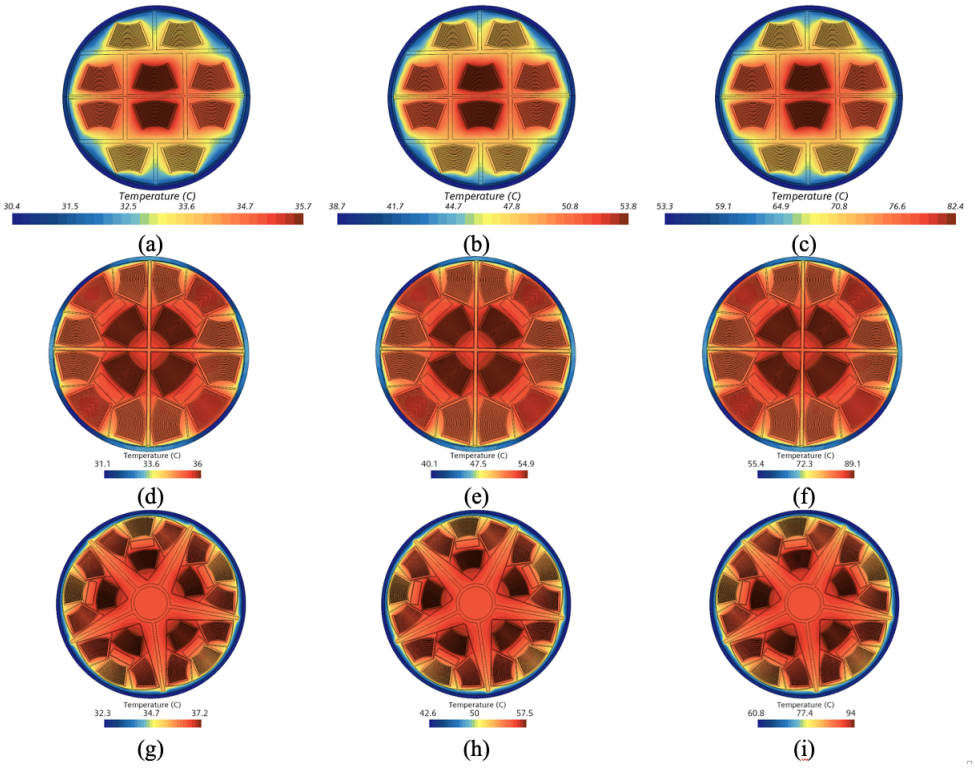


Figure 2: The steady-state temperature for (a) 6 watt, (b) 18 watt, and (c) 42 watt fuel elements in an 18 inch sealed base canister configuration; (d) 6 watt, (e) 18 watt, and (f) 42 watt fuel elements in an 18 inch sealed densely packed canister configuration; and (g) 6 watt, (h) 18 watt, and (i) 42 watt fuel elements in a 24 inch sealed densely packed canister configuration.

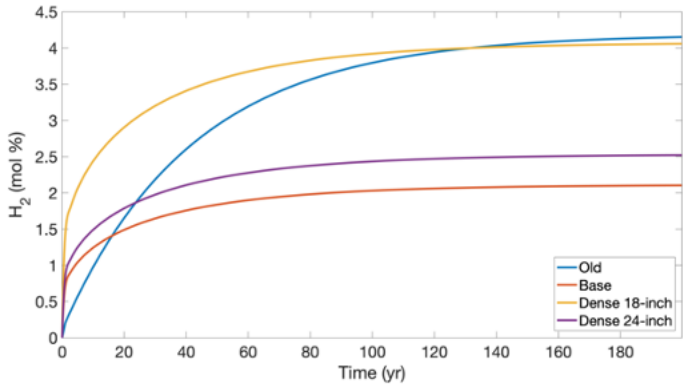


Figure 3: The hydrogen gas generation of the three packing configurations here against the old model data.

B.7 Improving the Modeling of Laminarization in High-Temperature Gas-Cooled Reactors Using RELAP5-3D

Report Participants

Steele, Robert W[1], Schultz, Richard R[1], Mesina, George L[2]
1 Idaho State University
2 Idaho National Laboratory

Scientific Achievement

Using experimental data and a comparative analysis of heat transfer correlations, modifications and correction factors are being developed to improve the calculational performance of RELAP5-3D. These correction factors will then be integrated into a standalone copy of RELAP5-3D and be validated with additional experimental data.

Significance

A data analysis has been performed on experimental data with correction factors developed. Additionally, an input deck has been made for the validation experiment. We are awaiting permission for limited code access, which will eventually lead to additional correction factors being offered for RELAP5.

Key Publications

Several future conferences and papers are being evaluated currently.

Sponsor/Program

INL RELAP5

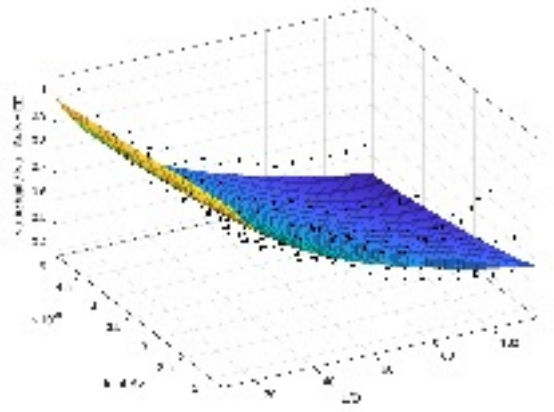


Figure 1: Using the experimental Nu vs. predicted Nu, vs. inlet Kv (acceleration constant) and L/D (axial position) in the development of the acceleration correction factor, which will improve the calculational precision of RELAP5-3D when acceleration induction deteriorated heat transfer is present.

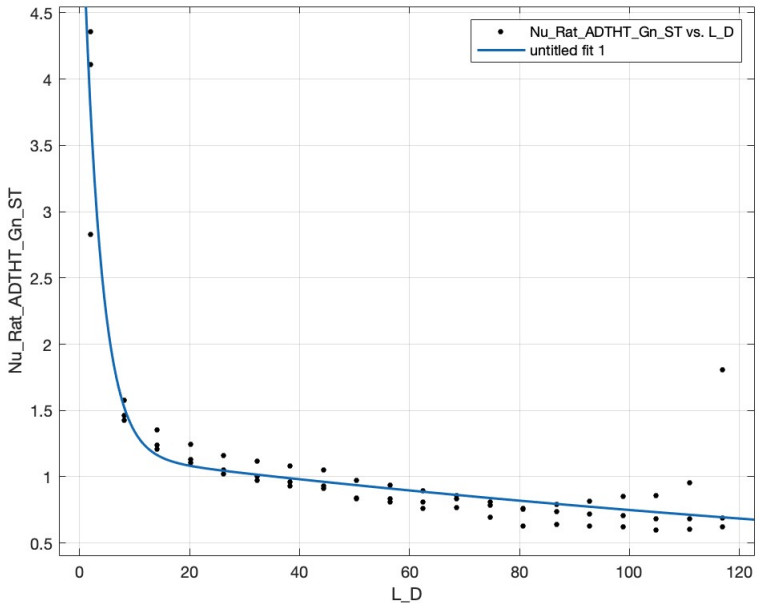


Figure 2: The ratio of experimental Nu vs. predicted Nu vs. axial position for acceleration-induced deteriorated heat transfer.

B.8 Machine Intelligence for Review and Analysis of Condition Logs and Entries

Report Participants

Mapes, Norman J[1]
1 Idaho National Laboratory

Scientific Achievement

Machine Intelligence for Review and Analysis of Condition Logs and Entries (MIRACLE), a 2022 R&D 100 winning technology, developed natural language processing and machine learning (ML) tools using data from 39 reactors operating in the United States to automate corrective action program related activities.

Significance

In a nuclear power plant, a committee of 5–10 people meets several times per week to sort through condition reports, as part of the plant corrective action program. Automating this process can significantly reduce the time, and consequently the cost, needed for screening. MIRACLE implements scalable ML models to expedite the industrywide adoption of collaborative models that perform better than utility-specific models. It can also synchronize keyword or trend code labeling across the industry and help better trend performance so as to operate more safely.

Key Publications

Publications to be submitted.

Sponsor/Program

DOE Light Water Reactor Sustainability

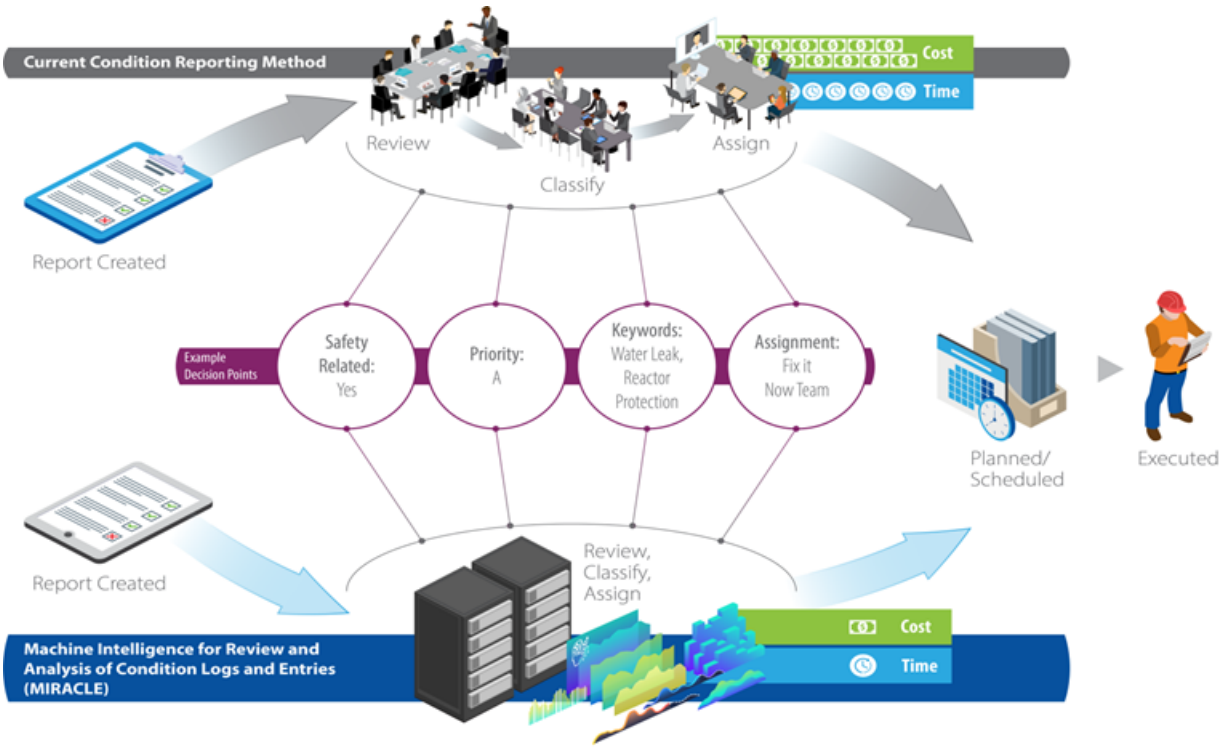


Figure 1: MIRACLE is used to replace or assist the current expensive, time-consuming condition report screening process.

B.9 Sensitivity Analysis, Reduced-Order Modeling, and Optimization of a Gas-Cooled Pebble-Bed Reactor

Report Participants

Prince, Zachary M[1], Balestra, Paolo [1], Ortensi, Javier [1], Schunert, Sebastian [1], Calvin, Olin W[1], Hanophy, Joshua T[1], Mo, Kun [2]
1 Idaho National Laboratory
2 Argonne National Laboratory

Scientific Achievement

This work presents and applies a workflow for performing design optimization on gas-cooled pebble-bed reactors (PBRs). Based on previous research, a representative equilibrium core of a PBR and a depressurized loss-of-forced-cooling model are created. These applications are built using MOOSE, specifically utilizing Griffin, Pronghorn, and BISON. After defining design-related parameters and quantities of interest (QoIs) regarding reactor safety and efficiency, this multiphysics model is sampled using the MOOSE stochastic tools module. The result is a comprehensive dataset of configurations, enabling the sensitivity analysis and generation of reduced-order models (ROMs). Subsequently, the dataset and ROMs are employed in an optimization study aimed at maximizing fuel utilization while adhering to safety and operational constraints. The optimization process leads to an improvement of fuel utilization by approximately 10%, compared to engineering-judgment-based nominal conditions.

Significance

Similar to any reactor design, PBRs encompass numerous design parameters that result in a seemingly endless array of possible reactor configurations. Design processes filter these configurations by considering both safety and economic factors. Safety constraints involve adhering to principles that enable certification and prevent system damage. Economic viability entails minimizing development and operational costs while maximizing energy output. Often, safety and economic considerations counteract each other. For instance, higher core temperatures enhance fuel cycle efficiency but also increase the risk of fuel damage and reduce the margin for system failure. Thus, identifying a viable and optimized design from the multitude of potential configurations is a complex task. This typically involves testing various design parameters, determining viable resulting configurations, and ultimately narrowing down to an optimized design. Given that experimental data is often limited and lacks generality in the parameter and output space, modeling and simulation play a crucial role in the design process.

This study emphasizes the development and application of an efficient workflow for design optimization, considering a significant design space and accounting for both safety and economic factors. Any choice of optimization algorithm would inevitably require numerous evaluations of the physics model. Depending on the model's complexity, performing more than a few dozen sequential evaluations could become intractable. Parallel execution of the model could allow for more evaluations, but many optimization algorithms require sequential evaluations, and computing resources for design processes often involve clusters with limited parallel processes. Consequently, there arises a need for generating fast-evaluating surrogates or ROMs of the multiphysics model. This study characterizes various ROM methodologies that accurately predict QoIs for a given design configuration, effectively reducing the burden of evaluating configuration performance for optimization.

ROMs are known to suffer from the so-called curse of dimensionality; when more system parameters are added to the model, exponentially more training data is required to maintain model accuracy. Therefore, performing a sensitivity analysis on the design parameters becomes valuable. A sensitivity analysis quantifies the impact of parameter perturbations on resulting QoIs, providing insights into how specific design considerations influence the system and potentially streamline the design process. It also offers a method to filter high-dimensional design spaces, simplifying ROM generation and improving their accuracy within a fixed dataset. In this work, a global sensitivity analysis is performed using Sobol indices, computed using polynomial chaos expansion.

Key Publications

Prince, Z. et al. In progress. Sensitivity Analysis, Reduced-order Modeling, and Optimization of a Gas-Cooled Pebble Bed Reactor using Equilibrium-Core and DLOFC Performance.

Sponsor/Program

Advanced Reactor Technologies
NEAMS

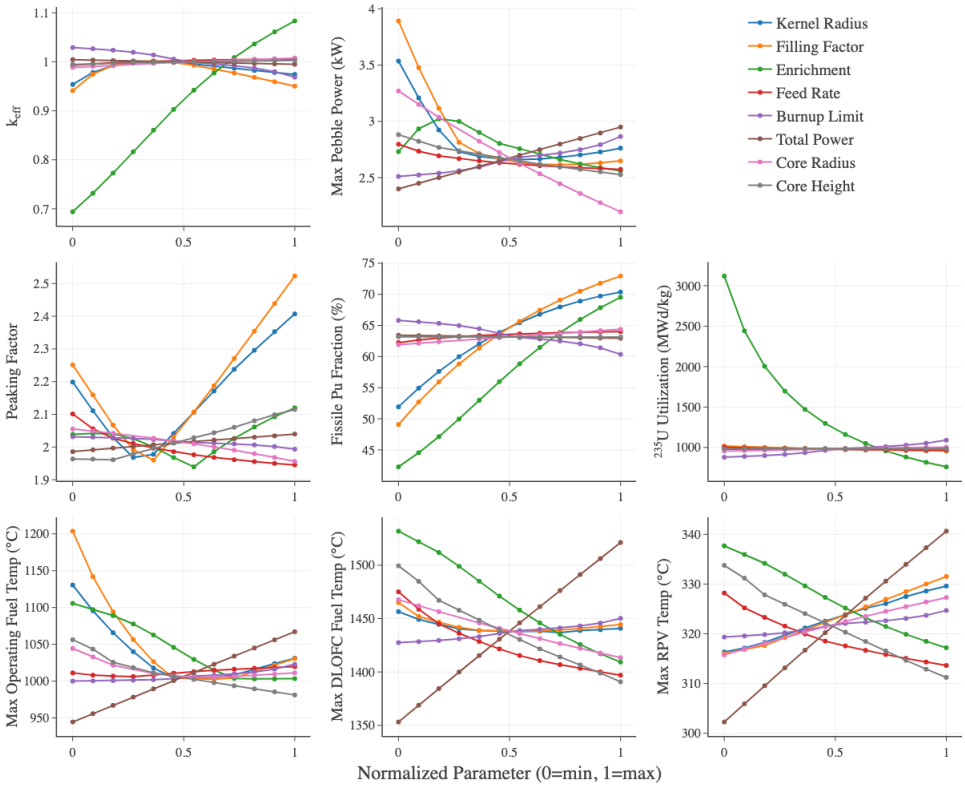


Figure 1: QoI versus design parameters from performing 1D grid sampling.

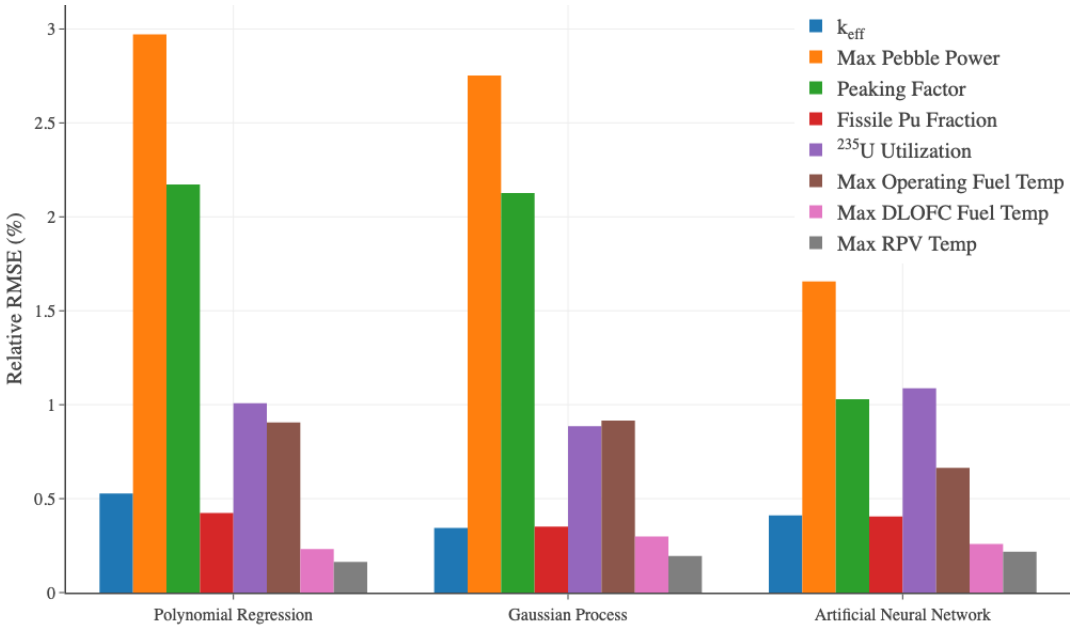


Figure 2: Comparing performance of ROM methodologies for each QoI.

Parameter	Nominal	Full Model	PR	GP	ANN
Kernel Radius	0.2125	0.28348	0.25128	0.2979	0.26386
Filling Factor	9.344	7.2802	7.5797	6.0249	6.933
Enrichment	15.5	16.025	15.774	15.067	14.276
Feed Rate	1.5	1.3136	2.1634	1.046	2.2308
Burnup Limit	147.6	163.98	163.2	158.61	147.74
Total Power	200	185.04	189.81	182.53	190.45
Core Radius	1.2	1.2767	1.2863	1.2963	1.2947
Core Height	8.93	9.6428	9.179	9.5896	9.5479

Quantity	Full Order Evaluation		ROM Evaluation with Relative Error		
k_{eff}	0.99961	0.994835	0.99839 - 0.0515%	0.99742 - 0.247%	0.99941 - 0.705%
Max Pebble Power	2.6742	2.2731	2.2518 - 0.865%	2.1967 + 7.59%	2.0952 + 0.723%
Peaking Factor	2.0145	2.1006	1.972 - 2.63%	2.0559 - 1.73%	1.935 + 0.132%
Fissile Pu Fraction	63.158	63.044	62.053 + 0.216%	59.14 + 1.36%	60.893 - 0.0201%
^{235}U Utilization	**984.18**	**1070**	**1063.1 - 0.183%**	**1087.1 - 1.23%**	**1084.9 - 0.912%**
Max Operating Fuel Temp	1006.2	941.72	989.46 - 0.561%	918.66 + 6.16%	977.56 + 0.741%
Max DLOFC Fuel Temp	1438.4	1341.7	1347.8 - 0.00344%	1358 - 0.675%	1328.3 + 0.298%
Max RPV Temp	321.97	309.31	311.36 - 0.0235%	311.06 - 0.758%	306.99 + 0.148%

Figure 3: Resulting parameters and quantities of interest from optimal configurations.

B.10 Burnup Correction Factors for Two AGR-34 TRISO-Particle Fuel Compacts

Report Participants

Sterbentz, James W[1]
1 Idaho National Laboratory

Scientific Achievement

The goal of this project was to calculate burnup corrections for two tristructural isotropic (TRISO) particle fuel compacts that had been irradiated in ATR. The nuclear fuel burnup is a key metric in the determination of the fuel performance. The burnup can both be calculated using computer simulations on the INL HPC supercomputers and by physical in-laboratory measurements using complicated chemical and isotopic separations of the neodymium isotopes. Comparing the calculated and measured burnups validates the compact burnups along with the simulations and measurements.

The calculated burnup was performed with the INL JMOCUP code software, the Los Alamos National Laboratory (LANL) MCNP transport code, and the Oak Ridge National Laboratory (ORNL) ORIGEN-2 computer codes. This project again used these same computer codes on the INL HPC systems to extend the simulation by calculating burnup correction factors needed specifically for the measured burnups. The burnup corrections factors for seven neodymium isotopes allowed the measured burnup to be adjusted to fall in line with the calculated burnups by accounting for the nuclear radiative capture reactions.

Significance

The calculated burnup corrections factors were calculated using the INL HPC computer systems and software. The correction factors were then transmitted to our colleagues at ORNL. ORNL performed the compact burnup measurements and used the correction factors to adjust their isotopic burnups. The result was very good agreement between the calculated and measured compact burnups.

Key Publications

To be published in an ORNL report: Grant W. Helmrich, John D. Hunn, Fred C. Montgomery, Darren J. Skitt, Tamara J. Keever, Benjamin D. Roach, Kayron T. Rogers, James W. Sterbentz, "Determination of Average Burnup in AGR-34 Compacts 1-4 and 7-4", ORNL/TM-2023/2969.

Sponsor/Program

INL, ORNL

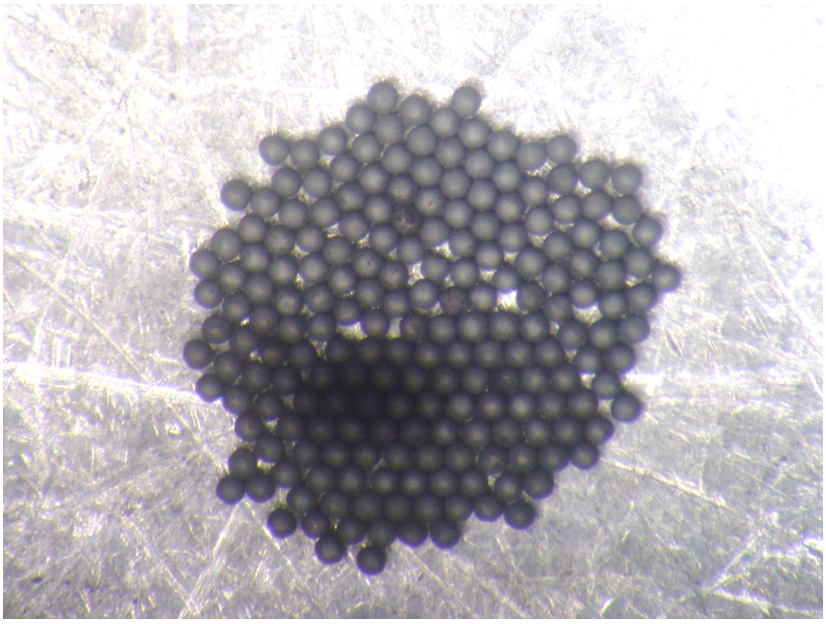


Figure 1: AGR-34 TRISO particles used to measure particle burnup from ATR irradiation.

B.11 Thermal Property Prediction at Thermal Interfaces Using First-Principles Phonon Transport Techniques

Report Participants

Harter, Jackson R[1], Greaney, Alex [2], Chevalier, Cameron [2]
1 Idaho National Laboratory
2 University of California – Riverside

Scientific Achievement

This work investigated the effects of multigroup phonon transport and scattering at internal material interfaces, using first-principles-based methods to derive the continuum material property spectra. A new mathematical model was developed that uses a localized temperature to set transmission and reflection coefficients that dictate the amount of phonons transmitted or reflected off of an interface. New software was developed, which was merged into the Griffin code.

We leveraged HPC to run most of our 3D calculations and some of the 2D work. We used the Griffin code, which can model phonon transport, with the new interface code developed for this project.

Significance

Based on the new interface model, we are able to properly predict the amount of interfacial thermal resistance (also known as Kapitza resistance) at an interface between two dissimilar materials. We are also able to predict temperature distribution, thermal conductivity, heat capacity, heat flux, and the amount of nonequilibrium behavior in each respective material.

We modeled supercell heterostructure of aluminum nitride (AlN) bulk and gallium nitride (GaN) impurities. We showed the presence of various concentrations of GaN impurities would reduce thermal conductivity in the bulk. Additionally, we showed that different physical configurations of GaN impurities have differing effects on thermal conductivity because the varying configurations trap heat in different ways.

Key Publications

Harter, J.R., Chevalier, C., Greaney, P.A. A first principles approach to spectral phonon transport in heterostructures. In Progress.

Conference: Materials Research Society Spring Meeting 2023 — "A first principles approach to spectral phonon transport in heterostructures", 4/12/2023, INL/CON-23-72025

Sponsor/Program

Laboratory Directed Research and Development 21A1050-052FP

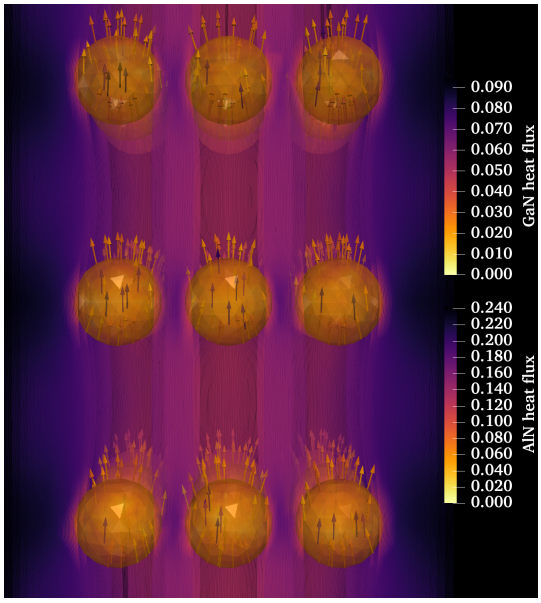


Figure 1: Heat flux streamlines in barricade geometry of GaN defects in AlN bulk, 15 axial layers.

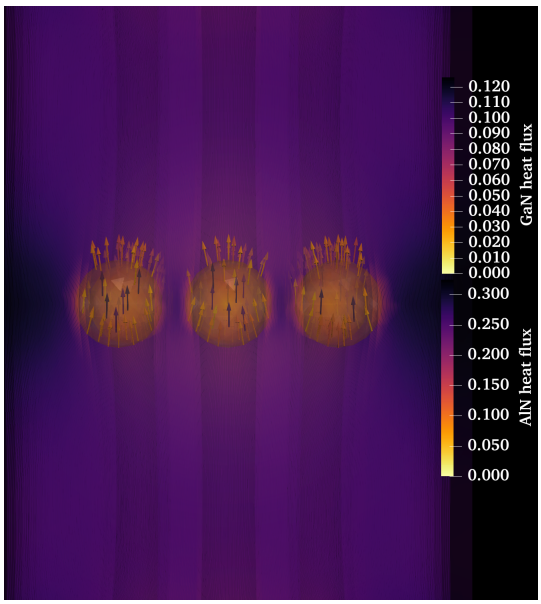


Figure 2: Heat flux streamlines in barricade geometry of GaN defects in AlN bulk, seven axial layers.

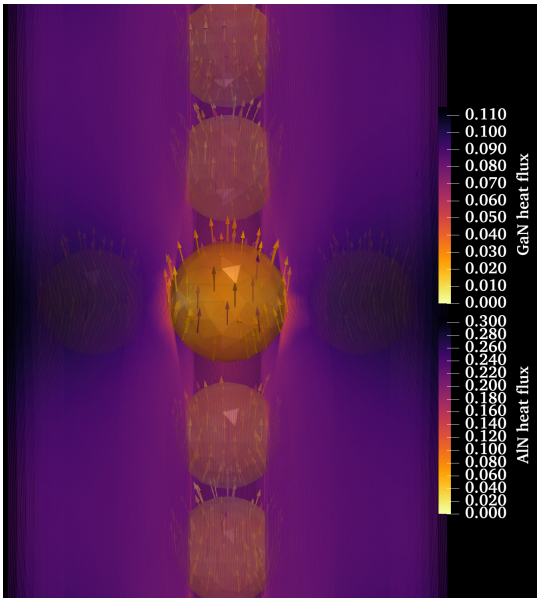


Figure 3: Heat flux streamlines in cruciform geometry of GaN defects in AlN bulk.

B.12 Discovering the Structures of Atomic-Scale Defect Clusters in Thorium Dioxide

Report Participants

Jiang, Chao [1], Hurley, David H[1], Marianetti, Chris A[2], Khafizov, Marat [3]
1 Idaho National Laboratory
2 Columbia University
3 The Ohio State University

Scientific Achievement

When subjected to the irradiation of high-energy particles, point defects and atomic-scale defect clusters will be generated in materials in large amounts. Although these small defects are hidden under transmission electron microscopy, they can have a large influence on material properties. For nuclear fuels, in particular, their thermal conductivities can be significantly degraded due to the scattering of phonons by atomic-scale defects. Using fluorite-structured thorium dioxide (ThO2) as an example, this project demonstrated the combination of DFT calculations and machine learning interatomic potential (MLIP) as a powerful tool that enables an exhaustive exploration of the large configuration spaces of small point defect clusters. Unraveling the ground-state configurations of these defects is an important step toward establishing the structure-property relationship for irradiated materials. By learning directly from large DFT datasets without assuming any fixed functional forms, a MLIP can reproduce DFT potential energy surfaces far more accurately than an empirical potential. This increased level of fidelity is particularly crucial since empirical potential-driven ground-state searches have been known to yield results that do not agree with DFT. Additionally, a MLIP is many orders of magnitude faster than DFT since it does not treat electrons explicitly, which makes ground-state searches computationally efficient.

Significance

The combined DFT+MLIP approach led to several unexpected discoveries, including ground-state polymorphism and ground-state structures that defy physical intuitions. The atomistic configurations of small interstitial and vacancy clusters as revealed in this project were used as inputs for nonequilibrium molecular dynamics simulations to assess their impact on thermal energy transport in ThO2. These results provide the physics basis for predicting the in-reactor performance of ThO2 as an alternative nuclear fuel.

Key Publications

Chao Jiang, Chris A. Marianetti, Marat Khafizov, and David H. Hurley, "Machine learning accelerated exploration of complex defect potential energy surfaces", In Progress.

Sponsor/Program

Laboratory Directed Research and Development 21A1050-078FP
Center for Thermal Energy Transport under Irradiation

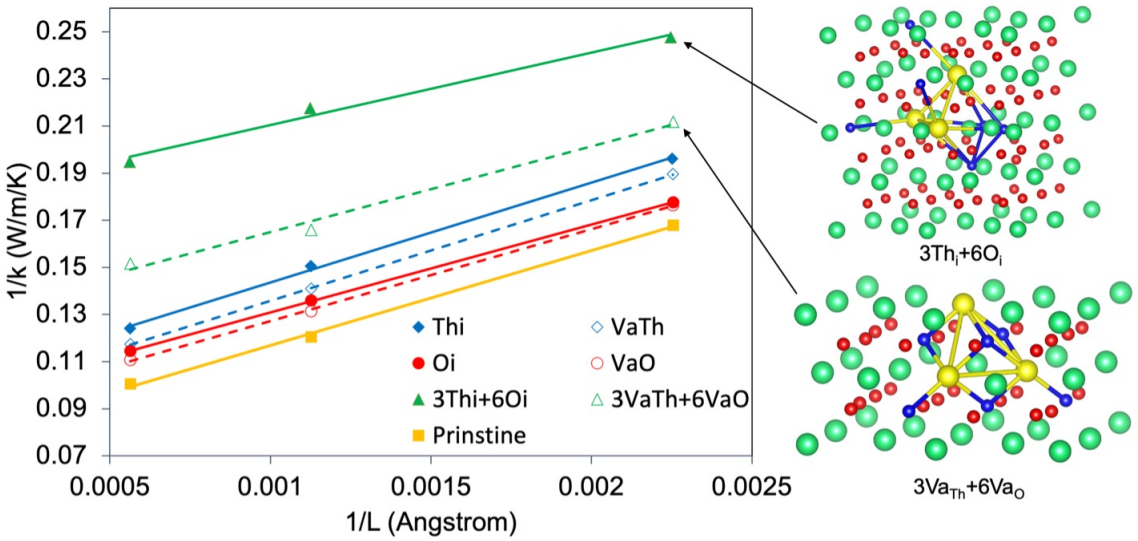


Figure 1: The impact of atomic-scale defects on the thermal conductivity of thorium dioxide.

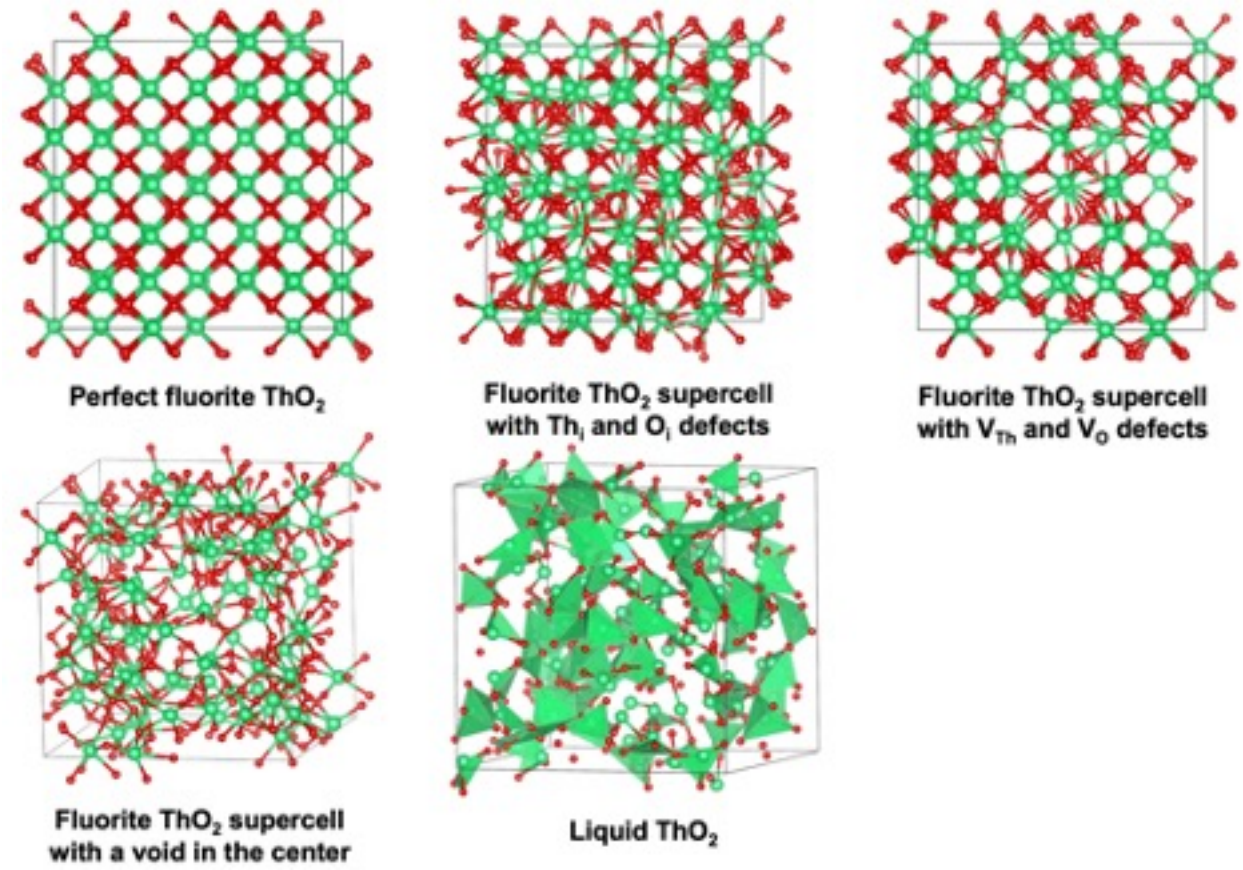


Figure 2: Structures included in the DFT-generated training database for ThO2.

B.13 Synthetic Transportation Fuel from Nuclear Energy

Report Participants

Garrouste, Marisol [1], Wendt, Daniel [1]
1 Idaho National Laboratory

Scientific Achievement

Case study analyses were performed to evaluate nuclear-powered synthetic fuel production in the United States. A Fischer-Tropsch fuel synthesis plant design and a methanol-to-diesel plant design were configured to produce a product slate of diesel fuel, jet fuel, and motor gasoline blend stocks from carbon dioxide and hydrogen feedstocks. The analysis specifies that power from either large reactors or small modular reactors is used to produce hydrogen via high-temperature steam electrolysis and to operate the synfuel production plant. The economic analysis calculated the net present value (NPV) for cases involving steady-state synfuel production for comparison with the NPV for a business-as-usual case in which nuclear power plants (NPPs) continues to sell only electric power to the grid. The calculations were performed with Risk Analysis Virtual ENvironment (RAVEN) and more specifically its economic analysis plug-in, the Holistic Energy Resource Optimization Network, on the INL HPC.

Significance

We show that the NPV of integrated energy systems coupling NPPs and low-carbon synthetic fuel production processes is higher than the business-as-usual case where the NPPs sell all their electricity to the grid.

Key Publications

In Progress: Integrated Production of Fischer-Tropsch and Methanol-to-Diesel Synfuels from Nuclear Power Plants and Small Modular Nuclear Reactors, Marisol Garrouste, and all

Sponsor/Program

INL

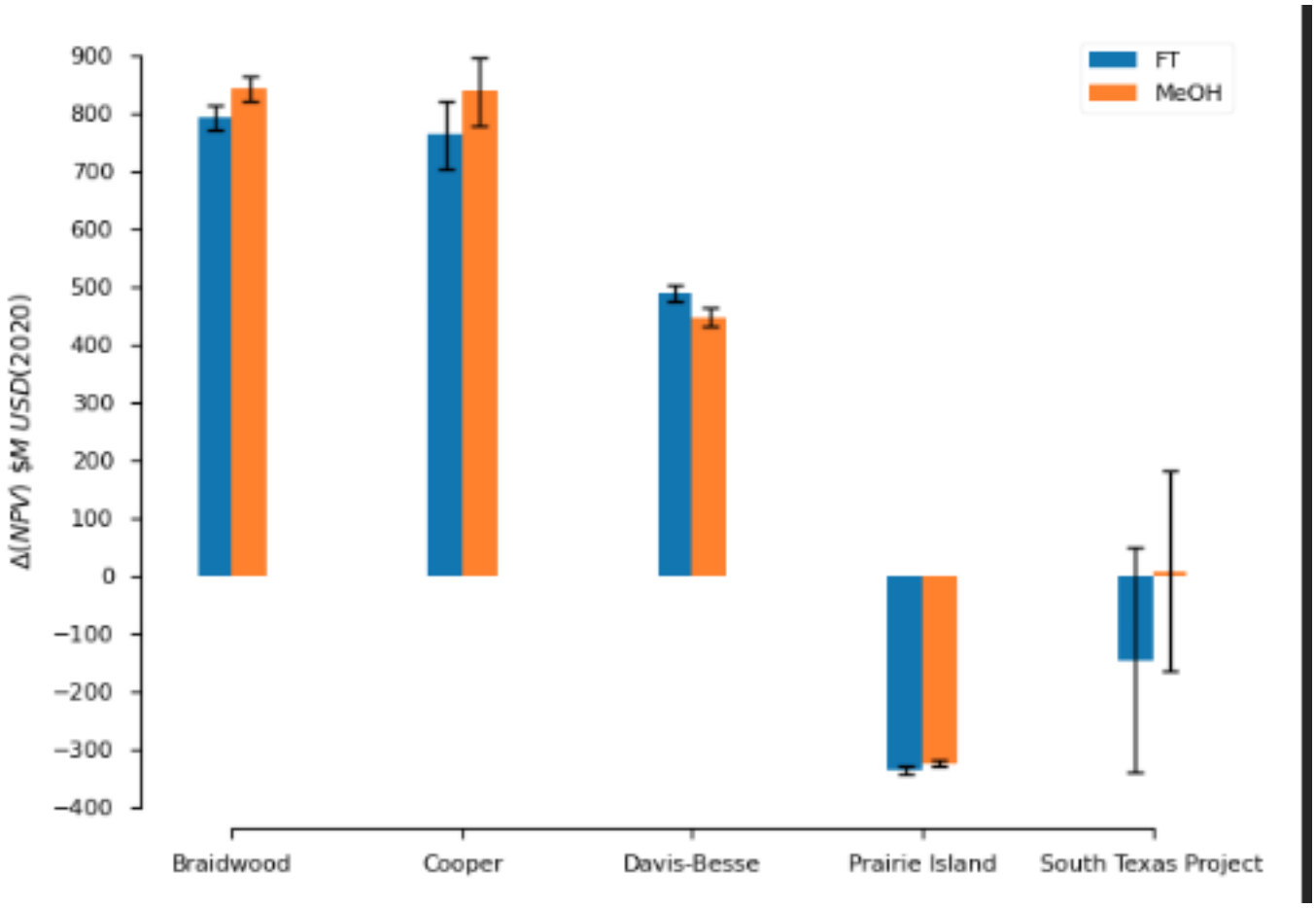


Figure 1: NPV for the synfuel integrated energy systems compared to the business-as-usual case at each NPP location.

B.14 FAST Fuel Performance Modeling

Report Participants

Swearingen, Alexander L[1], Paaren, Kyle M[1], Beausoleil, Geoffrey L[1]
1 Idaho National Laboratory

Scientific Achievement

The Fission Accelerated Steady-state Test (FAST) experiments have been modeled in BISON to get a baseline prediction of the strain expected from the experiments. As experimental data is collected, the results are being compared to the BISON simulations to find the conditions in which the models need work to increase the predictive accuracy. The FAST simulations will also be used to compare the effect of increased irradiation exposure on the cladding strain.

Significance

Work is currently still in progress for this project. We found that BISON is overpredicting the cladding strain in the fuel region and underpredicting cladding strain in the plenum region for the FAST experiments. The BISON-predicted burnup is also underpredicted when compared to MCNP simulations of the experimental parameters.

Key Publications

Beausoleil II, G.L., Capriotti, L., Paaren, K.M., Patnaik, S., and Swearingen, A.L. (2024, March 3-7) Fission Accelerated Steady-state Testing BISON Analysis and Profilometry Comparison [Conference Presentation (Submitted)] TMS 2024 Conference, Orlando, FL, United States. https://www.tms.org/TMS2024/TMS2024/Default.aspx

Beausoleil II, G.L., Swearingen, A.L., Paaren, K.M., Patnaik, S., and Capriotti, L. (In Progress) Parameterizing Irradiation Effects of HT9 Cladding & Fuel Performance Modelling of Accelerated Metal Fuels Tests.

Swearingen, A.L., Paaren, K.M., and Beausoleil II, G.L. (2023, November 28-30) Comparison of FAST Experiments to BISON Simulations [Workshop Presentation (Submitted)], MMSNF 2023 Workshop, Hamilton, ON, Canada.

Swearingen, A.L., Paaren, K.M., and Beausoleil II, G.L. (2023, December 10-14) Evaluation of Irradiation Creep Effects in HT9 cladding for FAST Experiments [Conference Presentation (Accepted)], MiNES 2023 Conference, New Orleans, LA, United States.
https://www.ans.org/meetings/mines2023/

Sponsor/Program

Advanced Fuels Campaign, Advanced Low Enriched Uranium

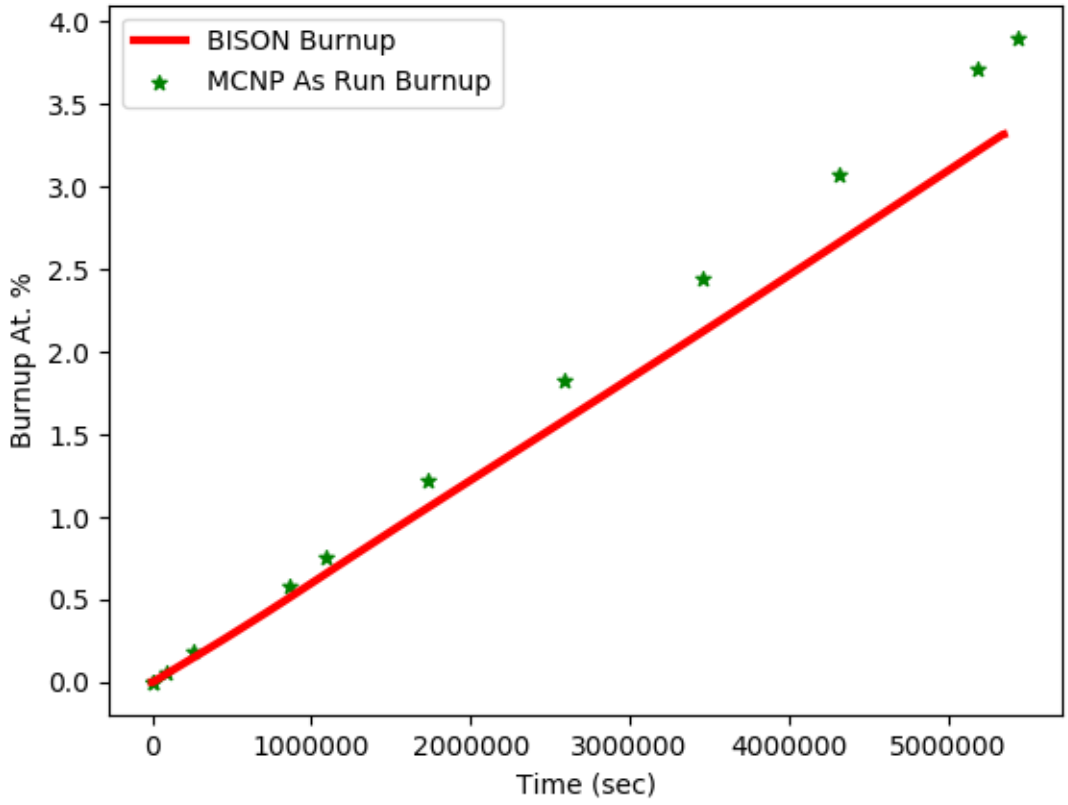


Figure 1: FAST-008 MCNP vs. BISON burnup comparison.

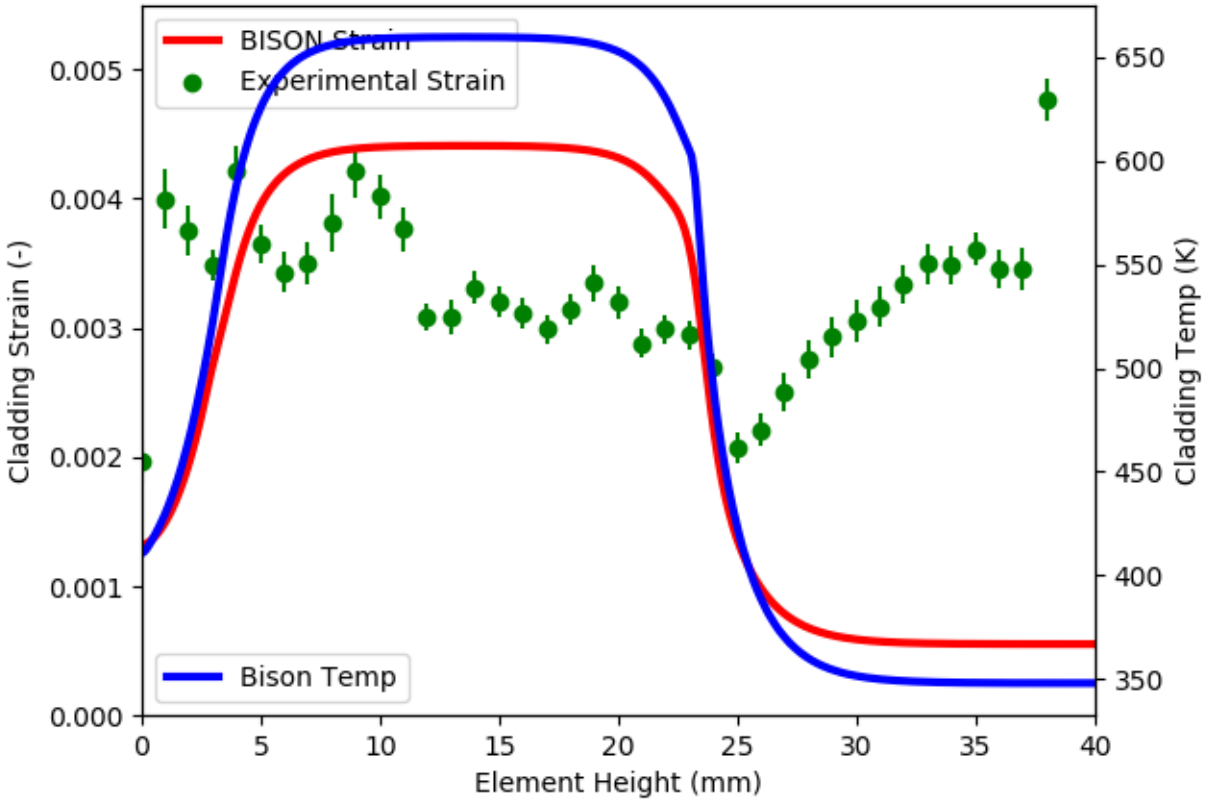


Figure 2: FAST-008 experimental vs. BISON-simulated strain comparison.

B.15 The Plant Reload Optimization Platform Development

Report Participants

Kim, Junyung [1], Abdo, Mohammad G[1], Wang, Congjian [1], Mandelli, Diego [1], Choi, Yong-Joon [1], Gutierrez, Juan Cristhian Luque [2], Nguyen, Khang H[2], Hou, Jason [2]
1 Idaho National Laboratory
2 North Carolina State University

Scientific Achievement

The Plant Reload Optimization Platform development project aims to build a reactor core design tool that includes reactor safety and fuel performance analyses and uses artificial intelligence to support the optimization of core design solutions. The Non-dominated Sorting Genetic Algorithm II optimizer was developed and tested within RAVEN to handle many constraints by using an augmented objectives methodology. The demonstration was performed with constrained multi-objective optimization of a 17×17 pressurized-water reactor core loading patterns to minimize fuel costs and maximize fuel cycle length using HPC.

Significance

The U.S. DOE Light Water Reactor Sustainability Program Risk-Informed Systems Analysis Pathway Plant Reload Optimization Project aims to develop an integrated, comprehensive framework offering an all-in-one solution for reload evaluations with a special focus on optimizing core design. Optimizing the fuel loading pattern is one of the most important considerations in reducing the amount of new fuel used in the core. Due to thousands of possible core configuration options, finding optimal solutions is an unachievable task for a human. The Plant Reload Optimization platform, which supports artificial-intelligence-based reactor core designing, is now fully capable of handling realistic problems.

Key Publications

Khang Nguyen, Jason Hou, Mohammad G. Abdo, Junyung Kim, Congjian Wang, Yong-Joon Choi. 2023. Optimization of Light Water Reactor Core Design Using a Genetic Algorithm in the RAVEN Framework. In Proceedings of American Nuclear Society Annual Meeting, Indianapolis, IN

Sponsor/Program

INL

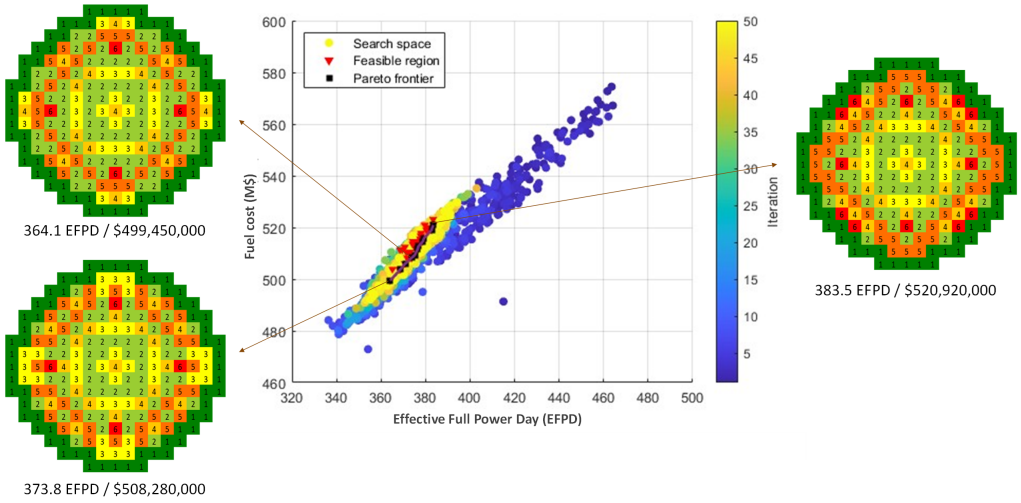


Figure 1: Search space, feasible region, and optimized solutions on the Pareto frontier of fuel loading patterns. Users can select one fuel loading pattern among the ones in the Pareto frontier.

B.16 Advanced Controls and Digital Twins

Report Participants

Al Rashdan, Ahmad Y[1], Farber, Jacob A[1], Montezzo Coelho, Maria E[1], Yadav, Vaibhav [1], Primer, Craig A[1], Oncken, Joe E[1]
1 Idaho National Laboratory

Scientific Achievement

The aim of this research is to demonstrate how control methods interface with digital twins of advanced nuclear reactors. The project focuses on developing a digital twin for Microreactor Applications Research Validation and Evaluation (MARVEL). Using MARVEL neutronics and thermal-hydraulic models and simulation results, we are developing digital-twin-enabled control modules to demonstrate autonomous operations of absorber drums and their impact to the reactor. We are using RELAP5-3D software to work with the RELAP5-3D model of MARVEL, create the MARVEL digital twin, and customize the digital twin to deploy control methods.

Significance

The work performed to date has connected the RELAP5-3D model of MARVEL to Python-developed control algorithms. Model simulation interacts with the control module feed system's current state information and intake control decisions. This research will contribute to the understanding of integrating control methods and digital twins for advanced nuclear reactors. Advanced nuclear reactors offer a new set of capabilities by using intelligent control to track dynamic power demands, make autonomous decisions, and reduce the need for human involvement. Control of advanced nuclear reactors will require a live model that can track and adapt to the actual process (i.e., a digital twin).

Key Publications

Al Rashdan, Ahmad Y., Farber, Jacob A., Montezzo Coelho, Maria Eduarda, Primer, Craig A., & Yadav, Vaibhav. Integration of Control Methods and Digital Twins for Advanced Nuclear Reactors. United States. https://doi.org/10.2172/1924292

Farber, Jacob A., Al Rashdan, Ahmad Y., Montezzo Coelho, Maria Eduarda, Primer, Craig A., & Yadav, Vaibhav. Integrating Control Methods and Digital Twins for Advanced Nuclear Reactors. United States. https://doi.org/10.13182/NPICHMIT23-41489

Sponsor/Program

INL

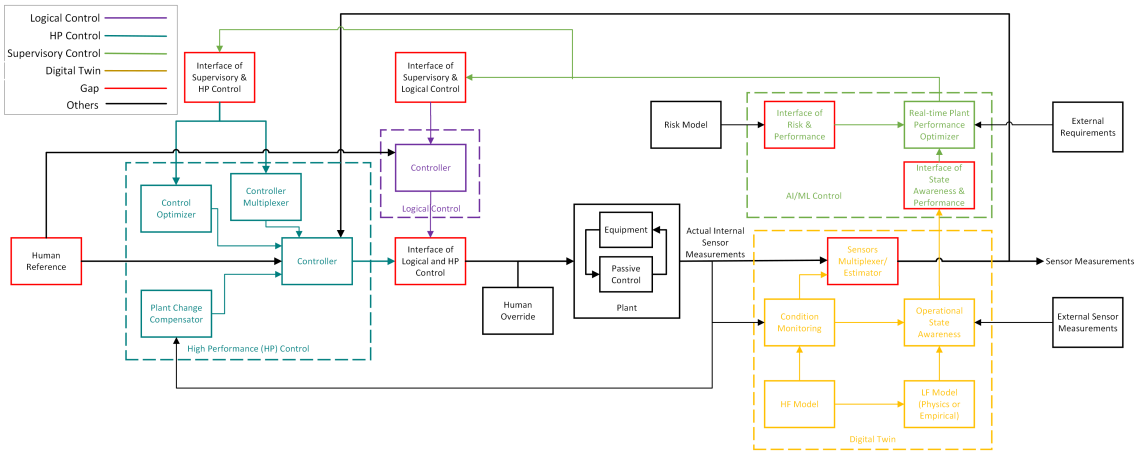


Figure 1: Operational approach to integrate advanced control methods and digital twins for advanced nuclear reactors.

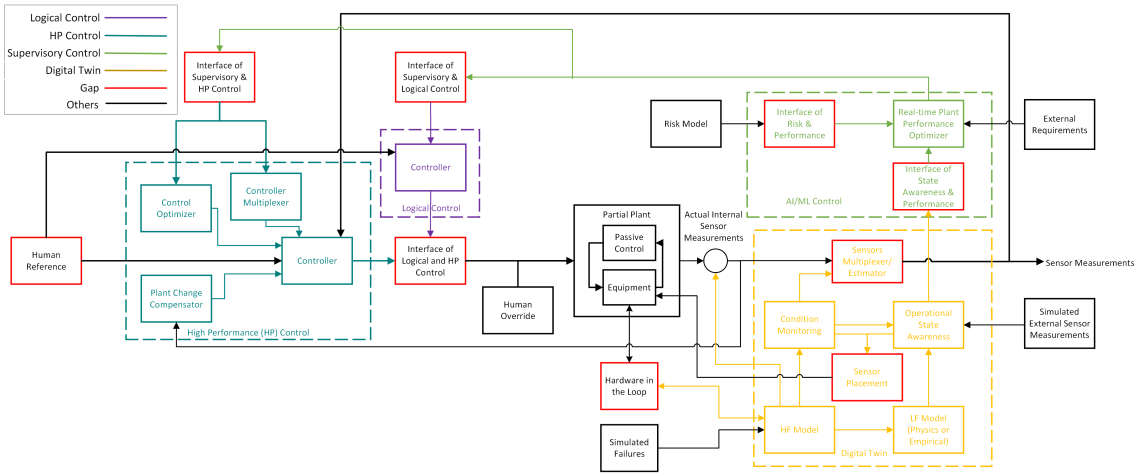


Figure 2: Design approach to integrate advanced control methods and digital twins for advanced nuclear reactors.

B.17 Phase-field simulation of Xe gas bubble evolution and elastic property degradation in U-10Mo fuel

Report Participants

Kadambi, Sourabh B[1], Aagesen, Larry K[1], Beeler, Benjamin W[2]
1 Idaho National Laboratory
2 North Carolina State University

Scientific Achievement

The burnup of U-10Mo fuel results in chemical and physical changes to the fuel microstructure. To gain a mechanistic understanding of Xe gas bubble evolution in U-10Mo, rate-theory-based multi-phase-field simulations were performed using the MOOSE/Marmot framework. We tested the effects of grain size, diffusivity of vacancy relative to Xe, faster diffusivities at the grain boundary and triple junction, and effective production rates of the defects. Furthermore, the mechanical properties of U-Mo fuel degrade during burnup due to significant microstructural changes. We assessed the impact of various microstructural features on the degradation of elastic constants. The phase-field microstructure models were combined with the finite-element-based asymptotic homogenization method to obtain effective elastic constants as a function of porosity and fission density.

Significance

During fuel burnup, smaller grain boundary face bubbles were found to dissolve, while larger triple junction bubbles were observed to grow and interconnect to form percolation paths for Xe and vacancy diffusion. Relatively fast vacancy diffusivity and smaller grain sizes prevent intragranular bubble formation. These results will help provide a mechanistic understanding of experimental porosity distribution, fission gas release to the fuel-cladding interface, and swelling behavior. In assessing mechanical property degradation, grain boundary face coverage strongly impacts mechanical property degradation. However, triple junction porosity causes the maximum degradation due to its predominant contribution to the total porosity fraction. The effective elastic constants assessed in this work are expected to be used by engineering models.

Key Publications

Benjamin, B, Aagesen, L. K., Cole, J., Hasan, ATM J., Hu S., Kadambi, S., Lavender, C., Majumder, S., Malakkal, L., Manzoor, A., Mao, Z., Mei, Z-G., Oaks, A., Okuniewski, M., Park G., Shu, S., Yacout, A., Ye, B., and Zhang, Y. (2023). "Microstructural-Level Fuel-Performance Modeling of UMo Monolithic Fuel." Idaho National Laboratory INL/RPT-23-74528.

Sponsor/Program

United States High-Performance Research Reactor (USHPRR) Program

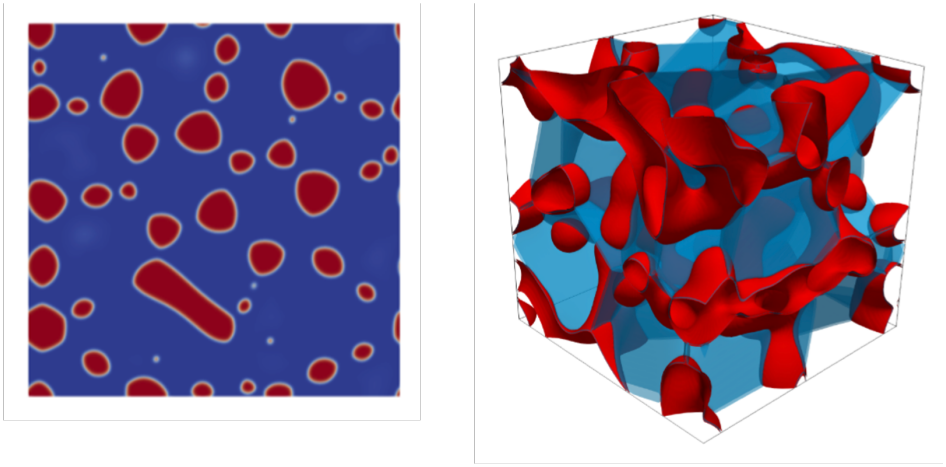


Figure 1: Evolved Xe gas porosity distribution in U-10Mo, showing predominant pores at triple junction points in 2D (left) and interconnected pores along triple junction lines in 3D (right).

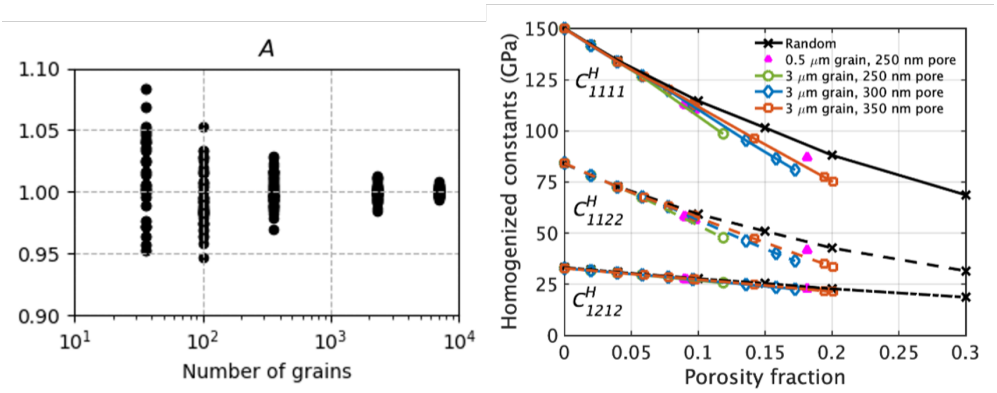


Figure 2: Effective elastic constants of U-10Mo, showing a convergence study for unirradiated fuel with different number of grains (left) and irradiated fuel with triple junction porosity of different pore sizes (right).

B.18 Extending Data-Driven Anomaly Detection Methods to Transient Power Conditions in Nuclear Power Plants

Report Participants

Farber Jacob, Aaron K[1], Al Rashdan, Ahmad Y[1], Reese, Randall D[1], Sundaram, Arvind [2], Abdel-Khalik, Hany [2]
1 Idaho National Laboratory
2 Covert Defenses

Scientific Achievement

The objective of the Advanced Remote Monitoring for Operational Readiness Program is to develop robust data-driven anomaly detection methods that can be implemented on NPP process data with minimal implementation effort and maximum detection performance. Historically, NPPs have operated predominantly at or near full power, meaning that data-driven anomaly detection methods can likely perform well during full power operations. This presents a challenge when the power drops (referred to as a transient) and may result in false alarms due to the lack of historical data at those new power levels. The objective of this specific effort was to develop anomaly detection methods that can extend to these transient conditions. The research hypothesis we tested is that anomaly detection methods can be extended to improve performance during the data-poor transient conditions compared with baseline methods trained on data from normal operation conditions. To test this hypothesis, multiple methods were developed, evaluated, and implemented on large synthetic time-series datasets. These methods ranged from relatively fast linear models to computationally expensive neural network and autoencoder models, each of which was trained many times with different datasets and different amounts of transient data.

Significance

The results of this effort showed that including full power data made a significant difference in anomaly detection methods when linear underlying patterns could be found within the data. This held true even when the main underlying physics of the system were nonlinear, so long as some linear patterns could be extracted. The methods developed could have significant impact on the nuclear power industry because plants are investing heavily into automated anomaly detection methods; however, it is likely they are currently only running at full power operations, reducing their effectiveness and impact. The methods developed here would enable increased monitoring to detect early signs of component malfunctions and anomalies, providing plants more time to anticipate and react to adverse conditions.

Key Publications

Farber, J., Al Rashdan, A., Reese, R., Sundaram, A., and Abdel-Khalik, H. Extending Data-Driven Anomaly Detection Methods to Transient Power Conditions in Nuclear Power Plants. Technical Report, Idaho National Laboratory, INL/RPT-23-73933, 2023.

Sponsor/Program

INL

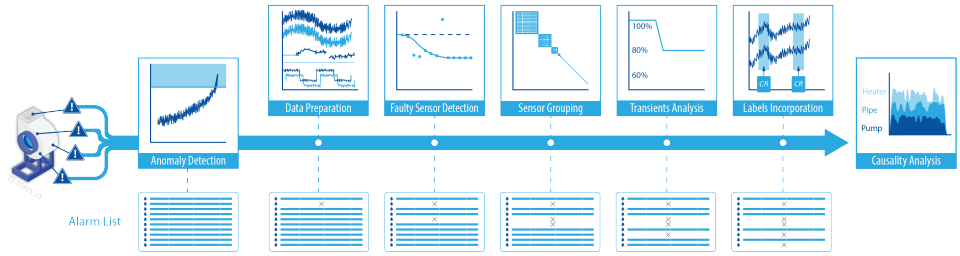


Figure 1: Developed anomaly detection modules, including the transient analysis module, to reduce false alarms and improve detection performance.

B.19 Development of Initial MOOSE-Based Crystal Plasticity Model for Irradiation Creep in 316 Stainless Steel

Report Participants

Pitts, Stephanie A[1]
1 Idaho National Laboratory

Scientific Achievement

Predictive simulation models for the behavior of austenitic 316 stainless steels under irradiation creep conditions are lacking. Our goal in this work is to develop a mechanistic, high-fidelity, crystal plasticity capability to assist in interpreting the scarce irradiation creep stainless-steel experimental data and to predict irradiation creep behavior of additively manufactured 316 stainless steel, which has a significantly different microstructure from conventional wrought material. Crystal plasticity is a well-accepted method to simulate the microstructure-sensitive mechanical response of a material. We selected dislocation glide and void swelling as the initial focus areas for developing an irradiation creep crystal plasticity capability in the MOOSE code. Models for these two mechanisms were implemented in MOOSE. A coplanar treatment of dislocation glide that groups dislocation slips, which share the same slip plane together, was selected; this model was developed by Hu and Cocks (2016, International Journal of Plasticity) for thermal creep simulations of 316 stainless steel. Volumetric swelling due to void growth was modeled as an eigenstrain, using the multiplicative decomposition of the plastic deformation gradient following Meissonnier et al. (2001, International Journal of Plasticity). In this model, an average void number density and average void radius were considered and the volume change due to void growth was calculated by assuming that the voids were perfect spheres. A series of verification simulations were preformed to evaluate the implementation of these models, and the HPC resource Sawtooth was used to perform these simulations.

Significance

The verification simulations demonstrated the correct implementation of the two crystal plasticity mechanisms in MOOSE. Results from a void eigenstrain verification simulation—using representative void evolution trends based on experimental data from Cawthorne and Fulton (1967, Nature)—are shown in the included figure. This initial implementation forms the basis of future irradiation creep simulation capability development focusing on deformation mechanisms directly connected to experimentally observed microstructure evolution. Irradiation creep—among other mechanical response behaviors—is dependent on the material microstructure. When fully developed and implemented, the MOOSE-based crystal plasticity model will be used to predict the mechanical response of 316 stainless steel under irradiation; this model will be among the first specifically targeting mechanism-based irradiation creep behavior predictions.

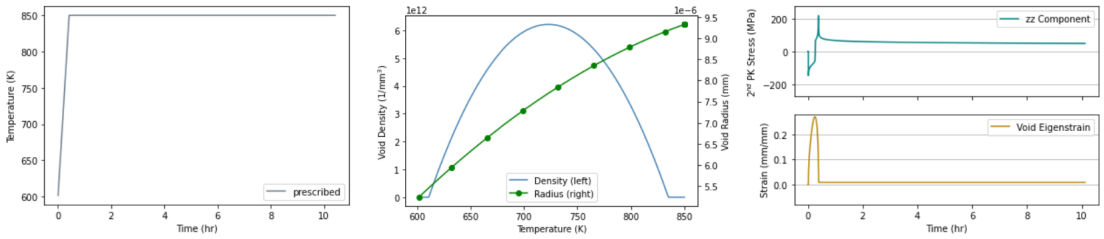
Additively manufactured material behavior predictions are of particular interest to the Advanced Materials and Manufacturing Technologies Program, and additively manufactured materials have significantly different microstructures from conventionally wrought materials. Because of the explicit focus on mechanism-based predictions, the irradiation creep crystal plasticity model under development in this current work will be applicable to simulations of additively manufactured 316 stainless steel.

Key Publications

Pitts, Stephanie A. and Andrea M. Jokisaari. "Development of Initial MOOSE-Based Crystal Plasticity Model for Irradiation Creep in 316 Stainless Steel." Milestone Report for the Advanced Materials and Manufacturing Technologies Program. August 2023.

Sponsor/Program

Advanced Materials and Manufacturing Technologies



(a) Applied temperature profile (b) Model void characteristics (c) Predicted stress response

Figure 1: Demonstration of the history-dependent impact of the void volumetric eigenstrain on the predicted crystal plasticity stress state. The crystal simulation, oriented with the Cartesian coordinate system, is constrained in the z-direction and allowed to expanding in the x- and y-directions; the primary stress response is thus in the z-direction. (a) The temperature is increased linearly over 25 minutes and then held constant, (b) a prescribed evolution of average void density and average radius represents—in a general sense—the expected evolution in this temperature range, and (c) the resulting volumetric eigenstrain and stress response, where the non-zero steady-state responses highlight the history-dependent impact of the void eigenstrain.

B.20 Statistical Analysis to Detect Material Changes in the Adjuster Rods of a Pressurized-Heavy-Water Reactor

Report Participants

Stewart, Ryan H[1], Wen, Shaw X[1], Bays, Samuel E[1], Gleicher, Frederick N[1], Reyes, Gustavo [1], Schanfein, Mark [1]
1 Idaho National Laboratory

Scientific Achievement

Pressurized-heavy-water reactors (PHWRs) utilize a continual refueling scheme fed by depleted natural uranium fuel assemblies. These assemblies are fed into process tubes, where on a given day approximately 12 process tubes are refueled. To maintain a relatively flat neutron flux profile, adjuster rods are used in the central region of the core to suppress the flux in this area. Recently, the adjuster rods have been examined as a potential source for generating cobolt-60 for its use in medical devices. This work focused on determining if changes to the adjuster rods could be detected using statistical methods to provide an analysis technique for detecting anomalous behaviors via monitoring techniques.

Significance

This work developed a PHWR model in Serpent that incorporates a refueling scheme to accurately capture the time-dependent material composition of the core. Along with this, adjuster rods were included in the core where the material composition of the adjuster rods was placed with either stainless-steel 304 (SS304) or dicobolt-boride (Co2B). The later material was placed as a potential for introducing a means to generate cobolt-60. The focus of this work was to determine if SS304 adjuster rods were accidentally replaced with C2B rods would subsequent changes in the assembly powers show this difference. To examine this, the first 360 days of a PHWR were modeled with both SS304 and Co2B, where the subsequent assembly powers were collected and analyzed utilizing two statistical methods. The Rank Sum and Komogorrov-Smirnov (KS) methods were utilized to examine the distribution of assembly powers in both cores to determine if the two materials produced a unique signature. We found that the KS method can distinguish between the two different materials with limited data (i.e., with few time steps and some assemblies removed). Along with this, an examination of the assembly burnup and activity (integral quantities of reactor operations) were statistically similar and did not provide evidence of the change in material. The KS method provided preliminary evidence that one could utilize statistical methods to determine deviation in the core due to accidental (or intentional) insertion of materials into the core and could likely ensure proper assembly power distribution.

Key Publications

* F. Gleicher, et al, "Analysis of Heavy Water Reactor Reactivity Device with a Dyadic Monte Carlo Model", Transactions of the ANS 2023 Winter Meeting, 2023. * S. Wen, et al, "Statistical Analysis to Detect Material Changes in the Adjuster Rods of a Pressurized Heavy Water Reactor," Annals of Nuclear Energy (in progress).

Sponsor/Program

INL

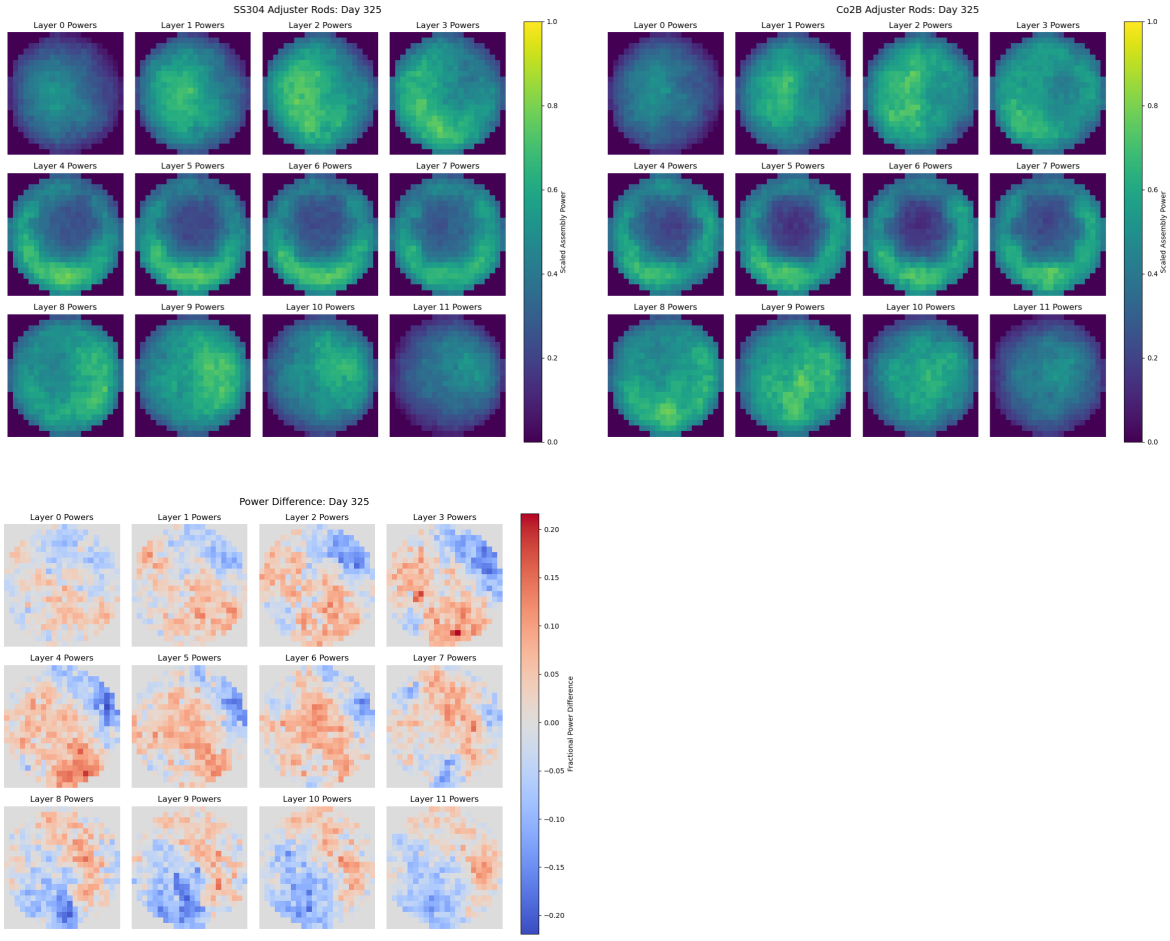


Figure 1: Comparison of assembly powers between the reference case (SS304) and perturbed case (Co2B).

B.21 Thermal Analysis of the AGR-5/6/7 Experiment Irradiated in the Advanced Test Reactor

Report Participants

Hawkes, Grant L[1]
1 Idaho National Laboratory

Scientific Achievement

A thermal analysis was performed to calculate the Advanced Gas-Cooled Reactor (AGR)-5/6/7 as-run daily temperatures of the fuel compacts. The experiment was irradiated in ATR for seven irradiation cycles. The experiment was composed of five separate capsules each with their separate control gas mix and temperature objective. Time-averaged, volume-averaged temperature data will be used to evaluate fuel performance. The AGR-5/6 portion of the experiment was for fuel qualification at prototypic temperatures, while the AGR-7 portion of the experiment was a margin test at very high temperatures. A separate thermal analysis was performed on the AGR-5/6/7 experiment detailing the consequences of not having the graphite holder perfectly centered and causing nonuniform gas gaps that control temperature. The model considered thermal expansion, graphite shrinkage and swelling due to fast neutron fluence, and various thermal properties varying with temperature and irradiation exposure. Daily temperature calculations were performed to obtain the time-averaged, volume-averaged temperature for the fuel compacts. The finite element structural analysis and heat transfer code from Dassault Systemes named ABAQUS was used.

Significance

As a result of this experiment and thermal analysis, the TRISO particle fuel has been qualified for use in reactors. The fuel performed very well at its standard operating temperature as well as at high margin temperatures. Thermal model predictions were compared to actual thermocouple measurements during irradiation. The thermal model was used to predict temperatures during irradiation and adjust irradiation operating parameters accordingly. The additional analysis showing the effects of not having the graphite holder perfectly centered shows peak temperatures about 100°C higher than the high and 100°C lower than the low when compared to perfectly centered graphite holders. An optimization routine was utilized to find the direction and magnitude of the offset for the top and bottom of Capsule 1 that best matched the thermocouple data.

Key Publications

A. J. Palmer, R. S. Skifton, M. Scervini, G. L. Hawkes, C. B. T. Pham, and T. L. Checketts, Summary of Thermocouple Performance In the Advanced Gas Reactor Experiment AGR-5/6/7 During Irradiation in the Advanced Test Reactor, paper ANIMMA2021-04-196, PRS/CON-21-01282, ANIMMA International Conference, Prague, Czech Republic, June 21-25, 2021.

G. L. Hawkes, Cylindrcity Sensitivity Thermal Model of the AGR-5/6/7 Experiment in the Advanced Rest Reactor, paper # IMECE2020-23329, INL/CON-20-59536 Rev:000, 2020 IMECE Conference, Portland, OR, Nov16-19, 2020, https://doi.org/10.1115/IMECE2020-23329 .

G. L. Hawkes, J. W. Sterbentz, Thermal Model Heat Rate Predictions of the AGR-5/6/7 EXPERIMENT, paper # 20136, INL/CON-19-55977, ICAPP 2021 Conference, Abu Dhabi, Oct 16-20,

2021.

G. L. Hawkes, Thermal Model Predictions of Gas Mixtures in the AGR-5/6/7 EXPERIMENT, paper # IMECE2019-12821 (presentation only), INL/MIS-19-54786, ASME IMECE Conference, Salt Lake City, UT, Nov 11-14, 2019.

G. L. Hawkes, J. W. Sterbentz, M. Plummer, Thermal Model Details and Description of the AGR-5/6/7 Experiment, paper # 000142, ICAPP 2019 International Congress on Advances in Nuclear Power Plants, Juan-les-Pins, France, May 12-15, 2019.

Sponsor/Program

DOE Advanced Reactor Technology

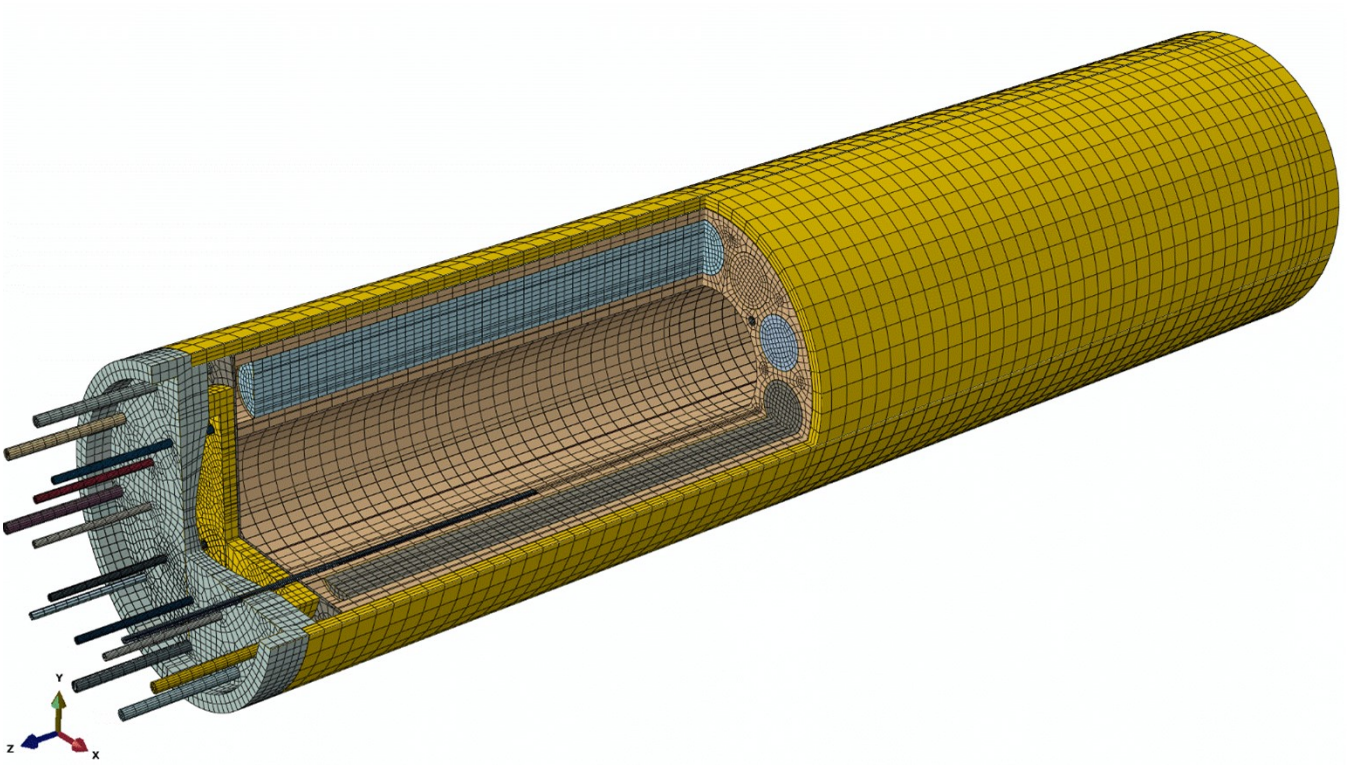


Figure 1: Finite-element mesh of Capsule 1 of the AGR-5/6/7 experiment.

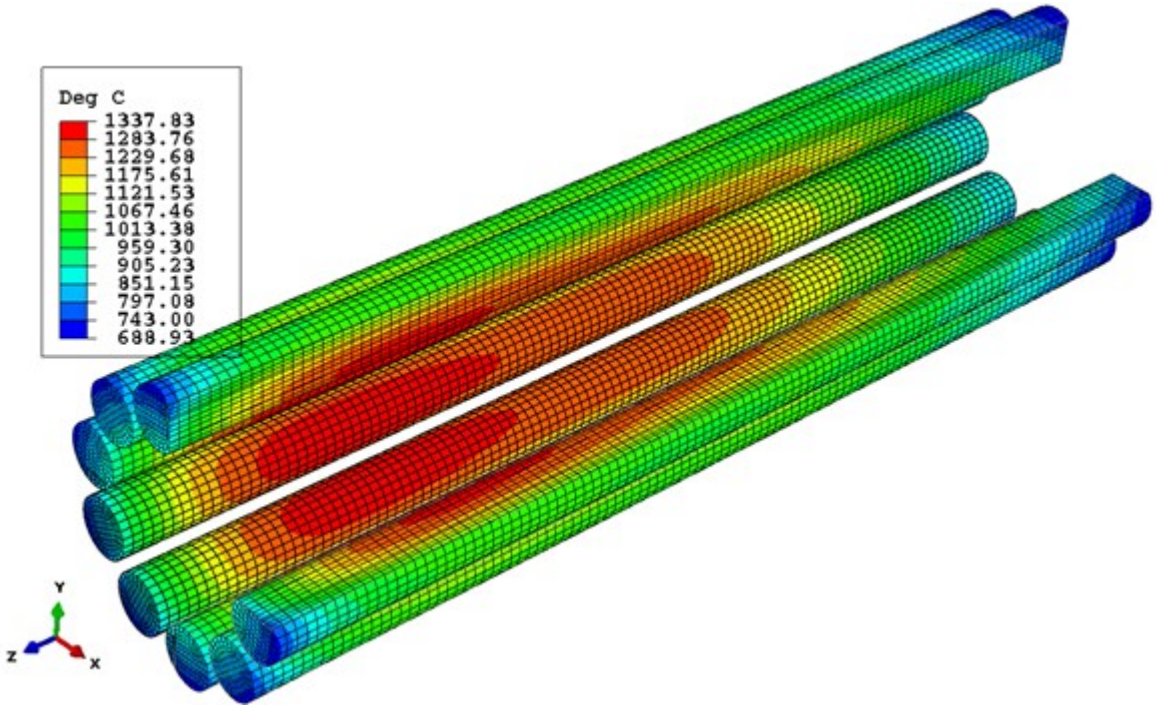


Figure 2: Typical temperature (°C) of the fuel in Capsule 1 of the AGR-5/6/7 experiment.

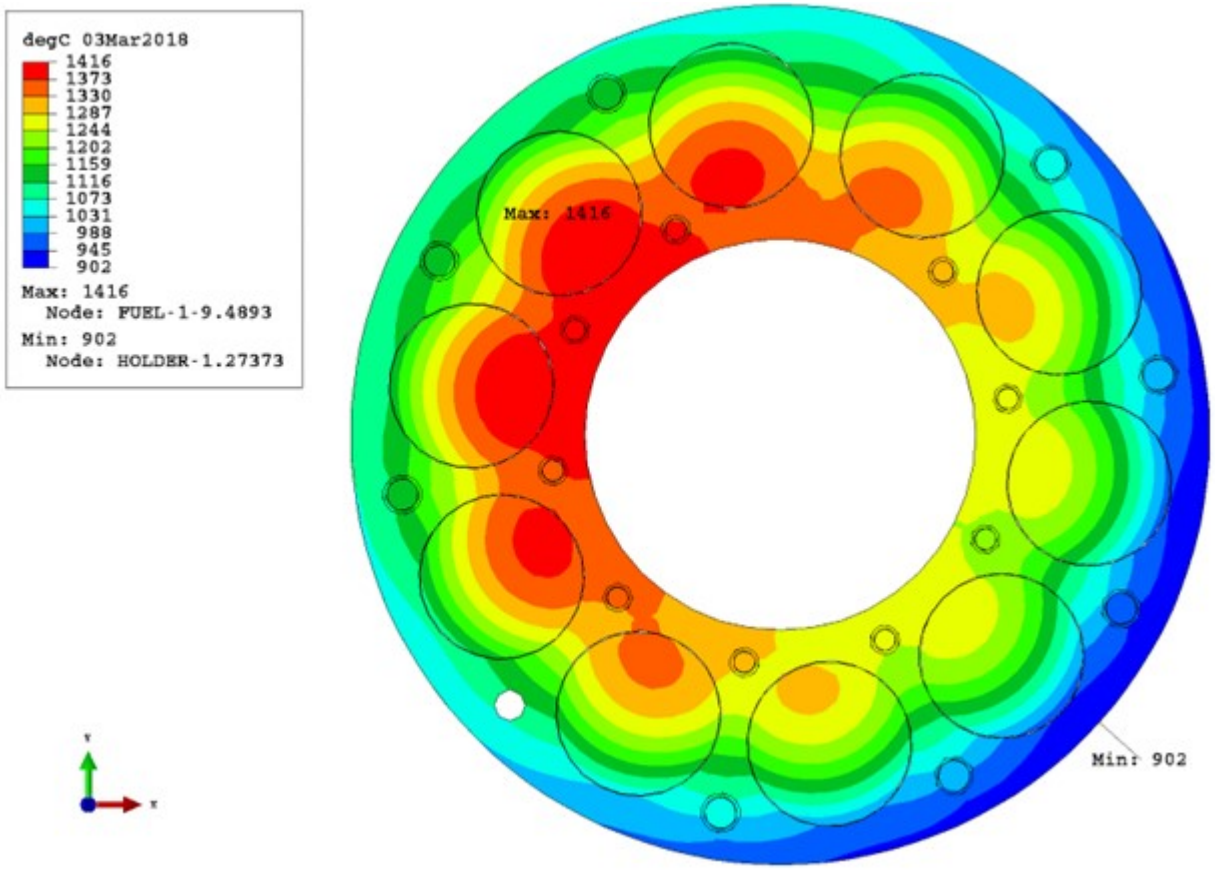


Figure 3: Cross-section temperature (°C) of The offset gap in NW for Capsule 1 of the AGR-5/6/7 experiment.

B.22 Effect of Material Composition on Collision Cascade Size and Production of Radiation-Induced Defects in Stainless Steel 316

Report Participants

Swisher, Mathew M[1]
1 Idaho National Laboratory

Scientific Achievement

There is a need to accurately predict the number of remaining point defects generated by irradiation damage cascades after their initial recombination to support quantitative predictions of the irradiation-driven microstructure evolution of stainless steel 316. In order to study the accumulation of radiation damage at an atomistic level, this study used molecular dynamics (MD) simulations to test the accuracy of several different potential models. Collision cascade simulations were performed both to analyze the maximum size of the cascade and the number of surviving Frenkel pairs at different energy levels, temperatures, and variations in material composition. Additional simulations were performed to study the partial diffusivity of vacancies and interstitial atoms in stainless steel (SS) 316 at a range of temperatures, both to confirm the accuracy of the molecular model and to investigate how strongly each of the component elements influence the diffusion of point defects. This work required a significant number of GPU-accelerated MD simulations to collect statistically significant data on the progression of collision cascades for various material compositions. The simulations were performed with the Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software package.

Significance

Quantifying the defect populations from the maximum extent of the collision cascade to the residual damage of the cascade is of vital importance for designing new materials and characterizing their lifecycles. In this work, MD simulations of collision cascades and the diffusion of point defects were performed to study the creation and diffusion of these point defects.

The performance of several different models for SS-316 were evaluated, and representing SS-316 with an Fe/Cr/C alloy using the Henriksson model was found to be the most successful. Collision cascade simulations have been used, along with the Wigner-Seitz method, to investigate the generation of point defects in SS-316 and how the composition of the stainless steel influences the progression of the collision cascade and the resulting impact on the number of Frenkel pairs that survive the subsequent recombination of defects. Our simulations showed that the effect of carbon on the number of generated defects was especially complex. We also found that a higher chromium content in the model material increased the generation of defects generated by collision cascade, possibly due to the segregation of iron and chromium atoms.

Additionally, MD studies on the diffusion of point defects in modeled SS-316 were performed. We were able to show that the Henriksson model can qualitatively reproduce the partial diffusivity of defects in the Fe/Cr/C system with reasonable accuracy. This makes it possible to study a number of important phenomena in the future, such as carbon atoms trapping vacancies, the sink strength and diffusion rates of defect loops and clusters, and the sink strengths of grain boundaries.

Key Publications

Swisher, M. M. and A. M. Jokisaari. In Progress. Effect of material composition on collision cascade size and production of radiation induced defects in stainless steel 316.

Sponsor/Program

Advanced Materials and Manufacturing Technologies

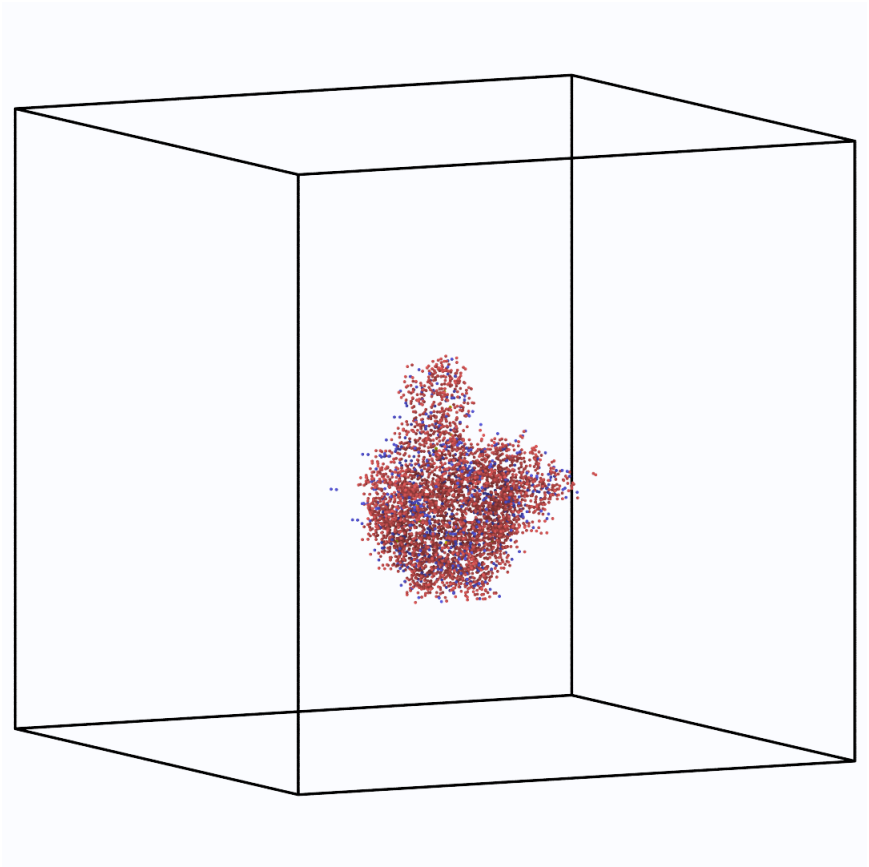


Figure 1: Distribution of interstitials in a Fe/Cr/C alloy modeling SS-316 at the peak of a 15 keV collision cascade.

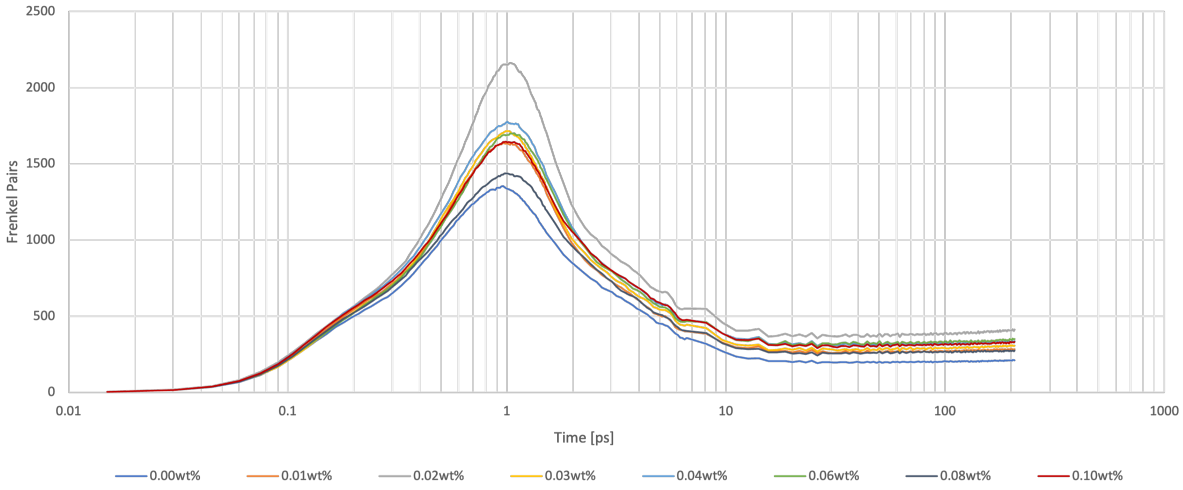


Figure 2: Number of Frenkel pairs making up the average 15 keV collision cascade as a function of time for a Fe/Cr/C alloy modeling SS-316 with a varying carbon content. Each profile is the average of 20 cascade simulations.

B.23 Hydrogen Migration in Hydrides for Microreactor Applications

Report Participants

Terlizzi, Stefano [1], Laboure, Vincent M[1], DeHart, Mark D[1], Faure, Quentin D[2]
1 Idaho National Laboratory
2 North Carolina State University

Scientific Achievement

This work assessed the current capabilities of MOOSE to model hydrogen redistribution and dissociation in hydrides. Emphasis was on yttrium hydride (YHx), which is the main candidate for moderating high-temperature microreactors. This work found that the redistribution of hydrogen within the hydride leads to a negative reactivity feedback due to hydrogen migration toward colder axial zones that are usually associated with lower neutron importance. The magnitude of the feedback, ranging from tens to hundreds of percent miles on the reactor eigenvalue, descends from the magnitude of the axial temperature gradient that determines the asymptotic hydrogen distribution in the hydride. To the best of the authors' knowledge, this was the first work in which the effect of hydrogen redistribution on microreactor reactivity was evaluated in a coupled multiphysics setting that included neutronics, heat-pipes flow, and heat transfer equations at a full-core scale. The dissociation of hydrogen at the hydride surface together with the leakage through the cladding was also modeled. Results from dissociation models are strongly influenced by the considerable uncertainty in YHx material properties. To further develop this insight, a rigorous uncertainty quantification study was performed to identify the main sources of uncertainty in YHx-moderated microreactors. We found that the epistemic uncertainties related to a lack of knowledge of material properties dominate over the aleatoric uncertainties, thus implying the need for additional experimental campaigns to characterize hydrogen dissociation dynamics and temperature-gradients-driven responses in YHx.

Significance

The project achieved three primary milestones. The first milestone was gaining a better understanding of the effect of hydrogen migration on YHx-moderated heat-pipe-cooled microreactors' performance by leveraging BISON. Subsequently, the influence of hydrogen migration on power density, eigenvalue, and temperature was determined through the integration of BISON inputs with full-core neutronic and heat transfer models established within the DireWolf software driver. Our findings demonstrated a negative reactivity feedback resulting from the migration of hydrogen toward colder axial zones. These axial zones are usually associated with low neutron importance, thus leading to a negative effect on reactivity. The magnitude of feedback on the effective multiplication factor was found to be "29 pcm for a prototypical heat-pipe-cooled microreactor. The modest scale of this effect is attributed to the minimal axial temperature gradient in heat-pipe-cooled microreactors. To the best of the authors' knowledge, this was the first work in which the effect of hydrogen redistribution on microreactors' reactivity was evaluated in a coupled multiphysics setting, including neutronics, heat pipes' two-phase flow, and heat transfer equations at a full-core scale.

As part of the second milestone, a BISON model was constructed to characterize hydrogen dissociation at the YHx and gap interface. Furthermore, a leakage model describing the hydrogen loss through the clad was implemented in BISON. The model's accuracy was validated against experimental data, demonstrating a good agreement between the computed and reference outcomes.

Notably, a non-negligible difference was found by employing different experimental data for the pressure-concentration-temperature curves definition.

The third achievement encompassed a rigorous assessment of the influence of uncertainties in YHx properties on temperature and stoichiometric ratio scalar fields. This evaluation was conducted through a two-step methodology employing Dakota, Griffin, BISON, and Sockeye. We found that the magnitude of the epistemic uncertainty of the heat of transport shadows the influence of the aleatoric uncertainties. To authors' knowledge, this is the first rigorous UQ analysis applied to microreactors and hydrogen redistribution feedback effect.

Key Publications

1. Terlizzi S., Labour, V., and DeHart M. (2022). Preliminary Observations on the Hydrogen Redistribution Feedback in YH-Moderated Monolithic Microreactors. 2022 ANS Annual Meeting. 2. Terlizzi S., Labour, V., and DeHart M. (2022). Selected results from full-core hydrogen redistribution asymptotic analysis in YH-moderated heat-pipe cooled microreactor. 2022 ANS Winter Meeting. 3. Terlizzi S. and Labour, V. (2023). Asymptotic Hydrogen Redistribution Analysis in Yttrium Hydride Moderated Heat-pipe-cooled Microreactors using DireWolf, Annals of Nuclear Energy, 186, 109735. 4. Faure Q., Labour, V., and Terlizzi S. (2023) Preliminary Results for Uncertainty Quantification on Asymptotic Hydrogen Redistribution in a Prototypical Yttrium-Hydride Moderated Heat-Pipe-Cooled Microreactor, ANS Winter Meeting, Washington DC, USA, November 2023. 5. Faure Q., Labour, V. Terlizzi S. (Expected Submission Date: 20 November 2023). Multi-Physics Uncertainties Quantification on Neutronics Response for a Prototypical Yttrium-Hydride Moderated Heat-Pipe-Cooled Microreactor, Annals of Nuclear Energy. 6. Terlizzi S., Faure Q., (Expected Submission Date: 30 October 2023) On the effect of hydrogen dissociation on the lifetime of hydride-moderated nuclear microreactors, Physor 2024, San Francisco, USA, April 2024.

Sponsor/Program

Laboratory Directed Research and Development 21P1056-010FP

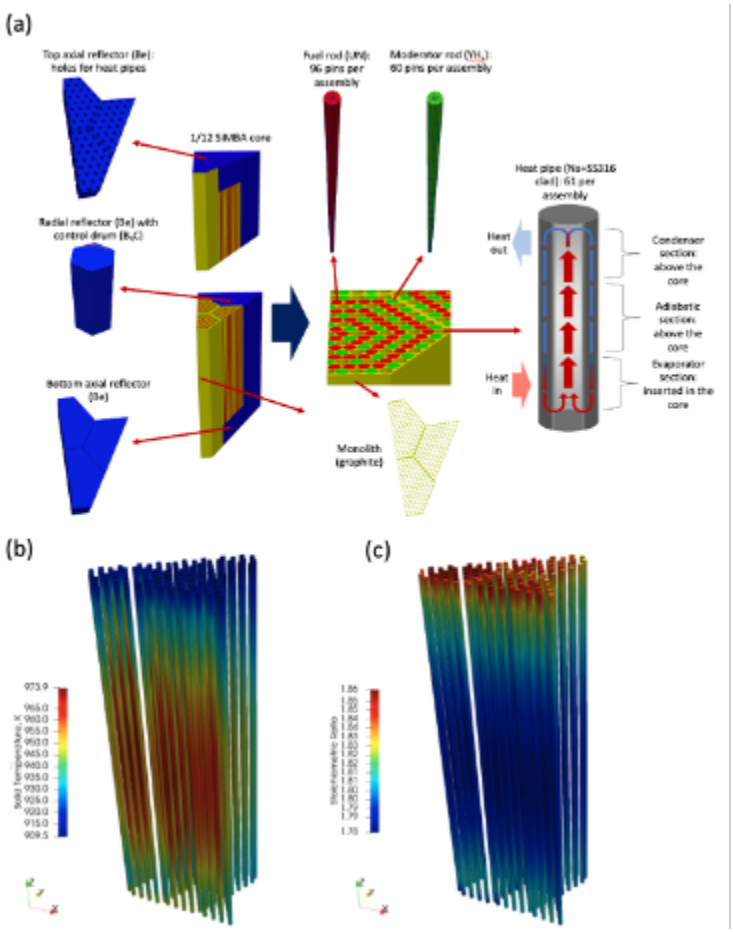


Figure 1: (a) Simplified microreactor benchmark assessment problem overview, (b) computed temperature, and (c) computed hydrogen stoichiometric ratio in the YHx moderator pins.

B.24 Modeling MARVEL with NEAMS tools

Report Participants

Terlizzi, Stefano [1], Trivedi, Ishita [1], Laboure, Vincent M[1]
1 Idaho National Laboratory

Scientific Achievement

In FY-23, the Nuclear Energy Advanced Modeling and Simulation (NEAMS) Multiphysics Applications Technical Area started a new research thrust aimed at using MARVEL to verify and validate NEAMS tools for microreactor evaluations. In fact, MARVEL will provide invaluable validation and benchmarking data to NEAMS tools once operating. The overarching objective of this activity is the development of a high-fidelity multiphysics MARVEL model using NEAMS tools to verify and validate NEAMS tools against MARVEL simulation and experimental data. The activity in FY-24 is expected to lay the foundations for comprehensive verification & validation activities in FY-25 and beyond.

Significance

BISON was used to model the full-core heat transfer and hydrogen redistribution in the fuel, while Griffin has been employed for the neutronics model development. The results from neutronics and heat conduction were verified against reference continuous-energy Monte Carlo calculations and literature values, respectively. Future work will be devoted to generate a thermal-hydraulic model of the core in SAM.

Key Publications

[1] Stefano Terlizzi, Ishita Trivedi, and Vincent Laboure'. (2023)."Status of NEAMS models for MARVEL" Presented on 05/17/2023, Idaho Falls, Idaho, USA. [2] Stefano Terlizzi and Vincent Laboure'. (2023). "Status Update: INL Microreactors Applications Driver", INL/ RPT-23-72501.

Sponsor/Program

NEAMS

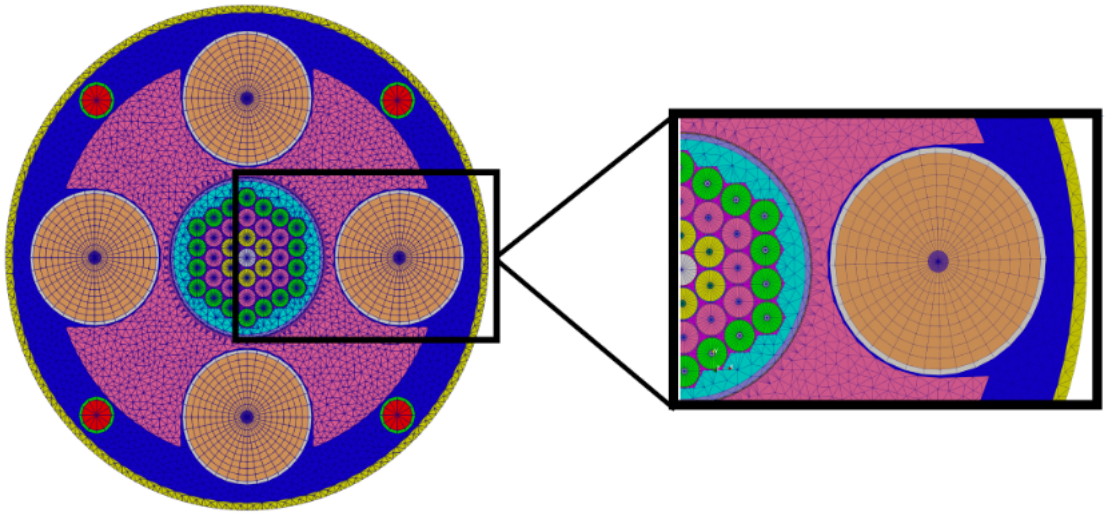


Figure 1: Radial view of the MARVEL core mid-plane.

B.25 Calibration of Advanced Test Reactor's Lobe Power Calculation and Indication System

Report Participants

Johnson, Matthew P[1]
1 Idaho National Laboratory

Scientific Achievement

A series of experiments was performed that measured the power distribution inside ATR using a variety of flux wires. These measurements were performed following the most recent core internals changeout (CIC). While the measured data from the CIC is very valuable, the measured core configurations only cover a small operating range of ATR. Simulations of the post-CIC experiments were compared to the experimental measurements and combined simulation past cycles in order to calibrate ATR's Lobe Power Calculation and Indication System (LPCIS).

Significance

Reactor operators use the lobe powers displayed by the LPCIS to drive the reactor to the lobe powers requested by experimenters. An accurate LPCIS output helps experiments achieve their desired irradiation conditions.

Key Publications

Reichenberger,et. al., "Fast and Thermal Neutron Spectrum Dosimetry Measurements in the Advanced Test Reactor Large-B and Small-I Positions Following the Sixth Core Internals Changeout," 17th International Symposium on Reactor Dosimetry, May 21, 26 2023.

Reichenber, et al., "Niobium Activation Measurements for Lobe Power Calculation Indication System Alignment at the Advanced Test Reactor," International Conference on Research Reactors: Achievements, Experience and the Way to a Sustainable Future, November 27 - December 1, 2023.

Sponsor/Program

ATR

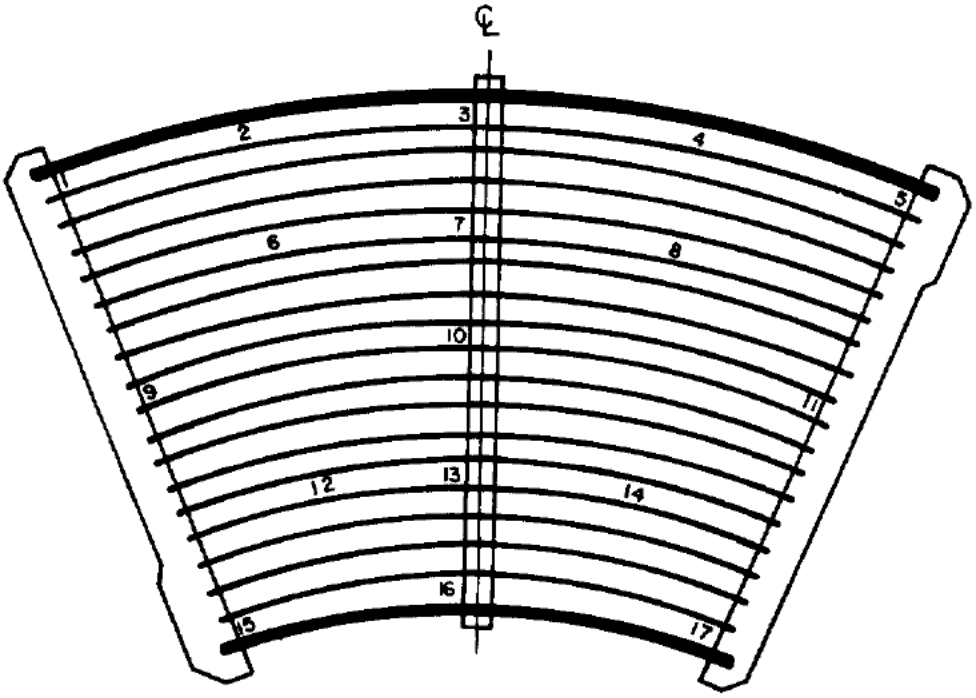


Figure 1: Location of the fission wires used to measure the fuel element power distribution.

B.26 The Electron Thermal Conductivity of Pu and Zr Substituted Gamma-Uranium

Report Participants

Yorgason, William T[1], Jokisaari, Andrea M[1], Muhich, Christopher L[2]
1 Idaho National Laboratory
2 Arizona State University

Scientific Achievement

DFT calculations are applied to gamma-U, U-Pu, U-Zr, and U-Pu-Zr compositions, followed by an application of the linearized Boltzmann transport equation under the relaxation time approximation [Madsen 2018] and a semiempirical electron relaxation time calculation method to calculate electron thermal conductivity for each composition (10 in total). The electrical and electron thermal conductivity are calculated using one of two methods based on literature: the direct method, which assumes electron relaxation time is independent of alloying, and the mixed method, which calculates conductivities by mixing alloying and host atom properties. Electron band structures are also calculated for gamma-U, U-Pu, and U-Zr compositions. The HPC Sawtooth at INL was used primarily, specifically the dual Xeon Platinum processors on the Sawtooth system. The Lemhi system was also used to a lesser degree, specifically the dual Xeon Gold processors.

Significance

Three important findings resulted from this work. First, the electron thermal conductivity decays more slowly with an increase in atomic percent Pu than with an increase in atomic percent Zr, both in the respective binary compounds with U and in U-Pu-Zr. This is especially important for U-Pu-Zr, as it implies more Pu can be recycled per fuel element of U-Pu-Zr. Second, of the two methods applied, the mixed method performs better if Zr is present and the direct method if Zr is not. This is attributed to the large mass difference and, to a lesser extent, electron band flattening that Zr induces. Therefore, we suggest that, if alloying and host atoms differ significantly in mass and or valance electron number (specifically, if the alloying atom has less valance electrons), the mixed method should be applied, while if they do not, the direct method is appropriate. This finding is applicable to all metallic alloys and can be applied for investigating the radiation resistance of high-entropy alloys, which often consist of at least four species. Third, when Pu content is doubled, from 12.5 to 25.0 at % (an increase of 100%) the electron thermal conductivity is lowered by only 7.7%. This again implies that greater Pu content in U-Pu-Zr is possible, allowing for a faster recycling of spent fuel. Fourth, because the mass difference of Am and Cm (other recyclable long-lived actinides) relative to U is similar to that of Pu and these elements have more valance electrons than U, Am and Cm should behave similar to Pu. Therefore, not only can Pu be recycled faster, increasing its content in U-Pu-Zr, but this is likely true for Am and Cm as well.

Key Publications

The Electron Thermal Conductivity of Pu and Zr Substituted Gamma-U (status: In Progress)

Sponsor/Program

Advanced Materials and Manufacturing Technologies

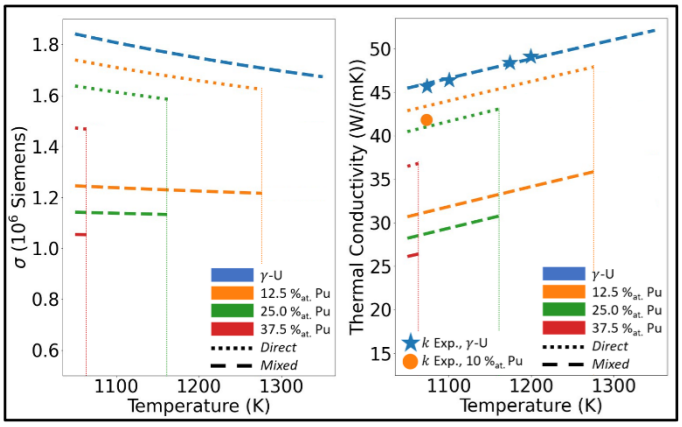


Figure 1: Thermal and electrical conductivity of U-Pu systems.

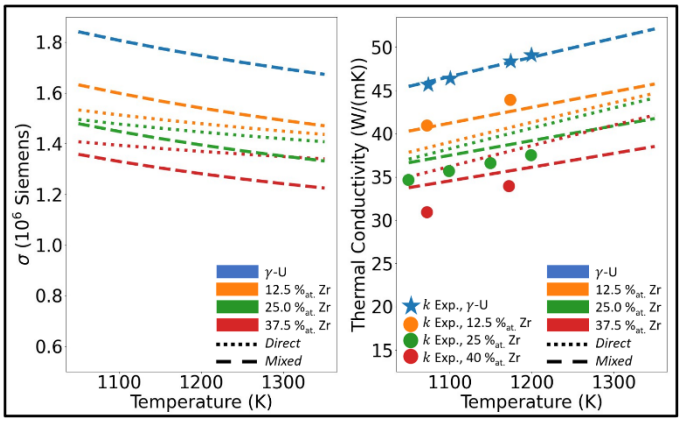


Figure 2: Thermal and Electrical Conductivity of U-Zr Systems: Left: Calculated direct and mixed for U-Zr systems, with direct and mixed for U for comparison. Right: Calculated ke direct and ke mixed are compared against experimental k [Touloukian et. al 1970], [ANL-87-19 1986] for U-Zr systems. Calculated ke direct, ke mixed, and experimental k [Ho et. al 1972] for U is included for comparison.

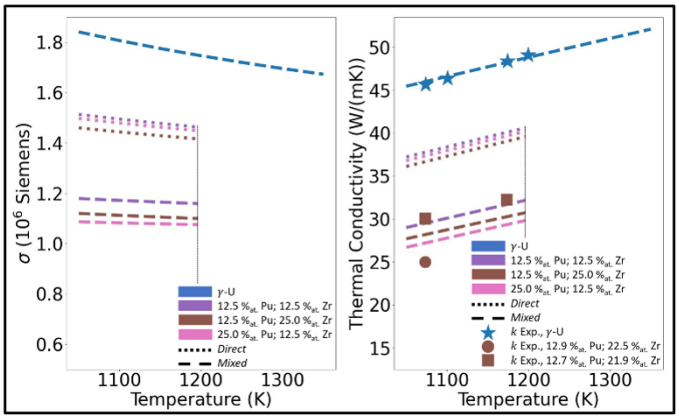


Figure 3: Thermal and electrical conductivity of U-Pu-Zr systems.

B.27 First-Principles Investigation of the Thermal Conductivity in Uranium Oxide

Report Participants

Zhou, Shuxiang [1], Gofryk, Krzysztof [1], Jiang, Chao [1], Marianetti, Chris A[2]
1 Idaho National Laboratory
2 Columbia University

Scientific Achievement

Computing thermal transport from first-principles in uranium dioxide (UO2) is complicated due to the challenges associated with Mott physics. We use irreducible derivative approaches to compute the cubic and quartic phonon interactions in UO2 from first-principles, and we perform enhanced thermal transport computations by evaluating the phonon Green's function via self-consistent diagrammatic perturbation theory. Our predicted phonon lifetimes at T = 600 K agree well with our inelastic neutron scattering measurements across the entire Brillouin zone, while our thermal conductivity predictions agree well with previous measurements. Both the changes due to thermal expansion and self-consistent contributions are nontrivial at high temperatures, though the effects tend to cancel and interband transitions yield a substantial contribution.

Significance

We have computed the scattering function and thermal conductivity of UO2 from first-principles using various levels of self-consistent perturbation theory and compared to our own inelastic neutron scattering (INS) experiments and existing thermal conductivity experiments. The relevant contributions of this work include accurately describing the phonon interactions in UO2 from first principles and illustrating the effects of improving the quality of the single particle phonon Green's function on the thermal conductivity. Favorable agreement between our theory and the INS experiment is obtained for the full width at half maximum (FWHM) of the scattering function across the Brillouin zone. In terms of quantitatively computing the thermal conductivity at high temperatures, we found that thermal expansion decreases the thermal conductivity while interband transitions increases the thermal conductivity, and these effects are of similar magnitude. Including quartic phonon interactions at the level of the bare sunset diagram causes a small decrease in thermal conductivity, while the self-consistent perturbation theory yielded moderate and appreciable increases for the quasiparticle and Hartree-Fock procedures, respectively. Aside from low temperatures where magnons play an important role, phonon thermal transport in UO2 is now well characterized from first principles.

Key Publications

S. Zhou, E. Xiao, H. Ma, K. Gofryk, C. Jiang, M. E. Manley, D. H. Hurley, C. A. Marianetti. "Phonon thermal transport in UO2 via self-consistent perturbation theory". In Progress.

Sponsor/Program

DOE-BES-EFRC Thermal Energy Transport under Irradiation

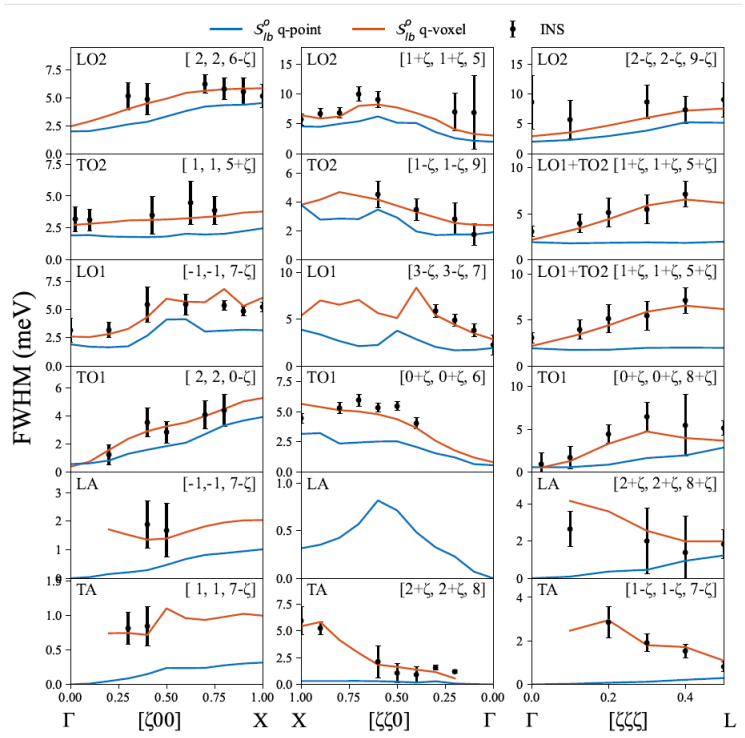


Figure 1: FWHM of scattering function peaks in various zones for UO2 at T = 600 K, comparing with INS data.

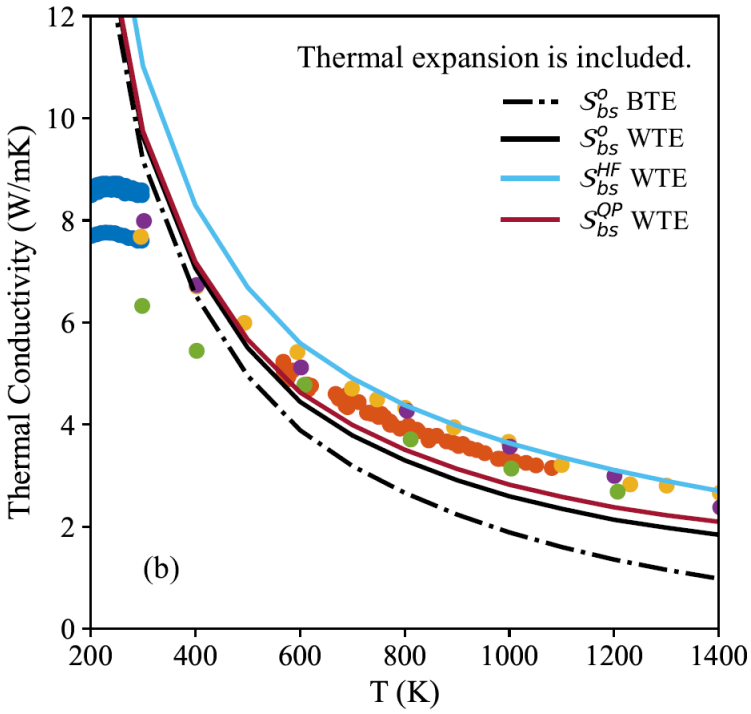


Figure 2: Thermal conductivity computed using GGA + U + SOC (U = 4 eV) and comparing with experiments. Thermal expansion is included. The self-consistent perturbation theory is applied.

B.28 VERA BWR Project

Report Participants

Asgari, Mehdi [1]
1 Oak Ridge National Laboratory

Scientific Achievement

The VERA (Virtual Environment for Reactor Analysis) computing suite was developed under the Consortium for Advanced Simulation of Light Water Reactors (CASL) program to advance the state-of-the-art modeling and simulating of light-water reactors (LWRs). The ability to model pressurized-water reactors (PWRs) using advanced coupled multiphysics computational tools was developed, and results were validated for over 100 cycles of PWRs. Past projects developed and extended the VERA capabilities to boiling-water reactors (BWRs) for analyzing the BWR fleet of reactors operated by Constellation. The capabilities developed have been and are being used by other projects for modeling and simulating BWRs. The results from some of these analyses are being used to compare with Nuclear Regulatory Commission (NRC) codes such as POLARIS/PARCS.

Significance

The VERA suite offers a significantly advanced modeling and simulation capability over existing industry simulation tools. The advanced capability includes detailed multigroup neutron transport for the entire core, detailed subchannel thermal-hydraulic solution over every fuel rod, and detailed pin-by-pin fuel temperature and depletion solutions.

These VERA features should yield substantial improvements over existing industry predictions of modeling void and depletion parameters on a rod-by-rod basis instead of a bundle-average basis and detailed modeling of different bypass flow regions. This enables a more rigorous calculation of within bundle power distribution. This is especially important in the presence of large power gradients, such as what occurs with the insertion of control blades. The feedback of the radial void distribution, particularly at high void, is expected to have a significant impact on calculated results. In addition, it is expected that the elimination of history models in the cross-section generation and inclusion of radial void distribution within bundles will improve eigenvalue and detector predictions.

Key Publications

" Amani Cheniour et al., A Structural Model of the Long-term Degradation of the Concrete Biological Shield , Nuclear Engineering and Design, 2023. " Robert Salko et al., Verification and Validation of the Alternative Nonlinear Two-phase Subchannel (ANTS) Code , Nuclear Engineering and Design, 2023 " Mehdi Asgari et al., Final Summary Report on the Feasibility and the Benefits of the Advanced Nuclear Fuel Pellet Designs with Radially Varying Fuel Zoning and Burnable Poison Concentration , ORNL/TM-2022/2541, Oak Ridge National Laboratory, July 2022 " Mehdi Asgari et al., Assessing UN Neutronic and Fuel Performance for Extended Cycle Lengths , American Nuclear Society Summer meeting, Jun 2023 " Mehdi Asgari et al., Final Report for Modeling and Analysis of Exelon BWRs for Eigenvalue & Thermal Limits Predictability , ORNL/TM-2021/2349, Oak Ridge National Laboratory, December 2021. " A. Graham, et al., Multiscale Thermal Hydraulic Coupling Methods for Boiling Water Reactor Simulation, PHYSOR 2022, Pittsburgh, PA, USA, May 15-20, 2022 " Kyle A. Gamble, et al., Pellet Cladding Mechanical Interaction as a Potential

Failure Mechanism During a Control Rod Drop Accident in a Boiling Water Reactor , PHYSOR 2022, Pittsburgh, PA, USA, May 15-20, 2022 " Sooyoung Choi, et al., Preliminary Simulation Results of Peach Bottom Unit 2 Cycles 1 and 2 with MPACT , PHYSOR 2022, Pittsburgh, PA, USA, May 15-20, 2022 " Chase Lawing, Scott Palmtag, Mehdi Asgari, BWR Progression Problems , ORNL/TM-2020/1792, Oak Ridge National Laboratory, September 2021. " R. Salko, et al., Oak Ridge National Laboratory Summary of CTF Modeling and Numerical Improvements for Boiling Water Reactor Simulation , ORNL/TM-2021/2004, Oak Ridge National Laboratory, April 2021 " Additional publications (including journal papers) are in progress.

Sponsor/Program

VERA is the primary modeling and simulation (M&S) capability for LWRs under the NEAMS program.

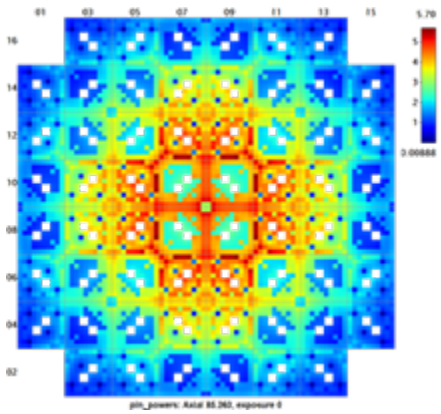


Figure 1: Radial 2D pin powers BWR mini-core.

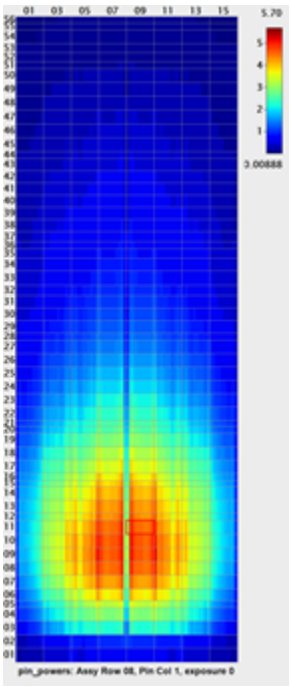


Figure 2: Axial pin powers BWR mini-core.

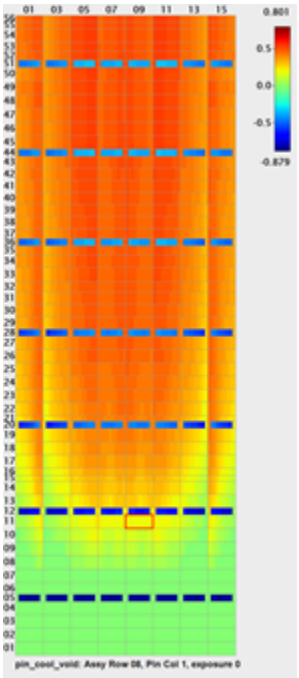


Figure 3: Axial void distribution BWR mini-core.

B.29 Modeling of Fuel Fragmentation in LWR Fuel during a Loss-of-Coolant Accident

Report Participants

Baldwin Oliver, Werner M[1], Brinkley, Walter C[1], Capps, Nathan A[2], Novascone, Stephen R[3], Wirth, B D[1]
1 University of Tennessee Knoxville
2 Oak Ridge National Laboratory
3 Idaho National Laboratory

Scientific Achievement

Fuel fragmentation occurs in fuel pellets in LWRs. Pellet cracking occurs due to thermal stresses during the initial rise to power, and fuel fragmentation can occur during power transients associated with anticipated operational occurrences and design-basis accidents. Oxide fuel is known to form both fragments, which form as the result of large radial and sometimes circumferential cracking, and pulvers, which form as the result of the disintegration of restructured, or partially restructured, fuel. Pulvers can be down to the size of individual grains (less than 1 mm), while fragments are notably larger. Figure 2 shows the fragment size distribution for available loss-of-coolant accident (LOCA) tests performed. During LOCAs, fission gas bubbles within the fuel become overpressurized due to the rapid temperature rise, which results in a high-stress field in the fuel, leading to pulverization. The effects of fuel fragmentation include fission gas release and fuel fragmentation, relocation, and dispersal (FFRD). For an accurate understanding of reactor performance, modeling of fuel fragmentation behavior is necessary. A new model is being developed to model results of fragmentation probability due to bubble overpressure and the thermal elastic stress within the fuel. A companion model will be fit to existing data from LOCA testing of fuel fragment size distribution in order to predict the volume of fuel susceptible to relocation and dispersal. These models will be implemented into the BISON fuel performance code.

Significance

This project aims to develop a high-burnup LWR nuclear fuel modeling capability to implement in the U.S. DOE fuel performance code BISON. The developed capability will enable the accurate and improved understanding of fuel fragmentation behavior, particularly during LOCAs. Notably, calculations of fragmentation probability will result in an improved understanding of the volume of the fuel susceptible to fragmentation and prediction of fission gas release as a result of this fragmentation. The new model to predict fragment size distribution will support understanding of fuel relocation and dispersal, and Figure 1 shows the probability for forming large fragments between 2 and 5 mm as a function of burnup. These models will aid in identifying rod life-limiting factors and understanding of the limits of safe reactor operation. This will culminate in a comparison of the model predictions to experimental data outside the fitting database and a discussion of next steps to improve the modeling of fuel fragmentation, relocation, and dispersal.

Key Publications

Capps, N., Aagesen, L., Andersson, D., Baldwin, O., Brinkley, W. C., Cooper, M. W. D., Harp, J., Novascone, S., Simon, P.-C. A., Matthews, C., & Wirth, B. D. (2023). Empirical and mechanistic transient fission gas release model for high-burnup loca conditions. Journal of Nuclear Materials,

584, 154557. https://doi.org/10.1016/j.jnucmat.2023.154557

Sponsor/Program

Nuclear Energy University Program Project DE-NE0009220

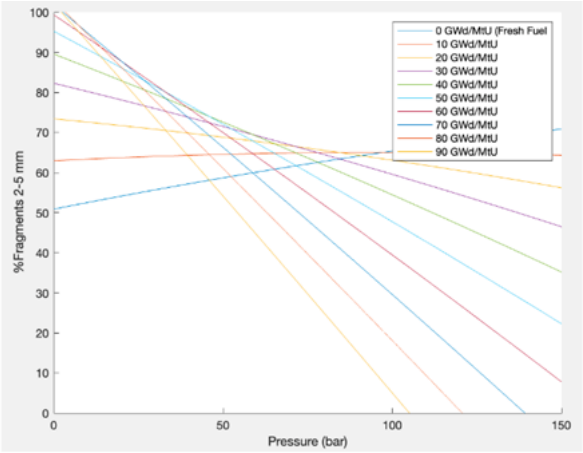


Figure 1: Preliminary fit for fraction of 2–5 mm fuel pellet fragments post-LOCA as a function of burnup.

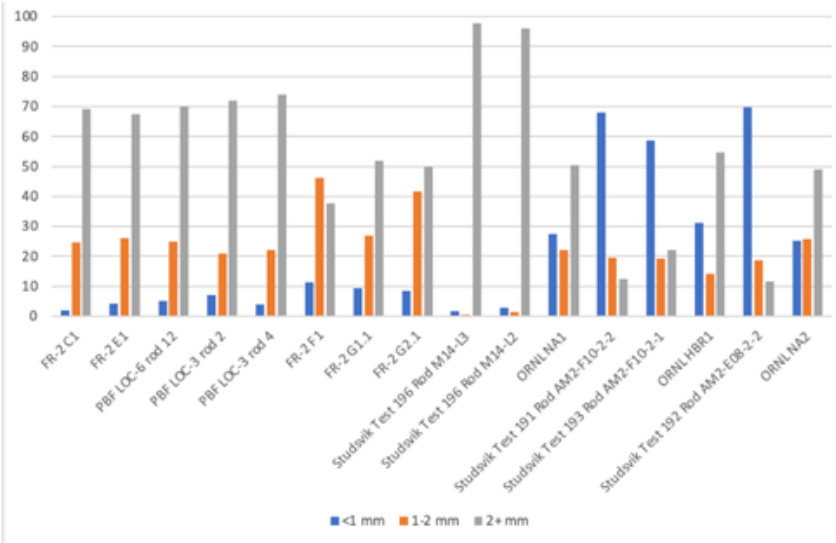


Figure 2: Existing fuel fragment size distribution data from LOCA testing.

B.30 Validation and Verification of RELAP5-3D Model of Molten-Lead Systems

Report Participants

Barthle, Jonathan L[1]
1 University of Tennessee Knoxville

Scientific Achievement

The goal of this project is to develop a complex RELAP5-3D model of an existing molten-lead system. This system was the Lobo Lead Loop Facility located at the University of New Mexico (UNM) (see Figure 1). RELAP5-3D has strong potential to be used in modeling molten-lead systems for advanced reactors (i.e., lead fast reactors) or fusion systems (dual coolant lead lithium blankets). However, validation and verification still needs to be done to ensure RELAP5-3D can accurately model these types of systems. Therefore, there has been an effort to model existing molten-lead systems to begin this process. This modeling of existing facilities is essential since it can be expensive and difficult to design new systems.

Significance

So far, a complex model of the Lobo Lead Loop has been developed in RELAP5-3D. The model continues to be improved upon to more accurately reflect the actual facility. Steps towards verifying the model have also begun. Code-to-code verification has been done with the computational fluid dynamics model of the loop developed by UNM. The pressure drop across the specimen holder region was calculated in RELAP5-3D and compared to the pressure drop calculated in CFD (see [1]) at various flow velocities. Figure 2 depicts the comparison of the pressure drops computed by both models, showing reasonable agreement between RELAP5-3D and CFD. The specimen holder region is important because there is an abrupt contraction in flow area, contributing to a large local pressure drop. In addition, a hypothetical loss-of-flow accident (LOFA) transient was imposed on the RELAP5-3D model to demonstrate the potential for the Lobo Lead Loop to do a similar experiment. Figure 3 illustrates the temperature in each major component during the transient. This provides an opportunity for potential experimental data for validation. Continued verification is currently being done with higher lead temperatures to observe effects of the pressure drop calculations. Validation studies are also planned once experimental data is obtained from UNM.

Key Publications

J. L. Barthle, G. I. Maldonado, N. R. Brown. 2023. Validation and Verification of a RELAP5-3D Model of the Lobo Lead Loop. 2023 ANS Annual Meeting

[1] K. Talaat, et al. 2021. Design of Specimen Holders for Flow Accelerated Corrosion Experiments in Molten Lead with Numerical Evaluation of Pressure Losses. Nuclear Engineering and Design 385

Sponsor/Program

Office of Fusion Energy Sciences under contract No. DE-SC0022308

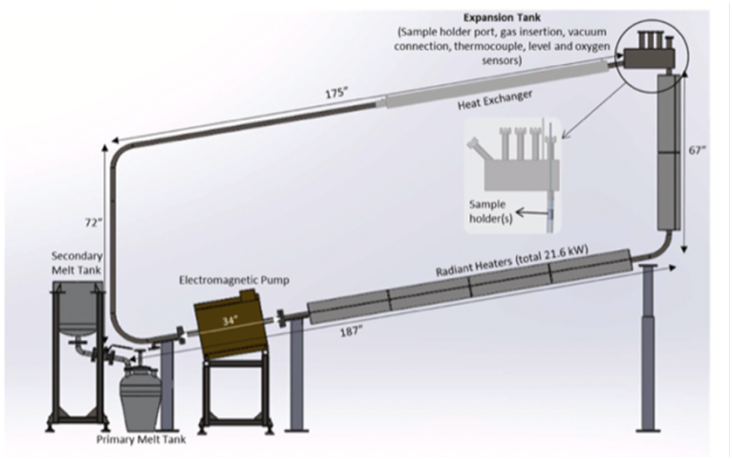


Figure 1: Diagram of the Lobo Lead Loop Facility [1].

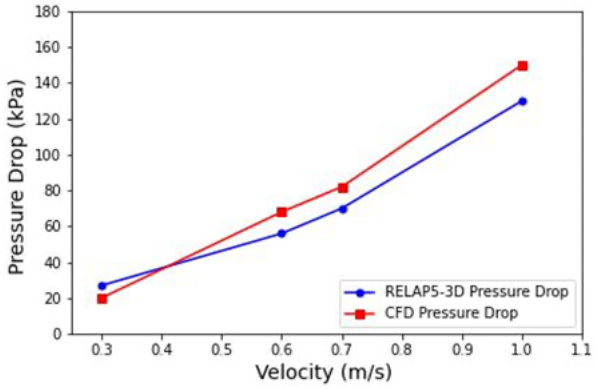


Figure 2: Comparison of pressure drop calculations between RELAP5-3D and CFD [1] in specimen holder.

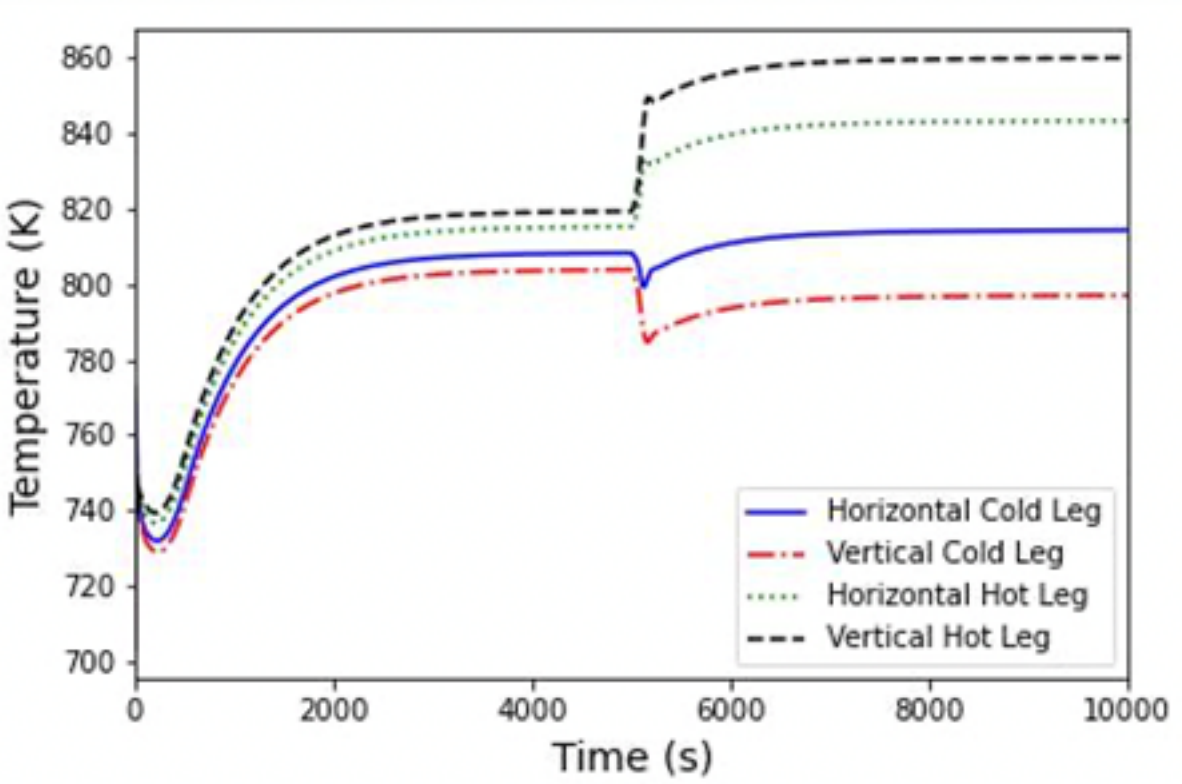


Figure 3: Hypothetical LOFA transient in RELAP5-3D model of loop.

B.31 CFD Modeling and Simulation of MARVEL Core Coolant Thermal Hydraulic Behavior

Report Participants

Biswas, Sutapa [1], Arafat, Yasir [2], Yoon, SuJong [2], Ali, Amir F[1]
1 Idaho State University
2 Idaho National Laboratory

Scientific Achievement

The project objective is to develop a CFD model temperature and fluid velocity distribution for the primary and secondary coolant behavior of MARVEL core using StarCCM+. The core circulates metal coolant using natural convection. This is a eutectic mixture of sodium-potassium (NaK) as the primary coolant and lead bismuth (LBE) as the secondary coolant. The MARVEL reactor thermal hydraulic core behavior has been investigated using RELAP5-3D. Though the results provided by RELAP5-3D convey significant information about the natural circulative and heat transfer capabilities of the MARVEL reactor core, flaws such as hot spots, dead circulative zones, and circulatory instabilities caused by geometrical primary coolant system (PCS) components are not detected. Traditional CFD software can provide a detailed description of the flow pattern and highlight potential locations for improvement to the current MARVEL PCS design in a 3D model analysis. Since the core is symmetric, to minimize the complexities, only of the core was modeled by using the boundary conditions provided by RELAP5-3D generated report. The geometrical flow domain and solid structure of the model of the core cooling system were generated in SolidWorks, then imported into StarCCM+ and sectionalized into following individual regions: argon cover gas, SCS intermediate heat exchanger wall, LBE fluid, NaK fluid, plenum wall, and Stirling Engine dome and tubes. Various sensitivity tests of mesh structure were also performed. Recent findings on LBE fluid leading to polonium formation has redirected the project in a different direction, where the usage and functionality of Galinstan (a eutectic mixture of alloy constituting gallium [Ga], indium [In], and tin [Sn]) as a secondary coolant being investigated to potentially replace LBE.

Significance

Improving MARVEL PCS geometrical design can lead to more robust designs for microreactor and small modular reactor (SMR) technologies. Additionally, a full understanding of natural circulation of the coolant flow in a nuclear reactor can pave the way for new features to be added. Some new potential features include scaling up MARVEL for commercial use.

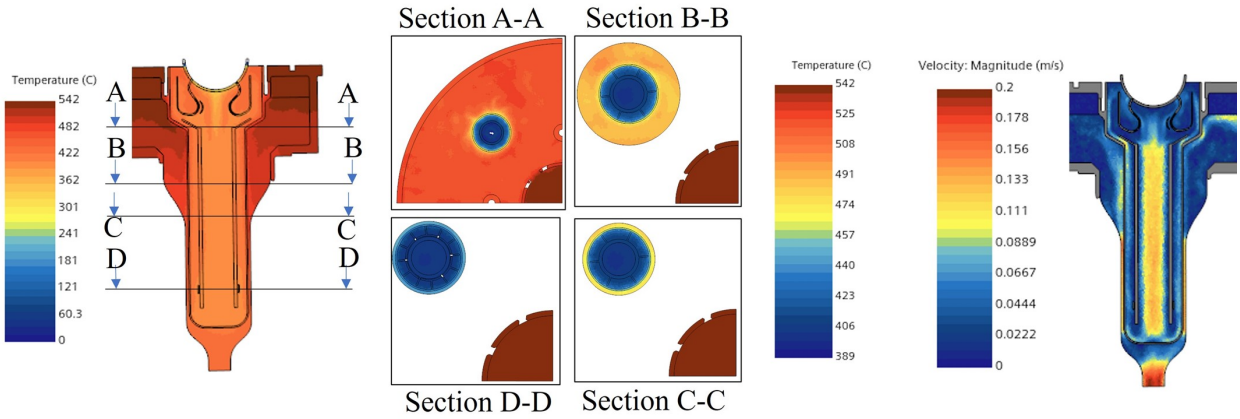
Key Publications

In progress; Understanding the impacts of seconday coolant on MARVEL Thermal-Hydraulic peformance (Paper is considered for submission to Annals of Nuclear Energy Journal)

Sponsor/Program

The ongoing research is funded through multiple CAES/INL awards in collaboration with Dr. Yassir Arafat, who originally sponsored our access to the HPC resources.
Dr. Arafat also serves as a thesis committee member at ISU and recently, Dr. Yoon has been added

to the committee.



B.32 Hybrid Model for Simulating Fission Gas in Uranium Oxide Nuclear Fuel

Report Participants

Blondel, Sophie [1], Kong, Fande [2], Biswas, Sudipta [2], Muntaha, Md A[3], Chatterjee, Sourav [3]
1 University of Tennessee
2 Idaho National Laboratory
3 University of Florida

Scientific Achievement

The objective of this project is to significantly advance the mechanistic understanding of fission gas behavior and release in UO2 nuclear fuel by developing a mesoscale simulator that takes advantage of leadership-class computers. Fission gas release within UO2 nuclear fuel occurs as gas atoms diffuse through grains and arrive at grain boundary (GB) bubbles; these GB bubbles grow and interconnect with grain edge bubbles; and grain edge tunnels grow and connect to free surfaces. In this approach, fission gas production, diffusion, clustering to form intragranular bubbles, and re-solution within grains are included using spatially resolved cluster dynamics in the Xolotl code. GB migration and intergranular bubble growth and coalescence are included using the phase field method in the MARMOT code. This hybrid model couples Xolotl to MARMOT using the MultiApp and Transfer systems in the MOOSE framework, with Xolotl passing the arrival rate of gas atoms at GBs and intergranular bubble surfaces to MARMOT and MARMOT passing evolved GBs and surface positions to Xolotl.

Significance

A strong scaling study was performed on four cases ranging from 10 to 100 grains in 3D. Each simulation was run for 50 timestep of 5 s each at 1800 K. Three different times were recorded at the end of the simulation: the total time, the “Xolotl" time representing the amount of time taken to run the multiApp part of the simulation (i.e., the intragranular part), and the “MARMOT" time taken to solve the intergranular part with the phase field model. The general trend is a departure from the ideal scaling when a larger number of MPI processes are used, with Xolotl performing less well than the phase field model. When the GrainTracker utility is used (50 and 100 grains), it seems that the phase field performs better than the ideal scaling. With 10 grains, the Xolotl component takes more time than the phase field, but this behavior is reversed with increasing number of grains included in the simulation. Additionally, we looked at how the problem scaled with a constant number of MPI processes, for 80, 120, and 160 Sawtooth nodes (each 48 processors). Due to the difference in computational techniques, each subcomponent (phase field, cluster dynamics) should scale in different ways as the problem size increases. Xolotl should scale with the total number of grid points composing the 3D mesh, while the phase field time should increase with the number of non-linear degrees of freedom (DOF) that takes into account both the number of mesh elements and the number of coupled variable to model the grains. Figure 2 shows the scaling for each of these subcomponents, where the dashed lines represent the ideal scaling taking the smallest size case run on the given number of nodes as reference. The phase field performs as expected while the cluster dynamic part seems to be a little faster than the total number of grid points scaling.

Key Publications

S. Blondel, D. Andersson, D. Bernholdt, S. Biswas, S. Chatterjee, P. Fackler, D.-U. Kim, F. Kong, M. A. Muntaha, M. Tonks, and B. Wirth. 2022. Coupling the phase field method and spatially resolved cluster dynamics to model fission gas behavior in UO2 Invited presentation at the NuMat 2022 Conference, Ghent, Belgium, October 24-28

Sponsor/Program

DOE Scientific Discovery through Advanced Computing (SciDAC) Program

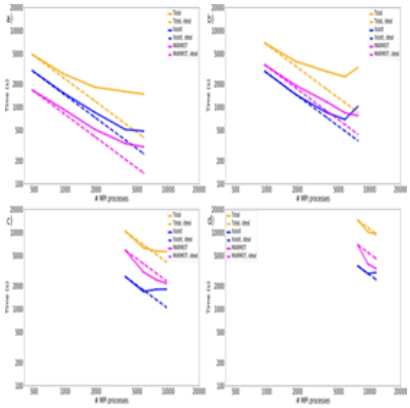


Figure 1: Strong scaling study for (a) 10 , (b) 20 , (c) 50 , and (d) 100 grains. For each case, the total time (orange), Xolotl time (blue), and MARMOT time (magenta) were recorded. The dashed lines represent the ideal scaling. The X and Y axis are the same for all four subfigures.

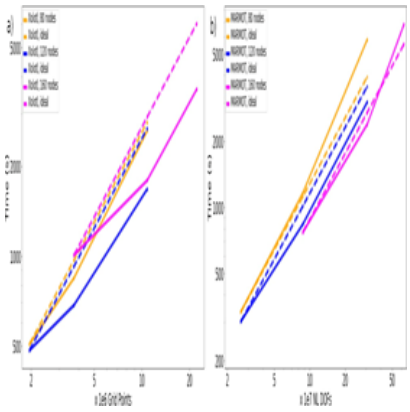


Figure 2: (a) Time taken by the Xolotl component as a function of total number of grid points and (b) time taken by the MARMOT component as a function of the number of non-linear DOF. Each color represents a constant number of HPC nodes; the dashed lines represent ideal scaling.

B.33 NEAMS—Shift and Griffin Development for LWR and Advanced Reactors

Report Participants

Bostelmann, Friederike [1], Pandya, Tara M[1], Ghaddar, T [1], Britt, Philip S[1], Johnson, S [1], Jessee, Matthew A[1]
1 Oak Ridge National Laboratory

Scientific Achievement

We have developed several TRISO-fueled reactor models for the Shift Monte Carlo code. Using these models, we performed a thorough runtime and memory performance assessment that eventually led to the addition of capabilities that enable user-friendly modeling options and dramatically improved the runtime for such double-heterogeneous models. This effort was conducted in preparation of the generation of multigroup cross sections for these types of reactors with Shift for Griffin.

Significance

This work will benefit NEAMS by expanding the capabilities of the NEAMS software suite, Shift and Griffin, as applied to LWR and advanced reactor multiphysics analysis. Comparisons of results from Griffin using Shift-generated cross sections and Serpent-generated cross sections serve as verification and validation.

Key Publications

Pandya, T., Bostelmann, F., Jessee, M., Ghaddar, T., Britt, P., Johnson, S. (2021). Modeling, Performance Assessment, and Nodal Data Analysis of TRISO-Fueled Systems with Shift. Oak Ridge National Laboratory Report ORNL/TM-2022/2601. https://info.ornl.gov/sites/publications/Files/Pub183158.pdf

Sponsor/Program

NEAMS

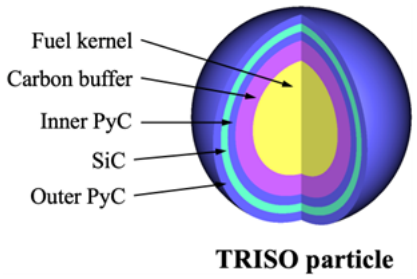


Figure 1: TRISO fuel particle.

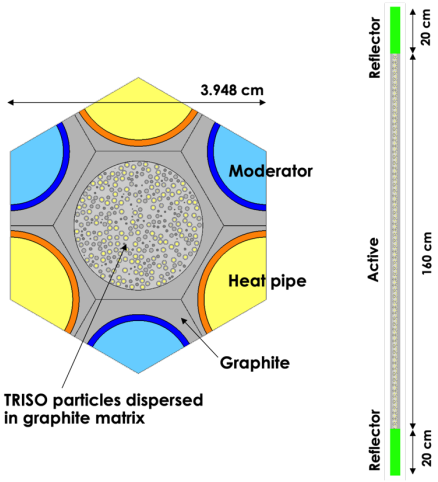


Figure 2: Heat-pipe reactor unit cell.

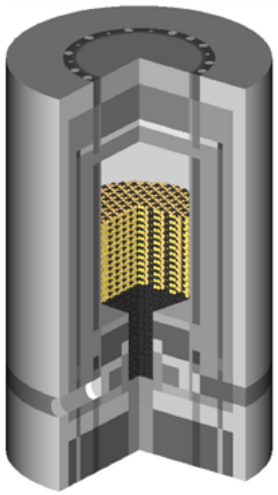


Figure 3: HTR-10.

B.34 Modeling High-Burnup LWR fuel under Normal Operating and Transient Conditions

Report Participants

Brinkley, Walter C[1], Baldwin, Oliver W[1], Capps, Nathan A[2], Novascone, Stephen R[3], Wirth, B D[1]
1 University of Tennessee Knoxville
2 Oak Ridge National Laboratory
3 Idaho National Laboratory

Scientific Achievement

The microstructure of uranium dioxide fuel changes with increasing burnup. Characterizing this restructuring remains a key challenge in developing modeling capabilities for high-burnup fuel. The formation of high-burnup structures (HBSs) is of particular interest because it is an overarching descriptor for the microstructural characteristics of a fuel pellet. Radially resolved pellet data from post-irradiation examination detailing fuel porosity, grain boundary characteristics (including grain size and misorientation angle), fuel fragmentation, and fission gas release has been obtained. This data will be used to develop semiempirical models predicting microstructural characteristics from a reactor power history. These microstructural parameters will be used to describe a total HBS fraction. These models will be implemented into BISON for modeling microstructurally dependent parameters in a fuel performance environment.

Significance

This project aims to develop a high-burnup LWR nuclear fuel modeling capability to implement in the U.S. DOE fuel performance code BISON, in order to provide a high impact in terms of informing the safety case and supporting the extension of burnup limits currently pursued by the U.S. nuclear industry. The developed capability will enable the accurate simulation and improved understanding of high-burnup fuel rod behavior during both normal reactor operation and transients associated with design-basis accidents (DBAs), such as loss-of-coolant accidents (LOCA) and reactivity-initiated accidents (RIAs). In particular, work modeling fuel restructuring will result in the ability to estimate the quantity of fuel susceptible to fragmentation and dispersal, fission gas release (FGR) and rod internal pressure, to ultimately identify the rod life-limiting factors and define the boundaries of safe operation. For this purpose, empirical and mechanistic engineering models will be developed for key phenomena controlling high-burnup fuel performance under normal operating and transient conditions. The focus will be on modeling the evolution and characteristics of the HBS, fuel fragmentation and pulverization (collectively referred to as high-burnup fuel fragmentation) during DBA transients, and FGR resulting from fuel fragmentation and transient responses.

Key Publications

Capps, N., Aagesen, L., Andersson, D., Baldwin, O., Brinkley, W. C., Cooper, M. W. D., Harp, J., Novascone, S., Simon, P.-C. A., Matthews, C., & Wirth, B. D. (2023). Empirical and mechanistic transient fission gas release model for high-burnup loca conditions. Journal of Nuclear Materials, 584, 154557. https://doi.org/10.1016/j.jnucmat.2023.154557

Sponsor/Program

NEUP Project DE-NE0009220

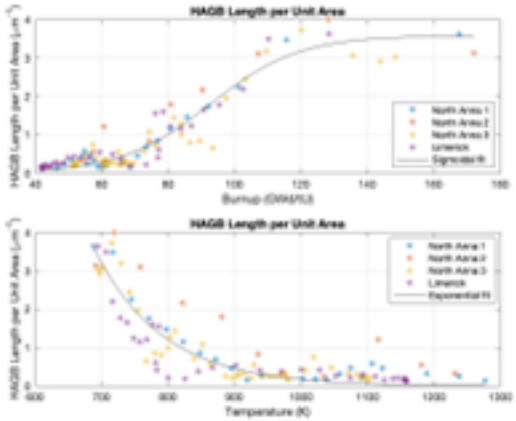


Figure 1: Preliminary fits of high-angle grain boundary data as functions of temperature and burnup (data from C. McKinney et al., J. Nucl. Mater. 585 (2023)).

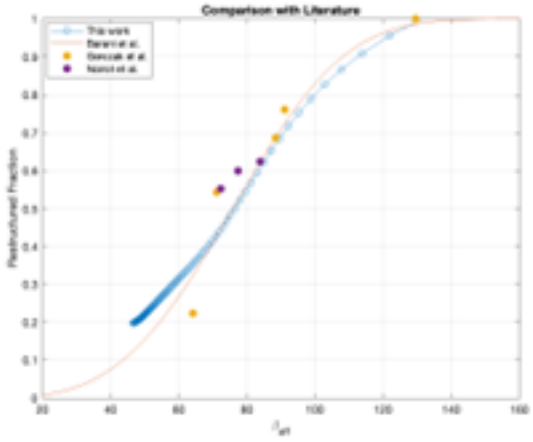


Figure 2: Comparison of a preliminary prediction of total restructured fraction with literature data and a model from T. Barani et al., J. Nucl. Mater. 539 (2020).

B.35 FIVSIM-Integration of Industry Techniques into a Fluid-Structure Interaction Simulation Tool

Report Participants

Brockmeyer, Landon M[1]
1 Argonne National Laboratory

Scientific Achievement

We are updating the existing coupled Nek5000-Diablo fluid-structure interaction simulation tool to suit industry pursuits. The new code, FIVSIM, is built from the research code Nek5000-Diablo, to leverage the existing high-fidelity research code to inform lower fidelity and computationally more efficient simulations. Increasing usability and portability is another significant goal of the project. To this effect, Nek5000 will be replaced with Cardinal, the MOOSE wrapper for Nek5000, so that the coupling can be handled by MOOSE. We have conducted Reynolds-Averaged Navier-Stokes (RANS) vs. large eddy simulation (LES) (industry methods vs. high-fidelity research methods) initial simulations on a simple nuclear fuel spacer grid geometry.

Significance

Flow-induced vibrations remain a significant failure mechanism for fuel rods in the nuclear reactor core and for the tubes in steam generators used in both nuclear and conventional power plants. Failures in either case lead to significantly higher plant operating costs. Even though flow-induced vibrations have been studied for a long time and empirical formulations are available for use in the nuclear industry, the underlining mechanisms for the onset of rod and tube instability when subjected to complex flow and boundary conditions remain unanswered. Understanding the particular set of thermal, mechanical, flow, and radiation conditions to which a fuel assembly is subjected and how the fuel assembly responds dynamically to those conditions is important in operational safety margin assessments, and in particular, in determining the risk of excessive wear. It will also enable further design exploration that can lead to better, safer, and more economical designs. The ongoing development of FIVSIM aims to produce a tool capable of simulation flow-induced vibration for geometries appreciable to industry. Existing fluid-structure interaction codes lack either the scalability necessary or the computational efficiency to simulate fuel rod spacer grid bundles. The current project is on pace to simulate a 5×5 fuel assembly in the coming year and even larger geometries thereafter.

Key Publications

Accepted conference publication: Brockmeyer, L., Saini, N., Tentner, A., Merzari, E. (2023). Evaluation of RANS vs. LES Simulation of Fluid Flow through 3x3 Rod Bundle with a Simple Spacer Grid as a Precursor to Coupled Fluid-Structure Interaction Simulations. 20th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (Nureth-20)

Sponsor/Program

NEAMS

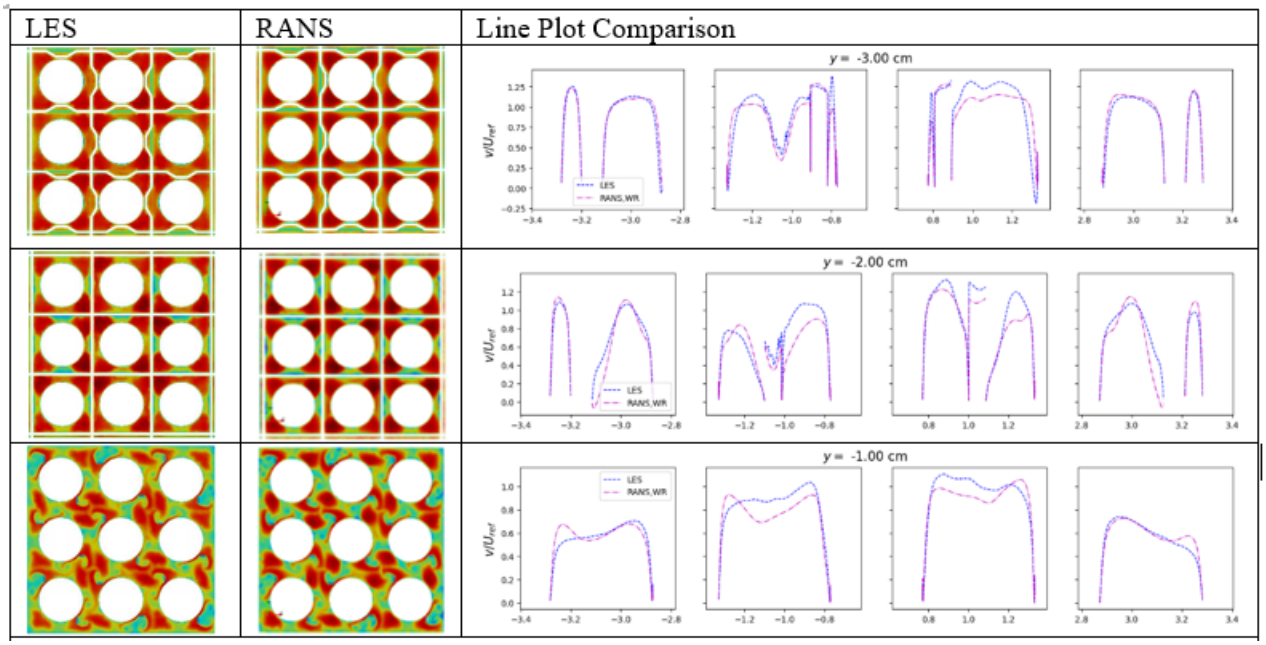


Figure 1: Column 1: LES axial slice of mean axial velocity at position specified on line plot. Column 2: RANS axial slice of mean axial velocity at position specified on line plot. Column 3: Line plot of mean axial velocity. Line horizontally across the axial slice (as shown on the first LES axial slice image). The single line plot is broken into four distinct curves as it passes through three pins. The black dotted line shows the results for wall-resolved RANS, and the blue dotted line shows the results for LES. Y = 0 is at the outlet of the spacer grid, just past the tips of the mixing vanes.

B.36 Multiphysics Coupling Analysis for Microreactor KRUSTY

Report Participants

Cao, Yan [1], Miao, Yinbin [1], Stauff, Nicolas [1]
1 Argonne National Laboratory

Scientific Achievement

Validation of the advanced numerical tools with experimental data is a crucial step for future applications of NEAMS high-fidelity tools to actual problems. In particular, the DOE-NE NEAMS Multiphysics Applications Microreactor team leverages the existing and developing NEAMS tools to model different microreactor concepts and assess these tools to ensure their capabilities can be used by the industry and DOE programs. The Kilowatt Reactor Using Stirling TechnologY (KRUSTY) is a microreactor recently designed, built and tested for space nuclear applications. Its steady-state and transient testing provided plentiful experimental data for validating multiphysics microreactor tools.

Significance

A steady-state multiphysics model, which couples Griffin for neutronics calculations, BISON for thermal mechanics, and Sockeye for heat transfer through the heat pipes, was developed in FY-22 based on initial work performed at LANL. In FY-23, the multiphysics model was significantly improved. The Griffin neutronics model was modified to follow the bechmark specifications in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) 2021 Handbook. The MOOSE mesh generator system has been tested extensively and deployed successfully to create the mesh shown in Figure 1. A new multiphysics steady-state model has been obtained using the new KRUSTY mesh model leveraging the computer resources available on the INL HPC cluster. Single neutronic calculations demonstrated that Griffin can be used to perform full core calculations using the most recent DFEM-SN solver with a CMFD acceleration technique. Multiphysics-coupled transient simulations will be performed to compare numerical simulation results with transient experiments.

Key Publications

Stauff, Nicolas E., Abdelhameed, Ahmed, Cao, Yan, Kristina, None, Miao, Yinbin, Mo, Kun, & Nunez, Daniel. Multiphysics Analysis of Load Following and Safety Transients for MicroReactors. ANL/NEAMS-22/1, September 2022, United States. https://doi.org/10.2172/1891258

Sponsor/Program

DOE-NE/NEAMS

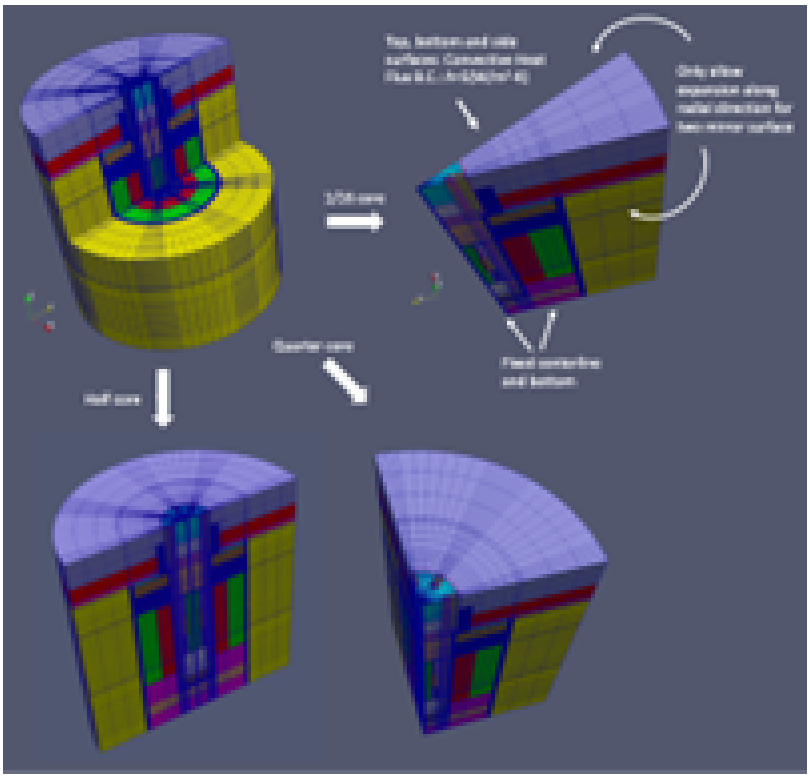


Figure 1: KRUSTY mesh generated by the MOOSE mesh generator system.

B.37 LOWE Fuel Transition Accident Safety Analysis

Report Participants

Burke, James M[1], Harroff, Brandon H[1], Brown, Curtis A[1], Hardtmayer, Douglas E[1]
1 MPR Associates

Scientific Achievement

To support developing the U-10Mo monolithic fuel concept and the design of ATR's low-enriched uranium (LEU) fuel element, LOWE, irradiation tests are planned with full-sized LOWE elements in ATR core driver positions. These tests are referred to as an element test (ET). Following the ETs, ATR will be qualified for unrestricted use of LOWE in ATR, allowing LOWE fuel elements to be used in any position and quantity in ATR. Addendums to the ATR safety analysis report (SAR) are being prepared to allow LOWE insertion for ET-3 and unrestricted LOWE operation. Accident analyses of LOWE in an otherwise highly enriched uranium (HEU) core are required to support SAR addendum development. Two postulated accidents are analyzed. First is the reflector block movement accident (RBMA), which occurs when an aging reflector block or its supports fail, allowing the beryllium reflector block to reposition towards the fuel elements, resulting in a reactivity insertion. Second is the slow power increase where the core power rises uncontrollably until the reactor scrams on total core power.

Significance

Currently, the ATR SAR includes the RBMA within a group of accidents that would result in reactivity and power distribution anomalies. These accidents are bounded by a hypothetical fault $0.50 step insertion. Figure 1 and Figure 2 show how Water Channel 20 was replaced with a beryllium reflector material to replicate a RBMA. Results from the RBMA found that, when using LOWE under the current lobe power limit, the accident caused a reactivity insertion less than $0.50. The slow power increase is still being analyzed, but once complete, the peak power densities and half plate power result in the accident will be compared to the allowable fuel limits.

Key Publications

MPR Associates. 2022. MPR Calculation 1129-0280-CALC-001, Rev. 0 MPR Associates. 2023. MPR Calculation 1129-0279-CALC-003, Rev. 0 (in progress)

Sponsor/Program

ATR
USHPRR Program

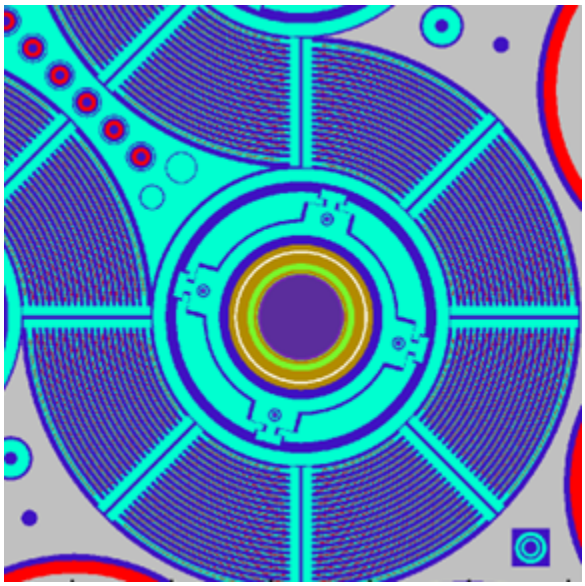


Figure 1: Standard ATR core.

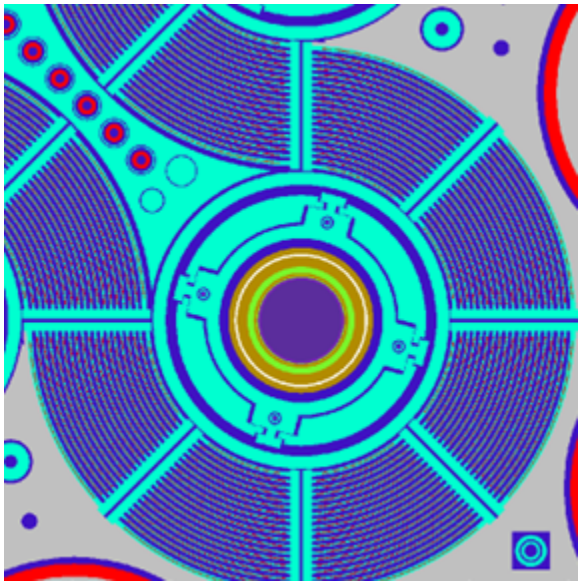


Figure 2: RBMA ATR core.

B.38 Revealing Hidden Defects through Stored Energy Measurements of Radiation Damage

Report Participants

Hirst, Charles [1], Kombaiah, Boopathy [2], Cao, Penghui [1], Middlemas, Scott [2], Kemp, R [1], Li, Ju [1], Short, Michael [1]
1 Massachusetts Institute of Technology
2 Idaho National Laboratory

Scientific Achievement

With full knowledge of a material's atomistic structure, it is possible to predict any macroscopic property of interest. In practice, this is hindered by limitations of the chosen characterization techniques. For example, electron microscopy is unable to detect the smallest and most numerous defects in irradiated materials. Instead of spatial characterization, we propose detecting and quantifying defects through their excess energy. Differential scanning calorimetry of irradiated Ti measures defect densities five× greater than those determined using transmission electron microscopy. Our experiments also reveal two energetically distinct processes where the established annealing model predicts one. Molecular dynamics simulations discover the defects responsible and inform a new mechanism for the recovery of irradiation-induced defects. The combination of annealing experiments and simulations can reveal defects hidden to other characterization techniques and has the potential to uncover new mechanisms behind the evolution of defects in materials.

Significance

We demonstrate in our recent study (Science advances 8.31 (2022): eabn2733) that radiation damage can be quantified. Instead of spatial characterization, defects can be identified and quantified through their excess energy. Fundamentally, all defects in a material contribute to its energetic structure, and therefore, all defects can be detected through changes in their population. Crucially, annealing experiments can be directly compared to MD simulations to gain insight into the defect reactions occurring. This also has the potential to experimentally validate atomistic simulations, thereby answering the key question that exists for all simulated observations. In conclusion, exploring microstructure through the lens of stored energy can be applied to the whole spectrum of material systems, can reveal defects unable to be detected by other characterization techniques, and can uncover new mechanisms behind the evolution of defects.

Key Publications

Hirst, C. A., Granberg, F., Kombaiah, B., Cao, P., Middlemas, S., Kemp, R. S., ... & Short, M. P. (2022). Revealing hidden defects through stored energy measurements of radiation damage. Science advances, 8(31), eabn2733. https://www.science.org/doi/10.1126/sciadv.abn2733

Sponsor/Program

NEAMS, NSUF

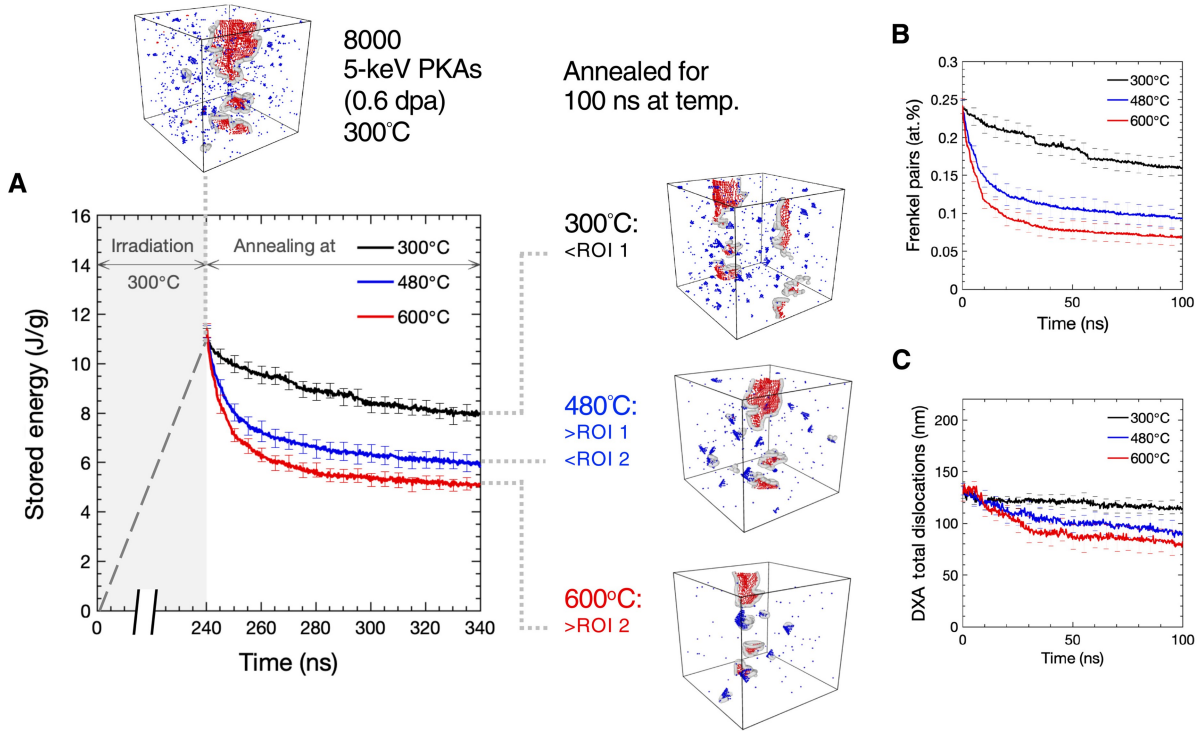


Figure 1: Simulations of 8,000 primary knock-on atom cascades generate defected microstructures. These are then annealed for 100 ns at 300, 480, or 600°C to determine the energy release (A) and the defects remaining. WS and DXA analyses show the defects as a function of time, with (B) a large decrease in the point defect concentration and (C) a minimal decrease in the total dislocation length. All data shown are means of 10 independent simulations, and the errors bars are SE. dpa, displacements per atom; at.atomic .

B.39 Multiphysics Coupling of Griffin and SAM for MSR Simulation

Report Participants

Fei, Tingzhou [1], Cao, Yan [1]
1 Argonne National Laboratory

Scientific Achievement

Validation of the advanced tools developed under the NEAMS program is essential for adopting these tools to solve real-world problems. Among many nuclear reactor designs, the MSR is unique in using flowing fuel. This results in a tightly coupled system between thermal hydraulics and neutronics, which makes the NEAMS multiphysics tool a perfect candidate for simulating the MSR behavior. However, it is also necessary to validate the newly developed tools. This can only be achieved through benchmarking and validating against experimental data. The Molten Salt Reactor Experiment (MSRE) data are employed for this purpose. This is an essential step to demonstrate the accuracy and capability of the NEAMS tools for MSR applications.

Significance

The objective of the work is to demonstrate the capability of the NEAMS tools for MSR applications and to validate the NEAMS tool by benchmarking against MSRE data to give more confidence to the potential users. The work is still on going. Previous efforts have focused on demonstrating the multiphysics capability for the MSR system. One of the MSRE zero-power tests (pump startup test) was also investigated using the Griffin-SAM coupling approach. Different modeling approaches were adopted, including simple one-way coupling with the lattice fuel model, simple two-way coupling with the lattice fuel model, and coupling with the full core model. Through these works, several coupling approaches have been developed for simulating the MSR thermal hydraulic and neutronics behavior. The preliminary results are shown in Figure 1. It should be emphasized that the work is ongoing to improve results.

Key Publications

Fei, T., Shahbazi, S., Fang, J., & Shaver, D.. Validation of NEAMS Tools Using MSRE Data. United States. https://doi.org/10.2172/1880993

Sponsor/Program

NEAMS

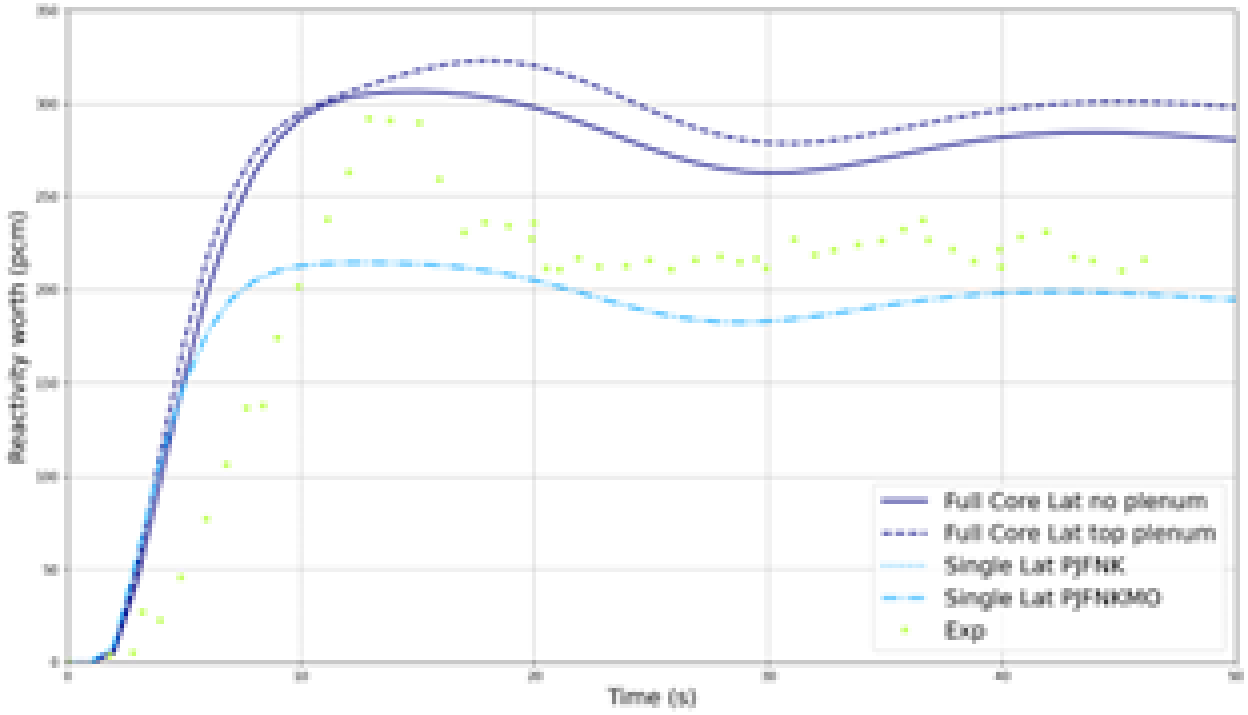


Figure 1: Pump startup simulation results compared to experimental data.

B.40 Full-Core LOCA Safety Analysis for a PWR Containing High-Burnup Fuel

Report Participants

Capps, Nathan A[1], Wysocki, Aaron J[1], Godfrey, Andrew T[1], Collins, Benjamin S[1]
1 Oak Ridge National Laboratory

Scientific Achievement

The objective of this work is to inform the high-burnup LOCA safety case for a core containing high-burnup fuel to help accelerate the nuclear industry's goals to extend cycle lengths to 24 months and increase peak rod average burnup to 75 GWd/MTU. Codes used to complete this work were BISON, VERA, and RELAP5-3D

Significance

VERA results identified the location and operating conditions of high-burnup fuel rods throughout the core. These conditions were in line with high-burnup depletion analyses. Best-estimate thermal hydraulic analyses indicated that high-burnup fuel would experience a peak cladding temperature (PCT) of 656°C. Additionally, a thermal hydraulic analysis was performed on a once-burned fuel rod, with the highest EOC LHR serving as a bounding condition. The thermal hydraulic analysis results were consistent with the literature. BISON evaluated the fuel rod performance prior to and during a LOCA. These results were used to calculate the total amount of fuel susceptible to pulverization throughout the core. The analysis was performed for a best estimate as well as for the highest temperature observed in the core. Best-estimate BISON results coupled with RELAP TH results identified cladding bursts in full-length commercial fuel rods are likely to occur at higher temperatures than burst conditions observed in the 12 inch cladding burst test. BISON did not predict cladding burst in high-burnup fuel rods, and as a result, cladding burst results for the highest power fuel rod was used to calculate the size of the cladding balloon. BISON results indicated that 106 kg of fuel will be susceptible to pulverization, while experimental cladding balloon data suggest 43–65 kg of fuel will pulverize. In an attempt to quantify the worst-case scenario, BISON evaluated pulverization susceptibility in high-burnup fuel rods using the RELAP cladding temperature for the highest power fuel rod in the core. The results indicated 182 kg of fuel would pulverize.

Key Publications

Nathan Capps, Aaron Wysocki, Andrew Godfrey, Benjamin Collins, Ryan Sweet, Nicholas Brown, Soon Lee, Nicholas Szewczyk, Susan Hoxie-Key, Full core LOCA safety analysis for a PWR containing high burnup fuel, Nuclear Engineering and Design, Volume 379, 2021, 111194, ISSN 0029-5493, https://doi.org/10.1016/j.nucengdes.2021.111194.

Sponsor/Program

NEAMS

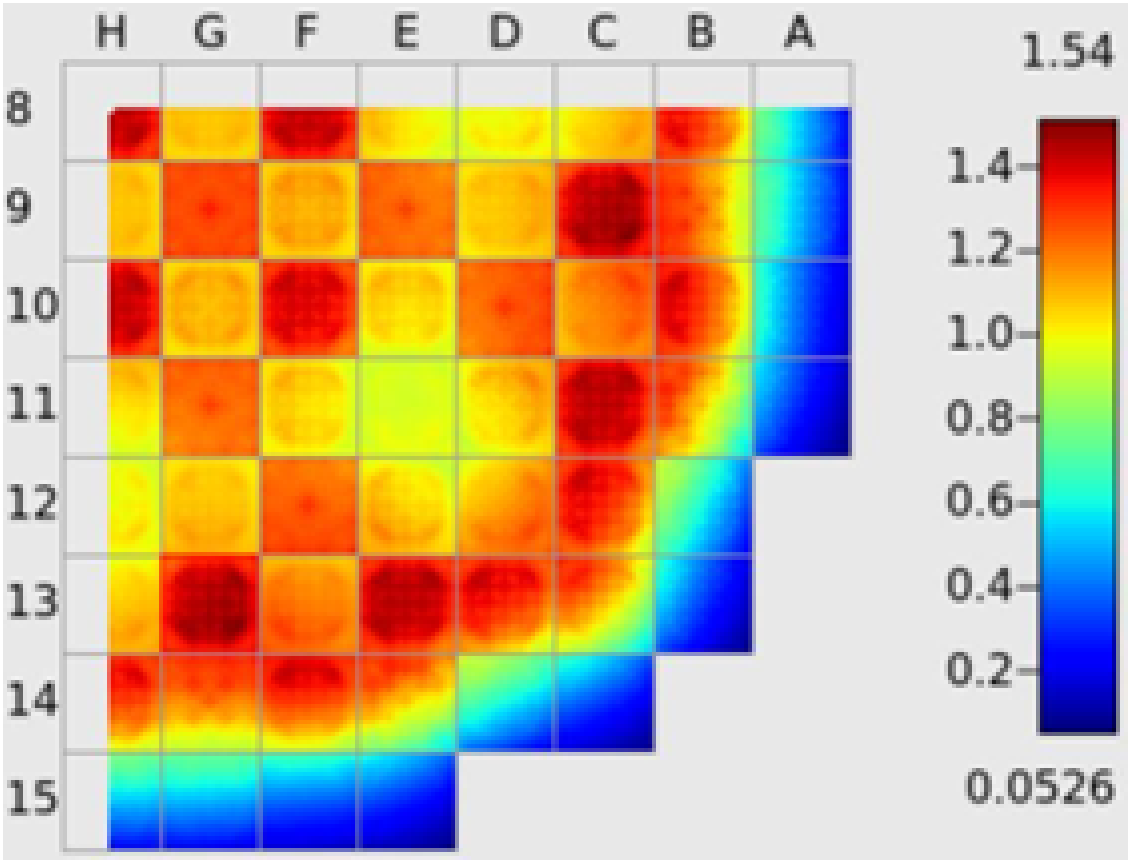


Figure 1: Radial rod-wise power distribution at the burnup where maximum Fdelta H occurs.

B.41 Machine-Learning Treatment of Pebble-Wise Cross Sections in Pebble-Tracking Transport Algorithm

Report Participants

Carlson, Liam N[1], Ragusa, Jean C[1], Balestra, Paolo [2]
1 Texas A&M University
2 Idaho National Laboratory

Scientific Achievement

Traditional neutronics calculations of PBRs, such as those used in codes like the Very Old Computer Program, rely on the homogenization of microscopic cross sections over regions called spectral zones. Since cross sections for pebbles of varying temperature and burnup are averaged over a region, there is a great deal of local information lost in a whole-core calculation that must be reconstructed using additional models to calculate peaking factors. The pebble-tracking transport (PTT) method in Griffin allows for a high-fidelity deterministic modeling of a PBR core by treating the pebble centers as nodes in an unstructured tetrahedral mesh. In PTT, macroscopic cross sections must be supplied for pebbles. These cross sections are currently being generated in Serpent using INL's HPC resources. It is very costly to generate new cross sections as pebbles change positions, burnup, and temperature during normal operation, so we are investigating the implementation of machine-learning algorithms to provide pebble cross sections for PTT simulations.

Significance

Several capabilities have been added to Griffin due to this research. Previously, the PTT algorithm has only been able to assign cross sections to pebbles within the same region or block. Now, cross sections may be assigned to groups of pebbles that share similar characteristics such as burnup, temperature, and neutronic environment. Additionally, pebble-wise reaction rates may be calculated for individual pebbles in a PBR core. It was determined that the incoming particles over a pebble surface may be recorded in Serpent for a whole-core eigenvalue simulation, which may be used to reliably reproduce the pebble-wise cross sections in a single pebble source calculation. A process for clustering pebbles into similar groups is currently being investigated.

Key Publications

Carlson, et al. (2022) Evaluation of Pebble-Wise Integral Values Using Pebble Tracking Transport in GRIFFIN. INL Intern Poster Session

Sponsor/Program

NEUP

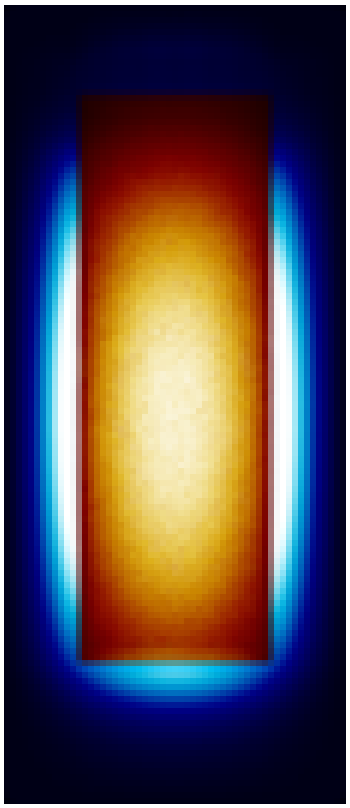


Figure 1: Thermal flux map for fresh isothermal gPBR200 model.

B.42 Metallic Fuel Performance Benchmarking

Report Participants

Casagranda, Albert [1]
1 TerraPower

Scientific Achievement

The BISON fuel performance code continues to be used to simulate the Experimental Breeder Reactor II (EBR-II) and other reactor experiments to inform the TerraPower fuel modeling capabilities. As additional metallic-fuel-related material models and benchmark analyses have been included in BISON, TerraPower reruns and updates analysis results to keep up to date. In addition, an INL and TerraPower collaboration on specific metallic fuel modeling needs is ongoing.

Significance

The main focus of this year was on evaluating the constituent redistribution, fuel-cladding chemical interface and HT9 creep material models. As code verification and validation efforts have continued at TerraPower, comparisons with BISON and other codes have proved useful to the development of Alchemy. In particular, since the EBR-II experiments were periodically removed from the reactor and examined, the inclusion of cooldown steps in analyses of these experiments provides a consistent way to compare predictions to both data and other codes. BISON was used to confirm this approach and update the code predictions.

Key Publications

In Progress

Sponsor/Program

Advanced Reactor Demonstration Program

B.43 Explainable Multifidelity Surrogate Modeling Strategy with Active Learning for Efficient Rare Event Simulations

Report Participants

Chakroborty, Promit [1], Dhulipala, Lakshmi N[2], Shields, Michael [1]
1 Johns Hopkins University
2 Idaho National Laboratory

Scientific Achievement

We developed a surrogate modeling framework that incorporates active learning and multifidelity modeling concepts to incorporate information from one high-fidelity model (highly expensive but accurate and complete numerical representation of system physics) and multiple low-fidelity models (comparatively cheaper and less accurate numerical representations of system physics). Gaussian process regression (an ML algorithm) was used to make up for accuracy lost by using low-fidelity model information as well as develop an assembly procedure to adaptively handle information from multiple sources. The surrogate modeling framework was embedded in a rare event simulation algorithm to efficiently and confidently estimate the failure probability of complex real-world systems where failure is a rare event, such as TRISO nuclear fuel. A journal paper on the methodology has been accepted for publication in the American Society of Civil Engineers Journal of Engineering Mechanics.

Significance

For complex-real world systems (such as nuclear reactors or fuel sources), evaluating the system response at each individual system state is often highly computationally expensive due to the need for solving complicated numerical models (can involve coupled multiphysics governing equations, large number of degrees of freedom, etc.). This makes estimating the failure probability of such systems using simple simulation methods, such as Simple Monte Carlo, prohibitively expensive, as such methods require thousands or millions of response evaluations, particularly when the probability is small. Therefore, it is necessary to use more efficient methods that reduce the computational expense by reducing the number of response evaluations necessary or approximating the response using cheaper models. Our method leverages both of these ideas to create a highly efficient algorithm for failure probability estimation. We applied the method to a TRISO nuclear fuel example and saw major reductions in computational time compared to a benchmark algorithm in the field for comparably accurate and confident estimates of the failure probability. These results promise wider applicability to the nuclear engineering community for rare event simulation and failure probability estimation.

Key Publications

Chakroborty, P., Dhulipala, S. L., Che, Y., Jiang, W., Spencer, B. W., Hales, J. D., & Shields, M. D. Forthcoming. General multi-fidelity surrogate models: Framework and active learning strategies for efficient rare event simulation. ASCE Journal of Engineering Mechanics. DOI: 10.1061/JENMDT/EMENG-7111

Sponsor/Program

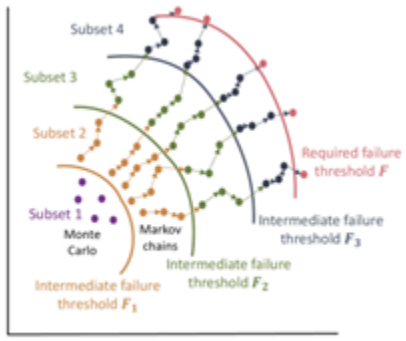


Figure 1. Visualization of Subset Simulation

Figure 1: Visualization of sampling strategy (subset simulation [Au and Beck, 2001]).

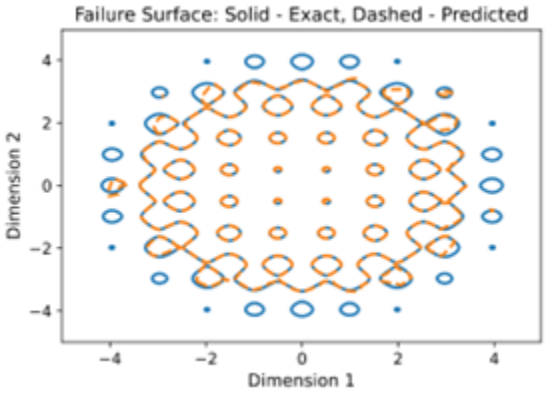


Figure 2: Comparison of predicted vs. true failure limit surface for Rastrigin function (benchmark analytical example).

	Estimated P_f (COV)	# HF calls (% of total)
Subset Simulation	9.99E-3 (0.07)	10000 (100%)
LFMC - LFDS	1.17E-2 (0.09)	58 (0.58%)

Table 6. Results for the TRISO Example (10,000 total samples generated for LFMC)

Figure 3: Results of proposed algorithm for TRISO fuel particle case study.

B.44 Assessment of Core Performance of Advanced LWR Fuel Concepts in Normal and Accident Conditions

Report Participants

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

Scientific Achievement

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

Significance

The neutronics and accident analyses are to screen candidate advanced fuel and ATF concepts to address the desired objective of ensuring that a proposed concept has at least equivalent performance and safety characteristics relative to current uranium dioxide (UO2) fuel and zirconium alloy cladding as well as offering potential performance and safety benefits. In FY-22, the analyses considered "LEU + fuels (enrichment above 5 and below 10 wt%) incorporating burnable absorbers directly in the fuel as opposed to the use of ZrB2 coating on fuel pellets, in a commercial PWR to increase burnup " advanced control rod options to complement ATF, for example, using hafnium as a replacement for AIC in a stainless-steel sheath in the standard PWR control rod geometry.

The assessment of the impacts of advanced fuels on reactor performance and safety characteristics will continue with a focus on a greater utilization of multiphysics computational platform provided the CASL suite of codes (e.g., VERA).

Key Publications

M. Todosow and A. Cuadra, Assessment of Core Performance of Advanced LWR Fuel Concepts in Normal and Accident Conditions Summary Report on FY22 Activities, BNL-AFC-2022-001, September 27, 2022.

Sponsor/Program

DOE NE Advanced Fuels Campaign

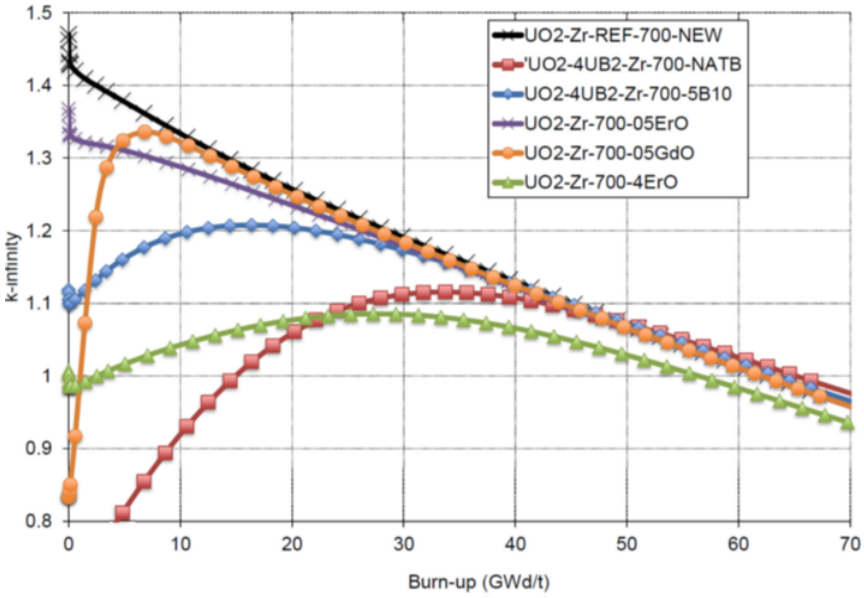


Figure 1: K-infinity vs. burnup.

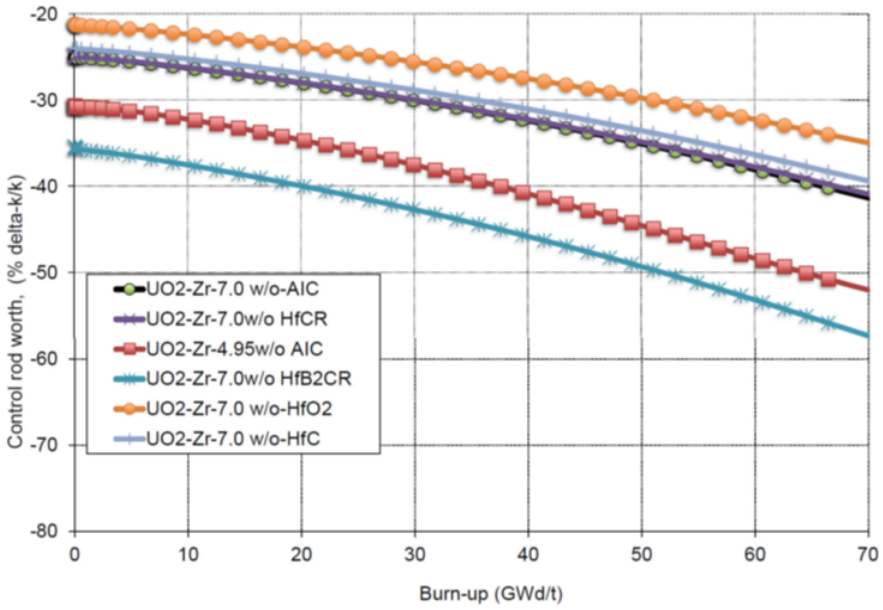


Figure 2: Control rod worth vs. burnup.

B.45 PN Source Expansion Nodal Method in MPACT for Boiling Water Reactors

Report Participants

Choi, Sooyoung [1], Kochunas, Brendan M[1]
1 University of Michigan

Scientific Achievement

This report describes the performance improvement results in MPACT by implementing the PN Source Expansion Nodal Method (SENM). We verified that the PN SENM can use more than a 1.5× larger axial mesh size than the PN Nodal Expansion Method (NEM) for the BWR 3D assembly problem.

Significance

Historically, the NEM solver has been used for the axial solver in MPACT for PWR analyses. However, the BWR has a more complex axial configuration of fuel and burnable absorbers. We observed that the NEM solver can be less accurate for some BWR applications. Therefore, we implemented the new PN-SENM solver, which has a higher spatial accuracy in the calculation of flux thanks to its additional hyperbolic functions in the flux representation. We have verified the PN-SENM solver for the 3D assembly problems. For the BWR GE14 3D assembly problem, we verified that the PN-SENM can improve the accuracy of the pin power distribution by 0.14% in RMS and 1.31% in the maximum difference compared to the PN-NEM for nomial axial dis cretizations. The PN-SENM is also able to use a 1.5× larger axial mesh than PN-NEM given a desired accuracy for BWR analyses. There was minimal difference in the eigenvalue. We also confirmed that the PN-SENM was less effective for the PWR since the PWR assembly does not have significant variations in its configuration for the axial direction.

Two conference papers were accepted and presented at PHYSOR2022 on May 2022.

Key Publications

1. S. Choi, A. Ward, A. Graham, B. Collins, B. Kochunas, M. Asgari Preliminary Simulation Results of Peach Bottom Unit 2 Cycles 1 and 2 with MPACT, In PHYSOR2022, Pittsburgh, PA, 2022, doi.org/10.13182/PHYSOR22-37699 2. S. Choi, B. Kochunas, PN Source Expansion Nodal Method in MPACT for Boiling Water Reactors, In PHYSOR2022, Pittsburgh, PA, 2022, doi.org/10.13182/PHYSOR22-37363

Sponsor/Program

We would like to thank Exelon Corporation for initiating this project with ORNL, INL, the University of Michigan, North Carolina State University, and the University of Illinois Urbana-Champaign under U.S. DOE Contract No. DE-AC05-00OR22725.

Method	Axial Mesh size (cm)			Compared to Serpent			Compared to finemesh calc.		
				k_{eff} diff.	Power diff.(%)		k_{eff} diff.	Power diff.(%)	
	Average	Max	Min	(pcm)	RMS	Max	(pcm)	RMS	Max
P_3-NEM	7.57	12.00	1.59	235	0.71	3.48	2	0.45	2.93
	5.23	8.00	1.59	235	0.72	3.15	2	0.43	2.39
	3.16	4.00	1.59	234	0.59	1.74	1	0.22	1.01
	1.77	2.00	1.07	234	0.52	1.54	1	0.10	0.37
	0.94	1.00	0.71	233	0.47	1.41	0	0.01	0.02
P_3-SENM	7.57	12.00	1.59	234	0.55	2.57	1	0.27	1.68
	5.23	8.00	1.59	234	0.58	1.84	1	0.27	1.30
	3.16	4.00	1.59	234	0.56	1.56	1	0.17	0.74
	1.77	2.00	1.07	234	0.51	1.52	1	0.09	0.30
	0.94	1.00	0.71	233	0.46	1.40	Ref.	Ref.	Ref.

Figure 1: GE14 3D assembly calculation results with different sizes of axial mesh.

B.46 Modeling of Particle Fuel for Nuclear Thermal Propulsion and Energy

Report Participants

Cluggish, Brian P[1]
1 General Atomics

Scientific Achievement

The goal of this project is to model the performance of coated particle fuel in reactors used for nuclear propulsion. These reactors will operate at much higher temperatures and much smaller burnups than conventional nuclear reactors. BISON is being used to first develop a one-dimensional (1D) model of a fuel particle that includes material properties and kinetic effects that are relevant in this parameter regime. The model will be extended to 2D and 3D as time and resources allow.

Significance

This is an ongoing project. Material property correlations have been developed for the high-temperature regime in which the reactor will operate. This includes correlations that include the transverse anisotropic nature of pyrolytic carbon. Figure 1 shows a stress profiles in a fuel particle using the anisotropic model for the material properties.

Key Publications

None yet

Sponsor/Program

This project is funded by an internal research and development grant from General Atomics Electromagnetic Systems

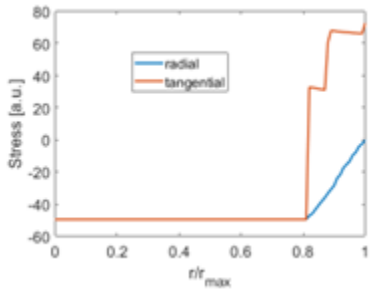


Figure 1: Stress profile in particle.

B.47 Convolutional-Neural-Network-Aided Temperature Field Reconstruction

Report Participants

Coppo Leitte, Victor [1]
1 Pennsylvania State University

Scientific Achievement

CFD are to be performed in the HPC using Nek5000 and nekRS, spectral elemental codes developed at Argonne National Laboratory (ANL). The results of the CFD analysis are applied in an ML algorithm targeted toward developing tools for physical field reconstruction based on sparse measurements in an arbitrary fluid domain (e.g., the temperature field in a nuclear reactor). After train and test data are generated by running the CFD simulations, a physics-informed convolutional neural network (CNN) is trained using the HPC's GPUs.

Significance

The study is being currently carried out with a strategy based on a physics-informed CNN with applications for the temperature reconstruction of the core in nuclear reactors of fourth generation. Current results demonstrated the ability of the CNN to reconstruct the temperature field of a molten-salt fast reactor (MSFR) design. Current efforts include extending this method for prismatic reactors, such as the PBR. This research is relevant as it allows the development of less invasive diagnostics tools for nuclear reactors operation as well as an improved monitoring system.

Key Publications

Conference publications: Coppo Leite, V., et al (2023). Application of a Physically Informed Convolutional Neural Network for Monitoring the Temperature Field During Accidents in Prismatic Reactors. 20th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-20), in preparation Jornal: Coppo Leite, V., Merzari, E. (2021), Ponciroli, R., Ibarra, Lander. (2022). Convolutional Neural Network Aided Temperature Field Reconstruction, an Innovative Method for Advanced Reactors Monitoring. 20th Nuclear Technology (ANS), under review

Sponsor/Program

NEAMS MS-22AN060101

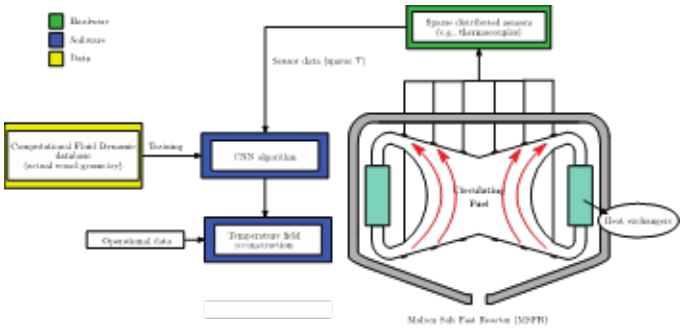


Figure 1: Temperature field reconstruction employing the novel CNN algorithm.

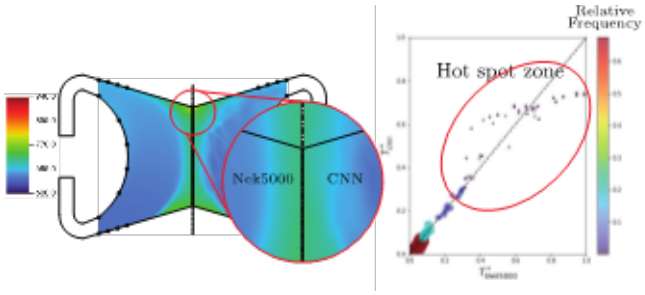


Figure 2: CNN field reconstruction at Re = 300k. A detailed view is shown for the peaking temperature region. The right-side plot compares the predictions from the CNN with the CFD solution. A red circle highlights probing points near the peaking temperature region, termed the hot spot zone.

B.48 Thermal Hydraulic Analyses of Low Enriched Fuel for Element Tests in the Advanced Test Reactor

Report Participants

Cowles, David [1], Saitta, Michael [1], Clark, Collin M[1], Roth, Gable D[2], Anderson, Nolan A[2]
1 MPR Associates
2 Idaho National Laboratory

Scientific Achievement

The HPC resources are used to execute verified thermal hydraulic codes for developing the LEU fuel safety basis during ATR operation. Specific details are excluded from this description due to the sensitive nature of the information.

Significance

The DOE National Nuclear Security Administration's (NNSA) Office of Material Management and Minimization (M3) mission is to convert, remove, and dispose of vulnerable nuclear material located at civilian sites worldwide. As part of its mission, M3's Office of Conversion works around the world to convert research reactors and isotope production facilities to non-weapon-usable nuclear material both domestically and abroad. In support of this effort, the Office of Conversion's USHPRR Conversion Program is working with INL to develop and qualify new LEU fuels and technologies for use in ATR, the Advanced Test Reactor Critical (ATRC) facility, High Flux Isotope Reactor, National Bureau of Standards Reactor (NBSR), Massachusetts Institute of Technology Reactor, and University of Missouri Research Reactor (MURR).

The USHPRR Program has selected a monolithic U-Mo fuel plate design of uranium-10 wt% molybdenum alloy (U-10Mo) foils clad in aluminum alloy 6061 as the best candidate for the USHPRR LEU fuel plates. The Fuel Qualification Pillar at INL is responsible for the development and qualification of the new U-10Mo LEU fuel plates. Major fuel development activities include the demonstration, thorough testing, and analyses of the new fuel that meet the operational safety, dimensional stability, thermal stability, performance, and other requirements for the reactors.

The work required to design, evaluate, and qualify a new LEU fuel element using the U-10Mo fuel plates for use in ATR and ATRC is directed by the ATR LEU Fuel Project at INL. The ATR LEU fuel element design (referred to as the LOWE element) has been selected as the best performing LEU fuel element design to use in place of the present HEU fuel element in ATR. Therefore, the LOWE fuel element design will be moved forward for further testing and evaluation to determine if the monolithic U-10Mo fuel plates are safe for use in ATR and ATRC.

Key Publications

" Anderson, N., January 2022, SASQUATCH (version 2.2) Software Verification Test Scenarios and Results, ECAR-3996, Rev. 3, Idaho National Laboratory. " Saitta, M., May 2022, Documentation of PROMETHEUS, INL/INT-21-61873, Rev. 0, Idaho National Laboratory. " Cowles, D., 2023, Operating Limits of Lead Test LOWE Fuel Elements for Pressurized Two Primary Coolant Pump Flow INL Document No. INL/RPT-22-69389, Rev. 0, Idaho National Laboratory.

Sponsor/Program

ATR

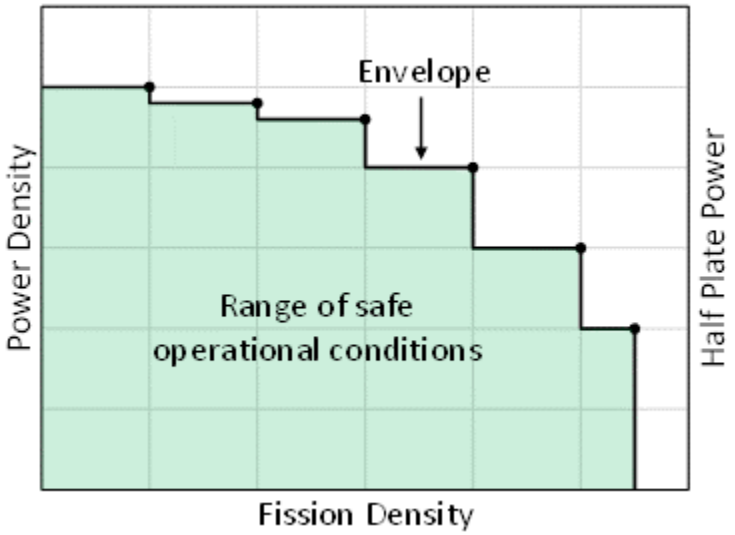


Figure 1: LOWE fuel operational criteria.

B.49 Advanced Reactor Fuel Performance Modeling

Report Participants

Everett, Patrick F[1], Kloiber, Brian T[1], Hanson, John P[1]
1 Oklo Inc

Scientific Achievement

Oklo is using BISON to model its advanced reactor fuel performance. In particular, Oklo is using BISON for modeling metallic fuel alloy swelling, fission gas release, plenum pressurization, cladding stress, cladding creep, and cumulative damage. Oklo has engaged with NRC staff throughout the past year to present findings from its fuel performance calculations and demonstrate margin to safety limits.

Significance

As Oklo continues to leverage BISON's fuel performance analysis capabilities, Oklo will advance its reactor design through the NRC licensing process to support initial deployment of its Aurora design at INL.

Oklo has additional projects underway (funded through a number of DOE awards) to develop commercial-scale fuel recycling capabilities. Oklo plans to work with INL BISON developers to develop capabilities to model recycled fuel performance methods, enabling a reactor fueled by recycled material to be qualified and licensed.

Key Publications

N/A license application(s) are under development

Sponsor/Program

Industry

B.50 CFD Modeling and Validation Experiment Design for HENRI

Report Participants

Warren, Austin M[1], Mignot, Guillaume [1], Race, Cody C[2]
1 Oregon State University
2 Idaho National Laboratory

Scientific Achievement

The TREAT Facility at INL is designing a helium-3 injection system to expand its capabilities for simulating LWR RIAs. The Helium-3 Enhanced Negative Reactivity Insertion (HENRI) capsule includes challenging physics to model due to its coupled nature. When the helium-3 is bombarded by neutrons in the reactor, it will release energy, which increases the temperature and pressure of the helium-3, causing the injection to slow down. The helium-3 is absorbing neutrons, which decreases the neutron flux and decreases this effect. However, the injection slowing down introduces less helium-3 into the reactor. The highly coupled nature of the HENRI injection system lead to the development of a model utilizing Serpent 2 for reactor physics and STAR-CCM+ for CFD coupled together. This model is now being used with validation experiments to confirm its predictive ability.

Significance

Since the last update provided a year ago, the coupled model using Serpent 2 and STAR-CCM+ was adapted to the Oregon State Unversity TRIGA Reactor (OSTR) to design experiments that can validate the coupled model before the HENRI system is installed in TREAT. The results of the coupled model for an OSTR experiment contain a measureable difference from the CFD-only simulations. Therefore, the coupled model can be validated using the OSTR and a HENRI-like experiment injecting helium-3 into the reactor. Figure 1 shows the pressure results over time for the coupled simulation of the OSTR experiment. There is an upward trend in the pressure that deviates from the CFD-only simulations and out-of-pile experiments. Additionally, there is a change in the frequency of the oscillations, which get closer together due to the added energy from the neutron absorption reactions. Both of these phenomena can be measured experimentally, proving the model can be validated with this experiment.

Key Publications

Warren, A. (2023). Validation of a Transient Coupled CFD-Reactor Physics Model: An Experimental Methodology to Quantify the Accuracy of CONSTELATION for the HENRI System. Oregon State University. Warren, A., Mignot, G., & Marcum, W. (2023). Scaled Experiment Design for Transient Coupled CFD-Reactor Physics Model for HENRI. 20th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-20). Washington, D.C.: American Nuclear Society. Warren, A., Mignot, G., Howard, T. K., & Marcum, W. (2022). Validation Experiment Design for HENRI Coupled Code CONSTELATION. ANS Winter Conference and Technology Expo. Phoenix: American Nuclear Society.

Sponsor/Program

NEUP, TREAT

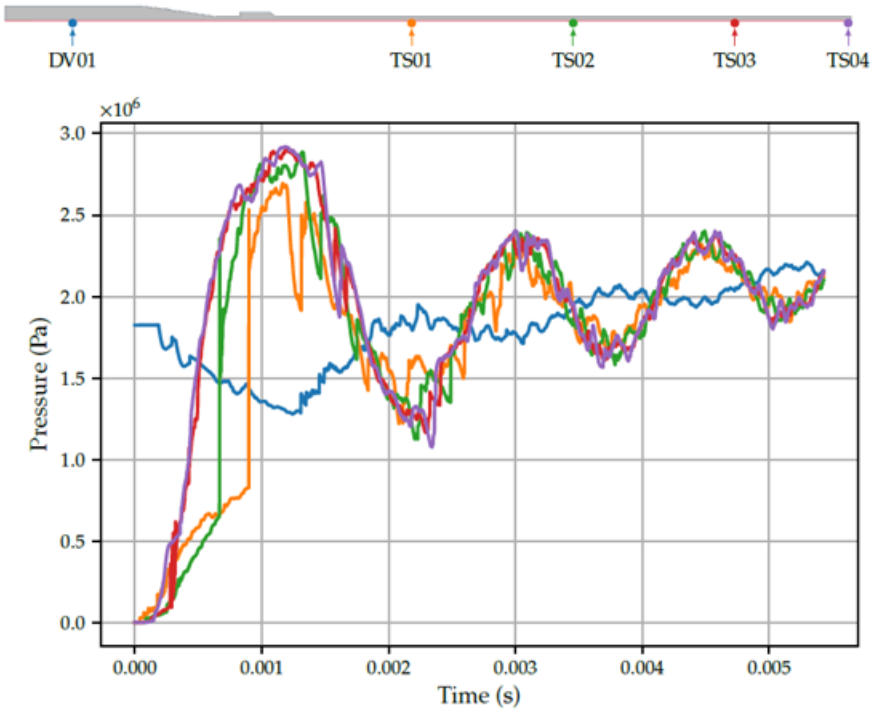


Figure 1: Coupled STAR-CCM+ Serpent 2 pressure results for the 250 psi initial pressure OSTR helium-3 injection experiment.

B.51 High-Fidelity Modeling Informs Safety Analysis Codes for Heat Pipe Microreactors

Report Participants

Da Silva Bourdot Dutra, Carolina [1], Merzari, Elia [1]
1 Pennsylvania State University

Scientific Achievement

The study conducted a comprehensive investigation into heat pipe behavior, particularly focusing on the sensitivity of heat pipe performance to variations in the wall-wick gap size. This research utilized the heat pipe MOOSE-based application, Sockeye, to model and analyze heat pipe behavior, incorporating experimental setup parameters and information from other numerical simulations.

Significance

By employing the Sockeye model, the study determined the capillary limit of the heat pipe under different conditions. In Figure 1, different liquid gap sizes are tested and compared with the manufacturer's value, and in Figure 2, the gap size is fixed, and the friction factor correlations are changed. These findings offer valuable insights into heat pipe behavior, enhancing our ability to design and optimize heat pipes for various applications. The study highlights the critical role of the liquid friction factor correlation and the liquid gap size in predicting the heat pipe capillary limit.

Key Publications

Bourdot Dutra, C. D. S., Merzari, E., Acierno, J., Kraus, A., Manera, A., Petrov, V., ... & Shaver, D. (2023). High-Fidelity Modeling and Experiments to Inform Safety Analysis Codes for Heat Pipe Microreactors. Nuclear Technology, 1-25.

Sponsor/Program

NA

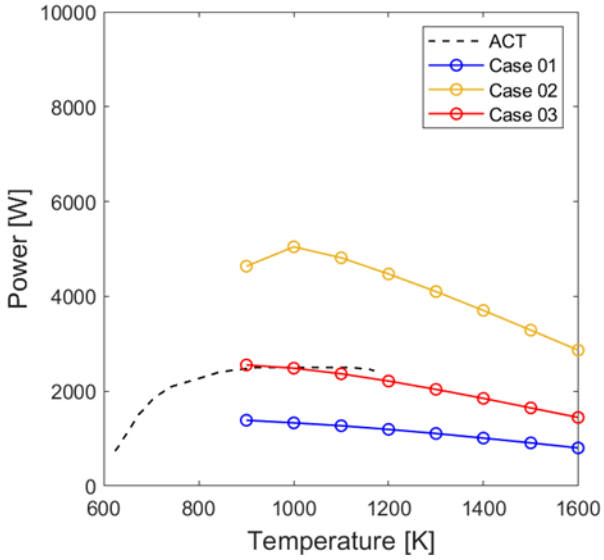


Figure 1: Capillary limit for Cases 01, 02, and 03 with different liquid gap sizes.

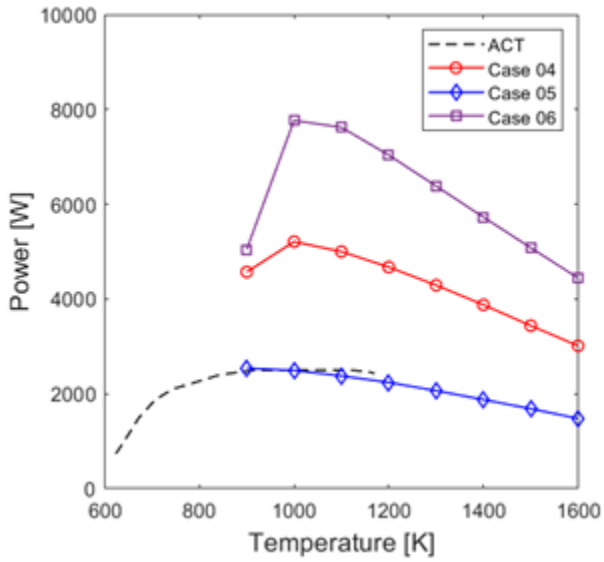


Figure 2: Capillary limit for Cases 04, 05, and 06 with different liquid friction factor correlations.

B.52 Predictive Time to Failure Modeling of U-Pu-Zr Nuclear Fuel

Report Participants

Daniell, James N[1]
1 Missouri University of Science and Technology

Scientific Achievement

A model of U-Pu-Zr nuclear fuel was developed using BISON to form the dataset for a time-series analysis using long short-term memory (LSTM) neural networks to predict the time until a partial melt for fuel in a similar system. ML techniques are used instead of traditional simulation to reduce the computational cost and draw correlations between direct operation using parameters commonly available during reactor operations.

Significance

Overpower analysis to reach melt was performed for multiple BISON models to generate a wider field of possible transients available in these systems. Parameters such as LHGR and coolant temperature were adjusted semi-randomly to increase the range of conditions during this event. Data collected from the BISON models was processed for use in an LSTM-based neural network. This neural network utilizes a piecewise activation and loss to provide operational flags as well as regression (time to failure) predictions and provide increased training capabilities while maintaining a smooth transition between regions (from neuron weight). Hyperparameter tuning and loss function finalization is ongoing.

Key Publications

Daniell, J., Kobayashi, K., & Alam, S. (n.d.). Partial Nuclear Fuel Melt Predictions Using LSTM as Surrogate Model. In 2023 ANS Winter Conference and Expo. American Nuclear Society. (in review, presenting at ANS winter 2023).

Sponsor/Program

DOE (funding for DT supporting modules)
NRC graduate fellowship (extended from work on deployable information and safety systems)

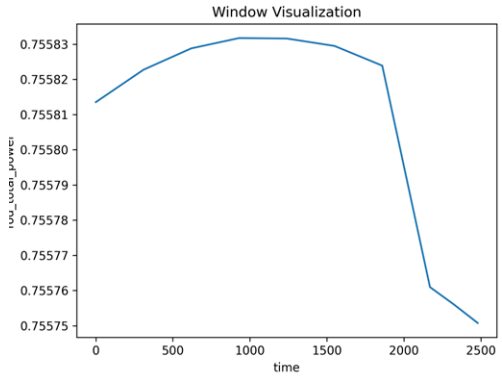


Figure 1: Example window for time-series analysis using LSTM module.

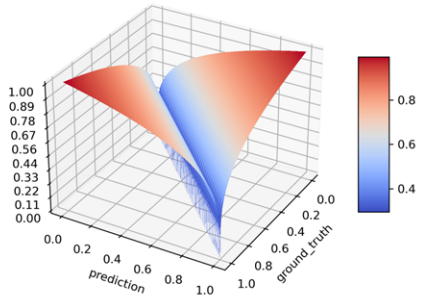


Figure 2: Loss surface used during time-to-failure prediction optimization.

B.53 Molten Salt Reactor Experiment Simulations Using Shift/Griffin

Report Participants

Hartanto, Donny [1], Davidson, Eva [1], Cao, Yan [2], Fei, Tingzhou [2], Tano, Retamales, M[3]
1 Oak Ridge National Laboratory
2 Argonne National Laboratory
3 Idaho National Laboratory

Scientific Achievement

This work focused on testing and demonstrating cross-section generation using the Shift Monte Carlo code for the MSRE model. These cross sections were used in Griffin, a MOOSE-based neutronics tool, to ensure that the solutions generated in Griffin using Shift cross sections are consistent with the cross sections generated by Serpent and OpenMC. Griffin was set up to perform depletion calculations for a 3D MSRE model using Shift, Serpent, and OpenMC cross sections. This effort was successful, and differences between the codes were identified and flagged for future code development needed to support MSR applications.

Significance

Shift is a Monte Carlo code being used by NEAMS to generate cross sections for Griffin. The ability to accurately generate cross sections with Shift to support multiphysics calculations using Griffin coupled with other MOOSE-based tools will be important in successfully benchmarking MSR models with experimental data to eventually support MSR deployment. In addition, the ORNL team was able to learn how to use Griffin by setting up depletion models to test the newly implemented depletion capability in Griffin.

Key Publications

There are no publications yet on this work. A report will be generated at the end of this fiscal year to document the milestone results, and a conference proceeding is being planned for next fiscal year.

Sponsor/Program

NEAMS

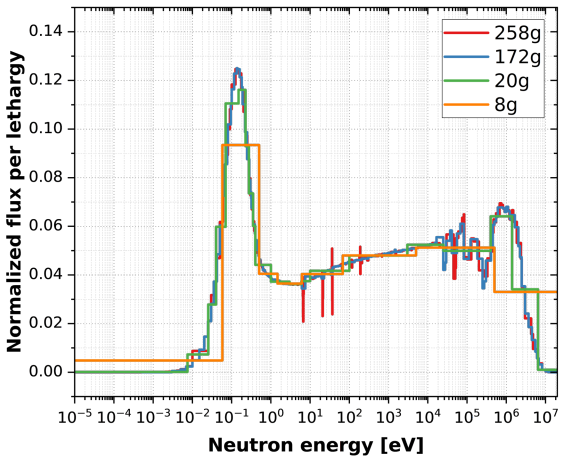


Figure 1: Normalized flux in Shift based on varied group macroscopic cross sections.

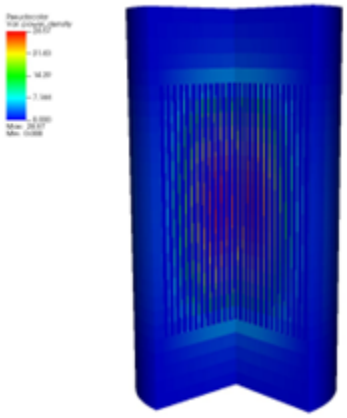


Figure 2: Power density in the Griffin MSRE model.

B.54 Parallel Low-Temperature Plasma Multiphysics Simulation using MOOSE and MOOSE-based Application Zapdos

Report Participants

DeChant, Corey S[1], Icenhour, Casey T[2], Shannon, Steven [1]
1 North Carolina State University
2 Idaho National Laboratory

Scientific Achievement

The objective of this work is developing a capability in the MOOSE framework ecosystem to model complex fluids and fluid-material interactions. These complex fluids are not only affected by the traditional fluid equations but also include the transport of species that can be affected by and form coupled fields in other physics domains, such as electric and magnetic fields due to volume charge separation and current flow in the fluid. Previous works presented in a paper that has been published this year involved addressing the current state of the verification process of codes for these complex fluids. When compared to other computational physics, such as traditional computational fluid dynamics, the verification methods for these complex fluids are underdeveloped, especially for low-temperature plasma codes. The work addresses this lack of sophisticated verification methods and suggests a methodology for verifying these codes. To demonstrate the verification methodology, the MOOSE framework and MOOSE-based applications, Zapdos and CRANE, were utilized. Current work focuses on coupling MOOSE's electromagnetic module with MOOSE's multifluid plasma application, Zapdos. Figure 1 shows 3D power deposition results for a one-way coupled simulation between the microwave-driven electric fields and a pseudo-plasma, which has a user-defined electron density profile, electron temperature, and pressure. Figure 2 is a radial slice of the same simulation, which shows a nonaxisymmetric power deposition for an axisymmetric electron density profile. This may suggest that higher-order modes of the electric field are present in these axisymmetric profiles. Next steps include a fully coupled simulation between the electromagnetic fields and plasma.

Significance

The work done on expanding the current state of verification methods for computational plasma will increase the confidence in such codes. This increased confidence is of interest to DOE-NE, since these codes can be used for the modeling and understanding of solvated electrons, which can be formed by radiation-induced detachment in LWR coolant channels. The current work focusing on coupling MOOSE's electromagnetic module with MOOSE's multifluid plasma application would be of interest for a variety of applications for very-high-frequency and microwave plasma (such as manufacturing processes).

Key Publications

DeChant, C. et al. 2023 Verification methods for drift diffusion reaction models for plasma simulations. Plasma Sources Sci. Technol. 32 044006 " DeChant, C. et al. 2023 Verification and Validation of the Open-Source Plasma Fluid Code: Zapdos. Submitted to Computer Programs in Physics, In Progress

Sponsor/Program

NEUP
Fellowship Project Number: FLW-18-16616

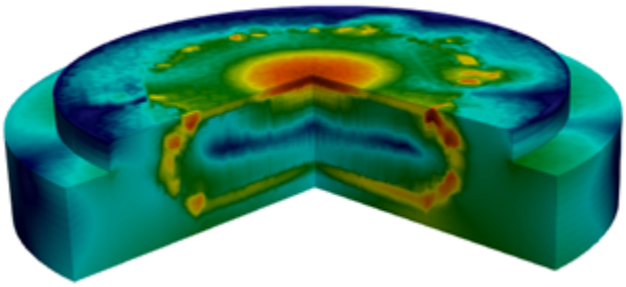


Figure 1: Power deposition [W/m3] for an axisymmetric electron density profile.

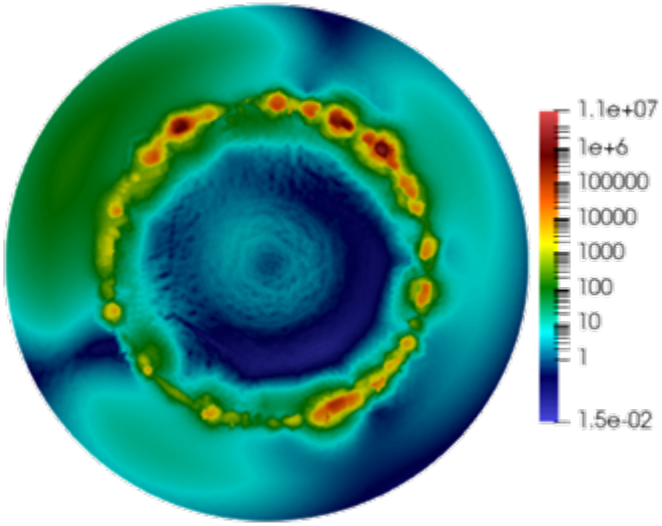


Figure 2: Radial slice of the power deposition [W/m3] for an axisymmetric electron density profile.

B.55 NEAMS Workbench on NCRC

Report Participants

Delchini, Marc-Olivier G[1], Lefebvre, Robert A[1], Baird, Mark L[1], Langley, Brandon R[1], Permann, Cody J[2], Gaston, Derek R[2], Shemon, Emily R[3]
1 Oak Ridge National Laboratory
2 Idaho National Laboratory
3 Argonne National Laboratory

Scientific Achievement

The objective of this project is to improve access to and usability of the NEAMS multiphysics software and associated advanced reactor analysis workflows. The addition of a language server to the MOOSE framework enables NEAMS MOOSE-based applications to provided integrated development environment features to users, which accelerates their editing, navigation, and understanding of the available capabilities deployed and under development in the NEAMS software and demonstrated via the Virtual Test Bed (VTB).

Significance

With the combination of INL's HPC OnDemand environment, NEAMS MOOSE-based multiphysics applications, and workbench capabilities, the targeted end-user and industry collaborator feedback cycles are shortened and better addressed. The NEAMS workbench provides a common analysis environment that accelerates user interactions and streamlines analysis and common workflows. This is significant in helping address the advanced modeling and simulation obstacles that need to be overcome to accelerate the deployment of advanced nuclear energy technologies.

Key Publications

Delchini, Marco, & Lefebvre, Robert Alexander. Documentation on How to Run the NEAMS Workbench GUI on Sawtooth. United States. https://doi.org/10.2172/1890289. Marc-Olivier G. Delchini, Robert A. Lefebvre, Brandon S. Biggs, Emily R. Shemon, Cody J. Permann, Enabling Remote Multiphysics Simulation of Virtual Test Bed Examples on Idaho National Laboratory High Performance Computing Resources Through NEAMS Workbench , American Nuclear Society, November 2022.

Sponsor/Program

DOE NEAMS

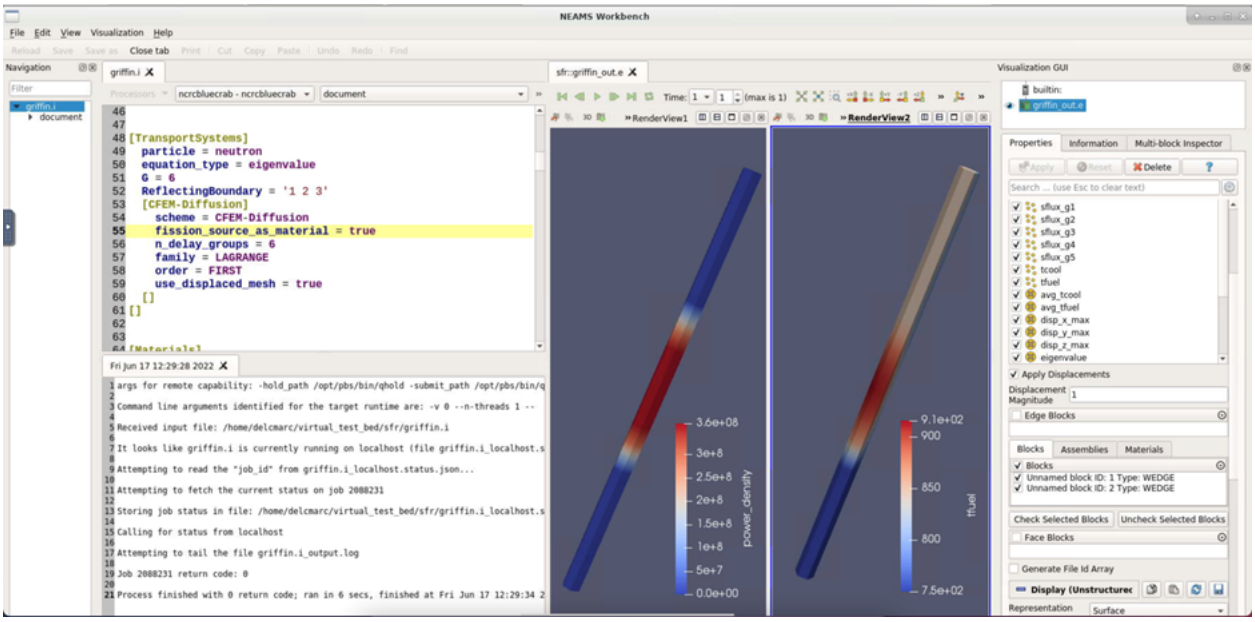


Figure 1: The NEAMS workbench GUI with griffin.i input file (top left), the output from the scheduler (bottom left), and the numerical solution visualized with embedded ParaView (right).

B.56 Benchmark Evaluation of Transient Multiphysics Experimental Data for Pellet-Cladding Mechanical Interactions

Report Participants

Delipei, Grigorios K[1], Faure, Quentin D[1], Ayramoya, M [1], Ivanov, K [1]
1 North Carolina State University

Scientific Achievement

Reactor physics M&S has benefited tremendously through high-quality experiments evaluated and documented in standard benchmark handbooks (such as the ICSBEP and International Reactor Physics Experiment Evaluation Project [IRPhEP] handbooks). However, there is a lack of similar quality data for integral transient multiphysics experiments. This project aims at providing the first evaluation of a multiphysics experimental benchmark using data from two cold ramp tests in the Studsvik R2 reactor. The experiments targeted pellet-cladding interaction and pellet-cladding mechanical Interaction (PCMI), fundamental multiphysics, and multiscale phenomena that require accurate and realistic M&S. As part of this overall project, BISON, a fuel performance code, is used in comparative benchmark evaluation studies and for developing uncertainty quantification approaches that account for both epistemic and aleatoric sources of uncertainties. The base irradiation of the fuel rodlet used in the ramp test was conducted with three different fuel performance codes, covering finite difference, volume, and element codes in 1D and 2D. In Figure 1, the results for the cladding outer diameter prediction with FAST, OFFBEAT, and BISON are provided and show very good results against the experimental data. The discrepancy of 15 um for BISON and OFFBEAT is attributed to the cladding oxidation models suited for PWR conditions, while the fuel rodlet was irradiated under BWR conditions. This result indicates the need for appropriate oxidation models for better predicting the initial fuel rodlet conditions. Follow up studies showed that these initial conditions will determine the onset of PCMI and the cladding axial elongation during the transient. Finally, together with initial conditions, the friction between the surfaces of fuel and cladding needs to be modeled to capture the PCMI behavior after contact accurately enough. This is why 1D fuel performance codes or codes that assume there is no slippage (e.g., FAST) will not be able to accurately predict the post-PCMI fuel behavior. Currently, the BISON contact models are being investigated, more particularly, the mortar model to provide reference high-fidelity fuel performance results for the benchmark. Additionally, uncertainty quantification and sensitivity analysis studies are being conducted for the two cold ramp tests as part of the benchmark evaluation. Finally, the end-goal will be to develop a GRIFFIN-RELAP7-BISON coupled reference calculation for the cold ramps.

Significance

Transient multiphysics benchmark evaluations are needed to support the U.S. DOE Office of Nuclear Energy mission of developing new reactors and improving the economic competitiveness of the current fleet. M&S is an integral part of these aspects that requires high-quality evaluated data to verify and validate the new developments. The results for the fuel performance M&S with various degrees of fidelity contribute directly to evaluating the transient multiphysics experimental benchmark. This will benefit not only the validation of fuel performance codes but also of multiphysics frameworks.

Key Publications

" Q. Faure, G. Delipei, A. Petruzzi, M. Avramova and K. Ivanov, Fuel performance uncertainty quantification and sensitivity analysis in the presence of epistemic and aleatoric sources of uncertainties , Frontiers in Energy Research, 2023, doi: 10.3389/fenrg.2023.1112978 " Q. Faure, G. Delipei, A. Scolaro, M. Avramova and K. Ivanov, Mutli-Fidelity Fuel Performance Comparative Analysis for the OECD/NEA MPCMIV Benchmark , (under preparation)

Sponsor/Program

NEUP Project No. 20-19590

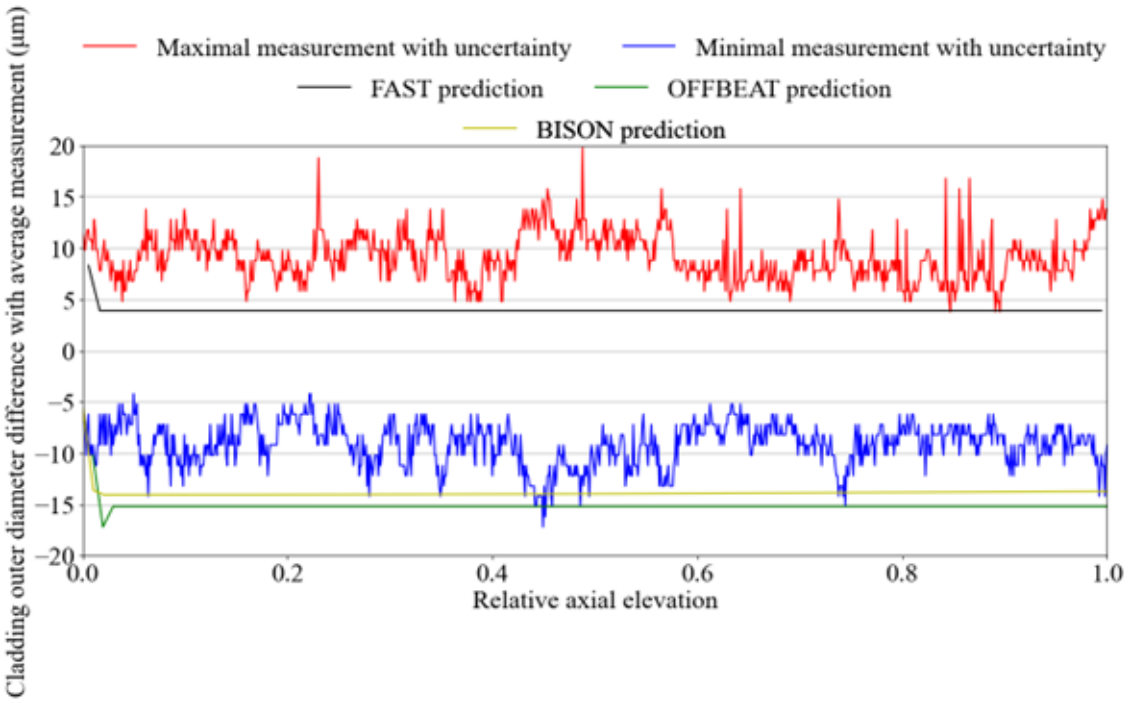


Figure 1: Cladding outer diameter comparison of measured and predicted values.

B.57 Post-DNB Thermomechanical Behavior of Near-Term ATF Designs in Simulated Transient Conditions

Report Participants

Dunbar, Cole J[1], Yeom, Hwasung [1], Jung, WooHyun [1], Armstrong, Robert J[2]
1 University of Wisconsin-Madison
2 Idaho National Laboratory

Scientific Achievement

Implementing ATF designs requires significant understanding of their performance during postulated DBAs, including LOCAs. In this project, we have used BISON, the fuel performance code, to investigate the effect of thin chromium coatings applied to Zr-alloy cladding on balloon and burst behavior using the Halden LOCA IFA-650.10 testing sequence. Calculations quantified the difference in performance during commercial irradiation and in the LOCA test sequence. A sensitivity analysis varied the coating material, thickness, mechanical, and creep model properties to better understand the behavioral differences exhibited during the transient.

Significance

The thin Cr-coating exhibits the negligible development of an oxide layer during normal operation leading to marginal decreases in fuel and cladding temperatures when compared to bare Zr alloy. Additionally, the application of a 30 m Cr coating shows a delay in the onset of significant clad deformation and clad failure by 30 seconds. Clad deformation during the LOCA scenario is driven by high-temperature creep, which depends on clad temperature and effective stress driven by the pressure difference between the internal and external cladding faces. The presence of a thin chromium coating alleviates the effective stress in the cladding, slightly delaying the onset of deformation through high creep strain rates. This work is part of a larger project that aims to quantify behavioral differences in high-burnup LOCA with ATF. Future simulations will characterize any differences in fuel pulverization and axial relocation during the postulated transient.

Key Publications

" WooHyun Jung, Cole Dunbar, Michael Corradini, Kumar Sridharan, David Kamerman, Robert Armstrong, Hwasung Yeom, 2022. Project Overview of Thermal-Hydraulic and Mechanical Behavior of Near-Term ATF Design in Reflood Conditions , ANS Winter Meeting 2022, Phoenix, (November) 2022.

Sponsor/Program

NEUP FC-2.1: Fuel-to-Coolant Thermomechanical Transport Behaviors Under Transient Conditions

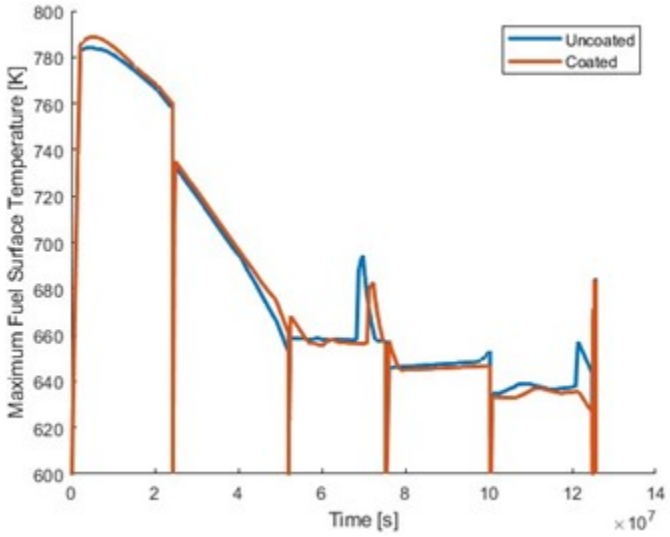


Figure 1: Maximum fuel surface temperature with and without a 30 m chromium coating during commercial irradiation of Halden IFA-650 Rod 10. Oxide growth on uncoated cladding increases thermal resistance from fuel to coolant, leading to higher temperatures at end of life.

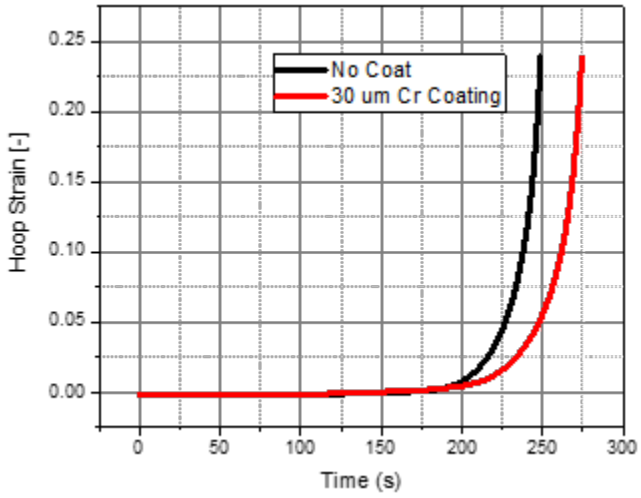


Figure 2: Maximum cladding hoop strain during the LOCA test sequence.

B.58 Design Optimization and CFD and Performance Analyses of Miniature Pumps for Circulating Molten Lead

Report Participants

El-Genk, Mohamed S[1], Schriener, Timothy [1], Altamimi, Ragai [1]
1 University of New Mexico

Scientific Achievement

Advanced nuclear reactors, accelerator-driven systems, and high-temperature industrial and experimental applications use liquid metal coolants and working fluids, such as alkali metals, lead, and lead-bismuth eutectic (LBE). The proposed Versatile Test Reactor (VTR) is a sodium-cooled fast spectrum reactor designed to conduct an accelerated irradiation testing and qualifying of fuels, materials, sensors, and instrumentation to support developing these Gen-IV advanced concepts. A conceptual design for the Extended Length Test Assembly-Cartridge Lead (ELTA-CL) loop has been developed which could be placed in the VTR core with lead coolant separated from, but thermally coupled to, the VTR primary sodium coolant. UNM-ISNPS investigated miniature pumping options of gas-lift pumping, direct current electromagnetic pump (DC-EMP), alternating current annular linear induction pump, and a novel axial-centrifugal flow mechanical pump (Figure 1). For the mechanical pump and DC-EMP options, the commercial CFD code STAR-CCM+, utilizing INL's HPC resources, is used to simulate the molten-lead flow and help determine the pump performance characteristics. The design methodology of the axial-centrifugal flow mechanical pump couples the STAR-CCM+ code with the commercial CAESES pump design software and the DOE DAKOTA design analysis software to optimize the pump's geometry to maximize pumping power, efficiency, or supplied pressure head. The design optimization analysis of the miniature DC-EMP combines finite-element magnetic field modeling with a developed Matlab optimization code. The STAR-CCM+ CFD code multiphysics magneto electrodynamics module is also used in this work to evaluate the pump designs' performance. This work validated the developed simulation approaches using reported experimental data for a lead axial flow mechanical pump and a DC-EMP designed for pumping liquid mercury.

Significance

The design methodologies were used to develop optimized designs for the mechanical pump and DC-EMP and evaluate their performance to determine if they meet the pumping requirements outlined for the ELTA-CL reference design. The CFD analysis of the optimized mechanical pump is used to calculate the pump's performance characteristics as functions of the rotation speed. The performed CFD results showed that the maximum blade tip velocity (Figure 2) is sufficiently low that the corrosion and erosion of the 316 SS impeller structural material in the molten-lead coolant is not likely to be of concern for the testing temperature of 500°C. The design methodology of the DC-EMP optimized the dimensions of the flow duct and Alnico-5 permanent magnets and Hiperco-50 pole pieces for the desired pump footprint diameters. These materials do not require active cooling for pumping molten lead or LBE at 500°C. Finite-element magnetic field analyses calculate the magnetic field strength for the pump's two pumping regions for use in the pump optimization models (Figure 3). Both the optimized mechanical pumps and DC-EMPs can achieve lead flow velocities over 3 m/s for the different investigated ELTA-CL options. These velocities are high enough

to support corrosion testing for the cladding materials of choice for the advanced molten-lead Gen-IV reactor concept.

Key Publications

El-Genk, M.S., T.M. Schriener, A.S. Hahn, (2022). Design Optimization and CFD and Performance Analyses of Miniature Axial-Centrifugal Flow Pumps for Circulating Molten Lead. J. Material Sciences & Engineering, 11(4), 1-14. Altamimi, R., El-Genk, M.S. (2022). An Assessment of the Equivalent Circuit Model for Predicting the Performance Characteristics of Direct Current-Electromagnetic Pumps. J. Material Sciences and Engineering, 11, 1-11.

Sponsor/Program

This work during 2022 was funded by The University of New Mexico's Institute for Space and Nuclear Power Studies and built off work which had been performed in support of the Versatile Test Reactor (VTR) program, Award No. DE-AC07-051D14517 to the University of New Mexico.

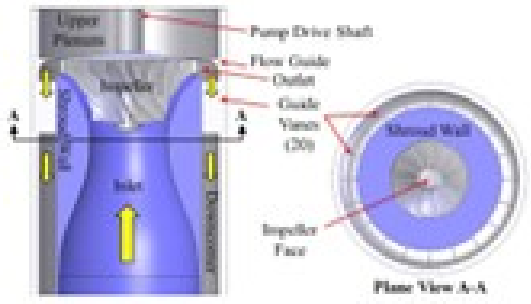


Figure 1: Section views of the developed centrifugal axial flow pump.

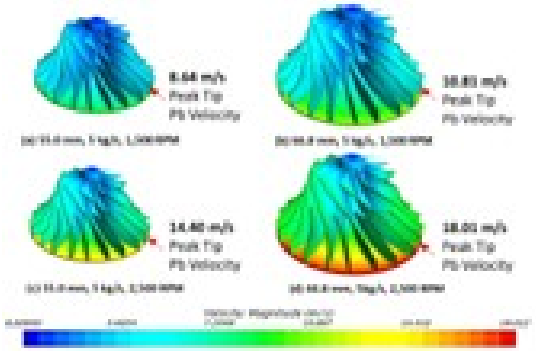


Figure 2: Lead surface velocity along impeller blades at shaft rotation speeds of 1,500 and 2,500 rpm and lead flow rates of 5 kg/s at 500°C

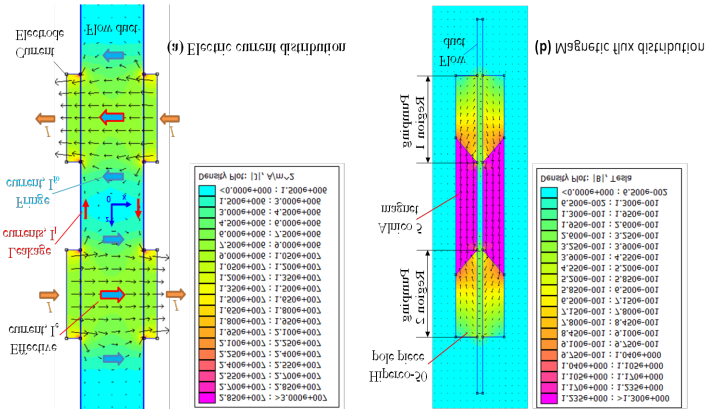


Figure 3: Calculated electrical current and magnetic field flux density distributions in the duct of miniature, dual-stage DC-EMP for lead at 500°C

B.59 CFD Simulations to Support Thermal-Hydraulics Research of Advanced Nuclear Reactors

Report Participants

Fang, Jun [1], Shaver, Dillon R[1]
1 Argonne National Laboratory

Scientific Achievement

This is an ongoing research project where we utilize the NEAMS signature CFD code, Nek5000/RS, to study the thermal-fluid problems crucial to advanced reactor designs, including MSRs and high-temperature gas-cooled reactors (HTGR). In the context of MSR research, we have performed extensive CFD simulations for the MSFR core cavity to support the industry's MSR design efforts. The CFD investigations conducted range from efficient 2D axisymmetric core modeling using the RANS approach to a 3D MSFR full-core model using a detailed LES. In our HTGR research, we are focusing on simulating flow mixing phenomena in the High Temperature Test Facility (HTTF) lower plenum. We have developed a detailed Nek5000 CFD case to study the complex flow physics involved in the lower plenum of HTTF.

Significance

Research on MSFRs and HTTF simulations is essential for advancing advanced nuclear reactor technologies. MSFRs offer promising advantages, such as improved passive safety characteristics and high thermal efficiency, due to the use of liquid fuel in molten salts. This paradigm shift from traditional solid fuel rods in other reactor designs presents unique challenges in terms of core flow configurations, which require extensive CFD simulations using high-fidelity solvers like Nek5000/RS. These simulations can provide insights into internal velocity distributions and help inform MSFR design efforts. Understanding the complex flow physics in MSFRs through CFD simulations is crucial for optimizing their performance and ensuring safe operation, which can accelerate the development and deployment of advanced nuclear reactors.

Similarly, HTTF research is significant for studying safety-relevant phenomena in HTGRs. The flow mixing in the outlet plenum of GCRs is a critical factor that can affect the thermal-fluid behavior and integrity of the lower plenum. Traditional 1D system codes are inadequate for capturing the complex flow mixing phenomenon in the lower plenum, and higher fidelity CFD codes like Nek5000/RS are required. The related simulations using Nek5000 have demonstrated the capability to capture the velocity and temperature distributions in the lower plenum and hot duct, providing insights into the thermal-fluid physics during mixing. These simulation results will be used in OECD/NEA benchmark exercises involving code-to-code and code-to-data comparisons, enhancing the accuracy of CFD modeling in GCR research and development. Overall, research on MSFRs and HTTF simulations is crucial for advancing the understanding and development of advanced nuclear reactor technologies, contributing to the safe and efficient operation of future nuclear energy systems.

Key Publications

Fang, J., Tano, M., Saini, N., Tomboulides, A., Coppo-Leited, V., Merzari, E., Feng, B., &

Shaver, D. (2023). CFD Simulations of Molten Salt Fast Reactor Core Flows. Invited for the publication on Nuclear Engineering and Design, Under review. Fang, J., Hua, T., Yuan, H., Ooi, Z. J., Zou, L. (2022). CFD Simulations of HTTF Lower Plenum Flow Mixing Using Nek5000. Transactions of 2022 ANS Winter Meeting, 980–983. Fang, J., Hua, T., Ooi, Z. J., & Zou, L. (2023). CFD Simulations of Flow Mixing Phenomenon in a Gas-Cooled Reactor Outlet Plenum. Proceedings of 20th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-20).

Sponsor/Program

DOE NEAMS

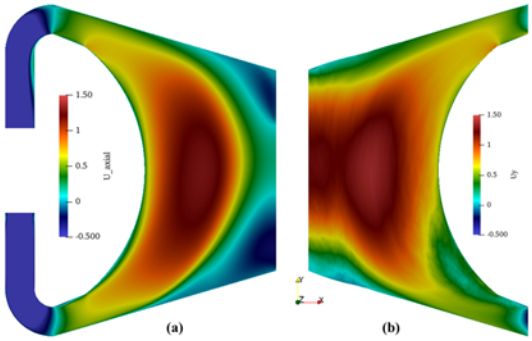


Figure 1: Comparison of the (a) RANS and (b) time-averaged LES results of axial velocity field.

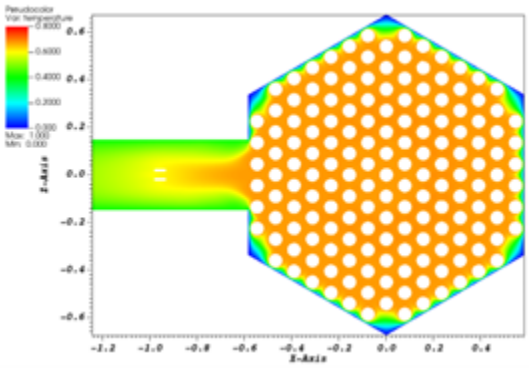


Figure 2: Time-averaged velocity field (nondimensional) in the lower plenum at y=-0.1 m.

B.60 Static and Depletion Benchmarking Simulations of a Plank Type FHR Reactor

Report Participants

Faulkner, Jonathon M[1]
1 Georgia Institute of Technology

Scientific Achievement

The fluoride-salt-cooled high-temperature reactor (FHR) benchmark is an OECD-NEA benchmark that covers the modeling of an AHTR-style FHR reactor. The plank-type fuel and triply heterogenous design of this reactor offers unique modeling challenges that are not apparent in simpler and more popular benchmarking exercises but may present themselves when running production-level calculations for advanced reactors. Also, preliminary simulations done in past work have indicated a high degree of discrepancy between different modeling methodologies, approximations, codes, and approaches for this reactor type. The objectives of this work therefore work to quantify and recognize sources of error for both steady-state and time-dependent depletion simulations of advanced reactors of this type. Work has thus been performed in modeling 2D steady state (eigenvalue) calculations using SCALE 6.2.4 and comparing results to Monte Carlo codes OpenMC and Serpent 2 from other benchmarking participants. Much work has also been done in performing 2D SCALE depletion simulations and comparing those results to depletion simulations from the state-of-the-art reactor physics code Serpent 2. In performing depletion simulations, the main source of error between different codes was found to be due to the different recoverable energy values used by each code. To further investigate this potential cause of error when performing depletion simulations, various OpenMC depletion simulations with different recoverable energy treatments and time integration schemes were performed using INL's HPC resources. Results were compared to past work by Serpent 2 benchmark participants and primary sources of error for depletion simulations between SCALE, Serpent, and OpenMC were quantized and reported to the community.

Significance

This work aimed to quantize and assess differences in benchmark-level calculations between state-of-the-art codes when modeling plank-type FHR reactors. This work falls under the modeling and simulation objectives of the University Nuclear Leadership Program (UNLP) fellowship that the author of this report is participating in. Depletion calculations found that a great deal of error may be attributed to the recoverable energy per fission and time integration scheme used in each code. This error can be eliminated by modifying the energy resource used in each code (sometimes including the source code) or by reducing the length of depletion burnup steps if the error is due to the time integration scheme. Detailed neutron-gamma calculations performed in OpenMC, when compared to SCALE and Serpent 2 results, have also been shown to contain considerable differences when compared to pure neutron-only depletion. This error has been found to be largely due to the high graphite content present in the FHR, and these modeling difficulties and inaccuracies are therefore expected to greatly affect the fuel cycle predictions of various other high graphite density cores. Methods to address the high computational cost of neutron-gamma depletion simulations through using a modified energy resource have been investigated and have been shown to be fairly accurate. Steady-state simulations have also been performed to benchmark and validate SCALE

FHR results with other Monte Carlo and deterministic codes.

Key Publications

Petrovic B., Faulkner, J. (2023). Fluoride-salt High-temperature Reactor (FHR) NEA Benchmark. Phase I-C: Fuel Element 3D, International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering. M&C 2023 (to be presented at conference).

Faulkner, J., Petrovic B., Ramey, K., Wu, Z., Lu, C., Losa, E., Chee, G., Mantecon, J,. Hill, I. (2023). Recoverable Energy per Fission Discrepancies in NEA FHR Benchmark Depletion Studies, International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering. M&C 2023 (to be presented at conference).

Sponsor/Program

UNLP fellowship

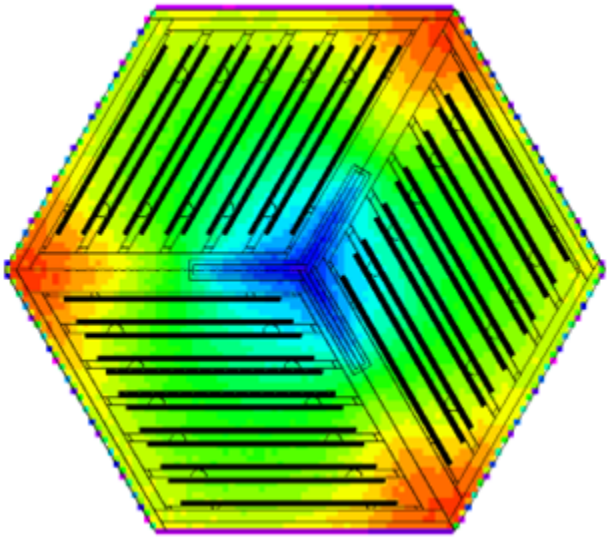


Figure 1: Thermal neutron flux in core midplane during control rod insertion, showing thermal flux shifting to assembly periphery due to thermal absorber placement.

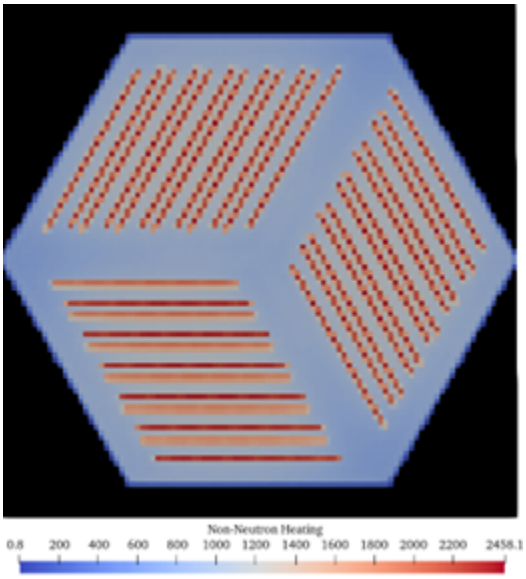


Figure 2: OpenMC gamma-induced energy deposition in the FHR core (arbitrary units), showing the relatively large graphite fraction in the FHR core as well as the complex distribution of gamma energy deposition.

B.61 Nuclear Energy University Program Project 20-19590: Benchmark Evaluation of Transient Multiphysics Experimental Data for Pellet-Cladding Mechanical Interactions.

Report Participants

Faure, Quentin D[1], Delipei, Geogory [1], Avramova, Maria [1], Ivanov, Kostadin [1]
1 North Carolina State University

Scientific Achievement

This project focuses on the multiphysics pellet cladding mechanical interaction validation benchmark. The benchmark consists of exercises modeling two cold ramp tests performed at the Studvisk R2 reactor and focuses on PCMI using multiphysics modeling. Following previous work on single physics fuel performance modeling using BISON, the models have been improved to obtain higher fidelity results. Standalone GRIFFIN and RELAP-7 models have also been developed and used in modeling the first exercises of the benchmark. Current work consists of coupling GRIFFIN and RELAP-7 while improving the results already obtained.

Significance

Guidelines and protocols for validating multiphysics modeling are currently missing in the nuclear reactor modeling industry. With the current shift toward multiphysics simulations using novel modeling and simulation tools, the need for such validation guidelines is becoming more important. The multiphysics pellet cladding mechanical interaction validation benchmark is aiming at partially filling this gap. This benchmark encompasses reactor physics, thermal hydraulics, and fuel performance in single physics simulations but also in multiphysics simulations. Uncertainty quantification and sensitivity analysis in single physics and multiphysics are also part of the benchmark.

Key Publications

Quentin Faure, Gregory Delipei, Maria Avramova, Kostadin Ivanov, "OECD/NEA MPCMIV Benchmark - Preliminary Fuel performance Results", PHYSOR 2022

Quentin Faure, Gregory Delipei, Maria Avramova, Kostadin Ivanov, Alessandro Petruzzi, "Fuel Performance Uncertainty Quantification and Sensitivity Analysis Methodology for Aleatoric and Epistemic Sources of Uncertainties , ANS WINTER 2022

Faure Q, Delipei G, Petruzzi A, Avramova M and Ivanov K (2023), Fuel Performance Uncertainty Quantification and Sensitivity Analysis in the Presence of Epistemic and Aleatoric Sources of Uncertainties. Front. Energy Res. 11:1112978

Sponsor/Program

NEUP

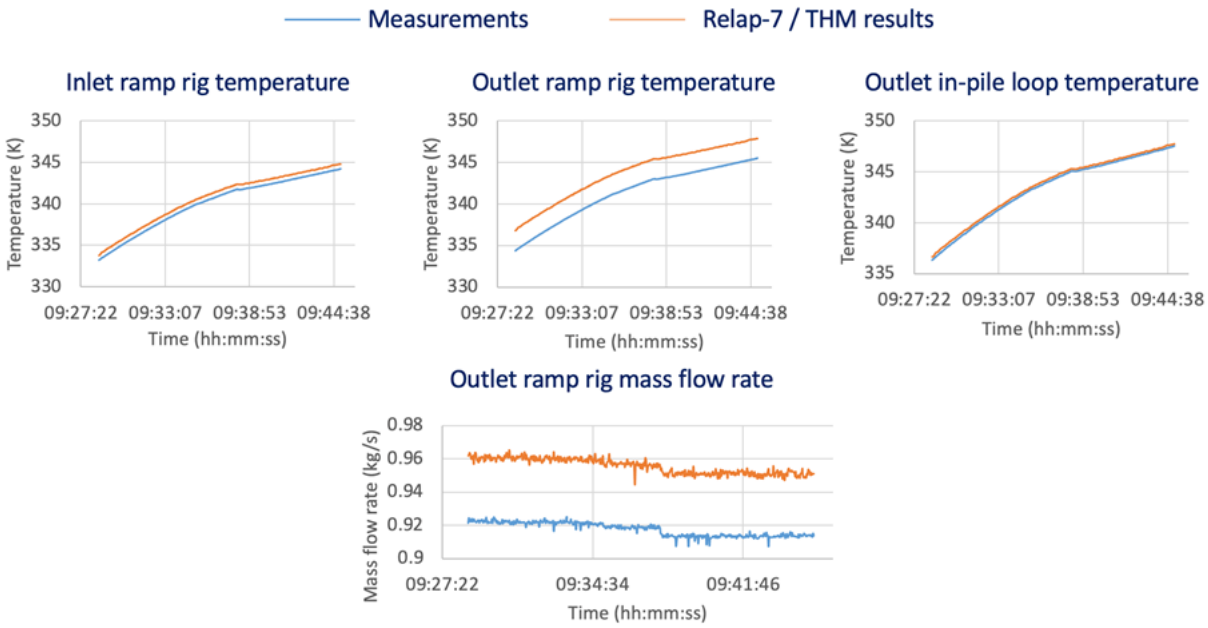


Figure 1: RELAP-7 and THM results, showing that some calibration of the loss coefficient is needed.

B.62 Multiphysics Coupling of Griffin and SAM for MSR Simulation

Report Participants

Fei, Tingzhou [1], Cao, Yan [1]
1 Argonne National Laboratory

Scientific Achievement

Validating the advanced tools developed under the NEAMS program is essential for the adoption of these tools to solve real-world problems. Among many nuclear reactor designs, the MSR is unique in using flowing fuel. This results in a tightly coupled system between thermal hydraulics and neutronics, which makes the NEAMS multiphysics tool a perfect candidate for simulating MSR behavior. However, it is also necessary to gain confidence in these newly developed tools through validation. This can only be achieved through benchmarking and validating against experimental data. The MSRE data are employed for this purpose. This is an essential step to demonstrate the accuracy and capability of the NEAMS tools for MSR applications.

Significance

The objective of the work is to demonstrate the capability of the NEAMS tool for MSR applications and to validate the NEAMS tool by benchmarking it against MSRE data to give more confidence to potential users. The work is still ongoing. Previous efforts have focused on demonstrating the multiphysics capability for the MSR system. One of the MSRE zero-power tests (pump startup test) was also investigated using the Griffin-SAM coupling approach. Different modeling approaches were adopted, including simple one-way coupling with a lattice fuel model, simple two-way coupling with a lattice fuel model, and coupling with a full-core model. Through this effort, several coupling approaches have been developed for simulating the MSR thermal hydraulic and neutronics behavior. The preliminary results are in Figure 1. It should be emphasized that the work is ongoing with efforts on improving the results.

Key Publications

Fei, T., Shahbazi, S., Fang, J., & Shaver, D.. Validation of NEAMS Tools Using MSRE Data. United States. https://doi.org/10.2172/1880993

Sponsor/Program

NEAMS

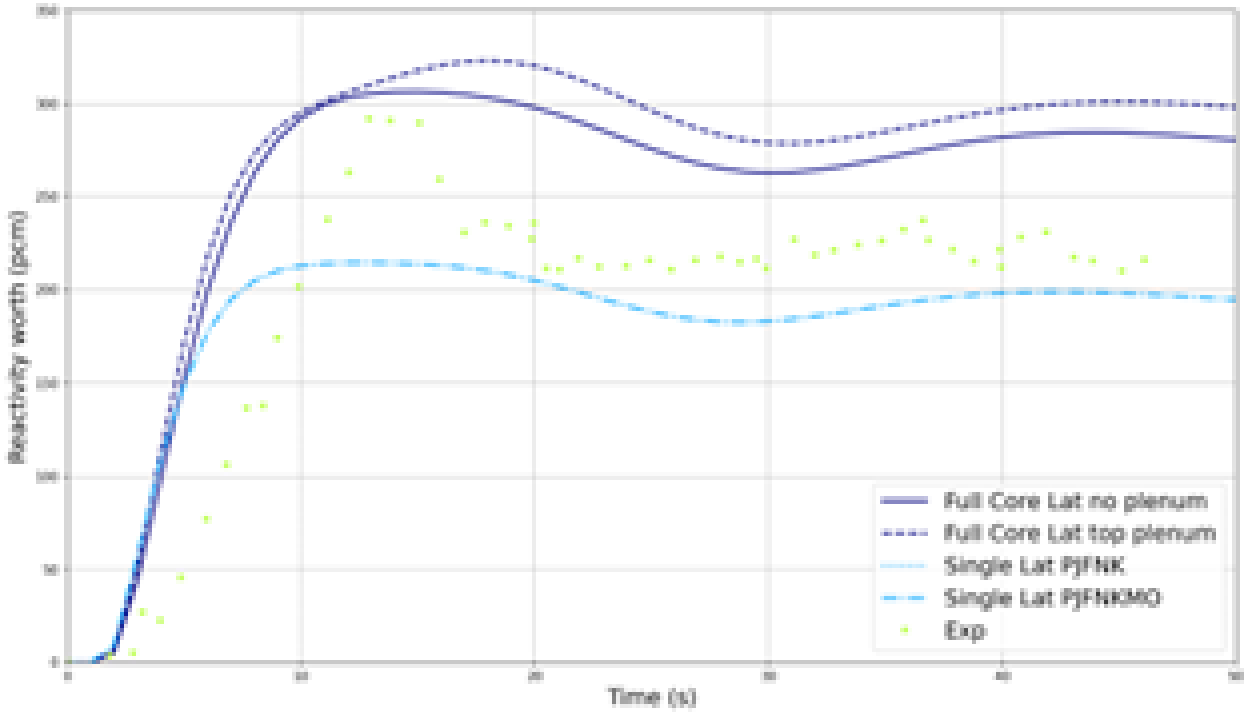


Figure 1: Pump startup simulation results compared to experimental data.

B.63 Fast and Rigorous Methods for Multiphysics SPn Transport in Advanced Reactors

Report Participants

Folk, Thomas H[1]
1 University of Michigan

Scientific Achievement

The HPC accounts will support DOE-funded research under the NEUP Program Project Number 22-26727 titled Fast and Rigorous Methods for Multiphysics SPn Transport in Advanced Reactors under DOE contract number DE-NE0009287. The objectives under this NEUP project are: 1. Develop a new discretization for the recently developed Generalized SPn equations 2. Develop the Hierarchical Poincare-Steklov solution algorithm for the multi-group GSPn equations 3. Establish error bounds on the current ISOXML interpolation procedures 4. Optimize procedures for case matrix construction for Monte Carlo Cross-Section Generation 5. Implement and evaluate Kernel Density Estimators into Shift for generation of few-group constants 6. Investigate relative efficiency and accuracy of SPH factors compared to Discontinuity Factors and potentially new equivalence factors. 7. Verification and Validation of the various methods developed in the project

Significance

By developing a fast and rigorous SPn methodology, NEAMS will gain a new capability for advanced reactor design and analysis with sufficient accuracy (e.g., $<$200 pcm on reactivity, and $<$1% RMS and $<$ 5% max difference on relative fission rate distributions) at an order of magnitude less computational resources (e.g., minutes with 10s of cores instead of hours with 100s of cores). This capability will enable NEAMS users to more quickly iterate on core designs to produce optimized results that can be verified by the existing high-fidelity capabilities. Through a rigorous approach, we expect to be able to fully characterize the numerical errors from each choice made in the development of the method. This will provide guarantees on accuracy and guidance on any future improvements.

Key Publications

None

Sponsor/Program

NEUP

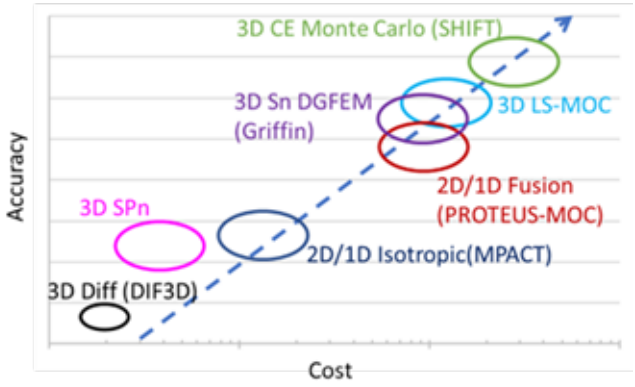


Figure 1: Accuracy vs. cost of various neutronics methods.

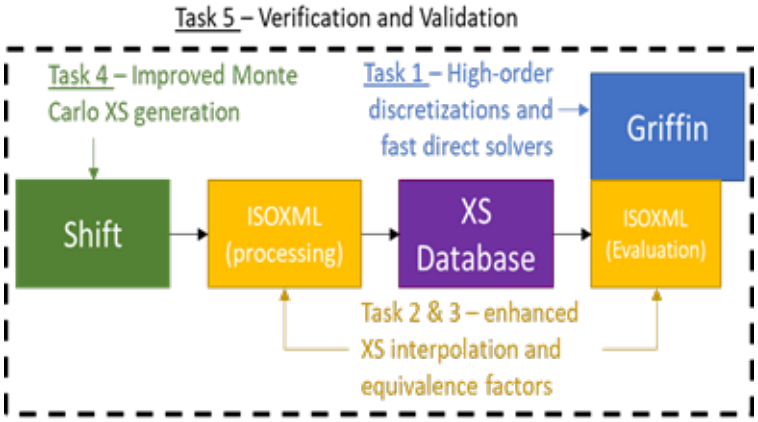


Figure 2: Overview of contribution of the project's tasks to NEAMS.

B.64 Safety Implications of High-Burnup Fuel for a 2 Year PWR Cycle

Report Participants

Fox, Mason A[1], Lindsay, Isabelle O[1], Brown, Nickolas [1]
1 University of Tennessee Knoxville

Scientific Achievement

Steady-state and transient safety analyses were performed for two proposed PWR core loadings capable of achieving a 24 month cycle length. These analyses emphasized performance during RIAs and anticipated operational occurrences. A multiphysics approach allowed the application of high-fidelity transient neutronics, systems-level thermal-hydraulics, and fuel thermomechanical performance models from PARCS, RELAP5-3D, and BISON to the analyses. This work identifies further opportunities and challenges for developing high-burnup LWR fuels, as well as high-priority needs in computational models and experimental data for improving predictive fuel performance capabilities.

Significance

A POLARIS-SCALE lattice physics model was developed for a proposed Gd2O3-doped high-burnup core design for depletion analysis and few-group cross section generation. Capabilities for control rod ejections were implemented into a PARCS model, and the model was extended for the analysis of a high-burnup core design using gadolinia-doped fuel. A RELAP5-3D model was modified to permit an analysis of control rod withdrawal and control rod ejections of PWR designs loaded with both ZrB2 Integral Fuel Burnable Absorber (IFBA) fuels and Gd2O3-blended UO2. Both core designs demonstrated the ability to achieve a 24 month cycle and satisfactory safety performance under typical design-basis RIAs. Boundary conditions from both PARCS and RELAP5-3D were provided to BISON for the fuel performance analysis. A detailed thermomechanical fuel performance analysis using BISON has been performed for control rod withdrawals, and an additional analysis is in progress to confirm and extend these findings.

Key Publications

Fox, M. A., Brown, N. R., Hu, J. & Mertyurek, U. (2023). Reactivity-Initiated Accident Analysis of a High Burnup PWR with a 24- Month Fuel Cycle. 20th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-20). (Submitted). Lindsay, I. O., Fox, M. A., Brown, N. R., & Capps, N. A. (2023). Evaluation of High-Burnup Fuel Coolability during a Control Rod Withdrawal. 20th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-20). (Submitted). Lindsay, I. O., Fox, M. A., Seo, S., Sweet, R. T., & Brown, N. R. (2023). Pressurized Water Reactor Control Rod Ejection Analysis Using PARCS, RELAP5-3D, and BISON for High Burnup Fuel. Transactions of the American Nuclear Society, ANS Annual Meeting. (Submitted).

Sponsor/Program

NEUP DE-NE0009212
DOE Office of Nuclear Energy UNLP fellowship.

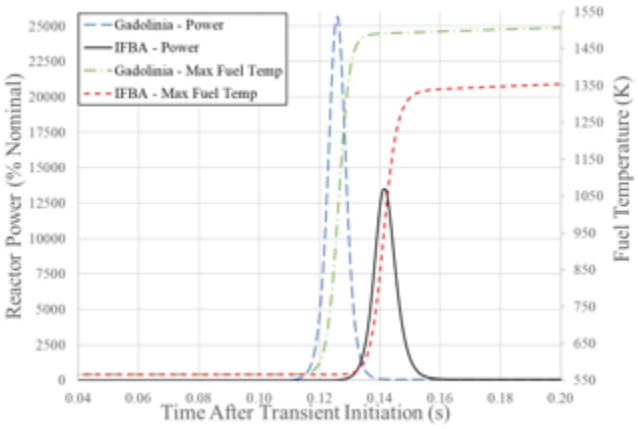


Figure 1: Control rod ejection transients of IFBA and gadolinia core.

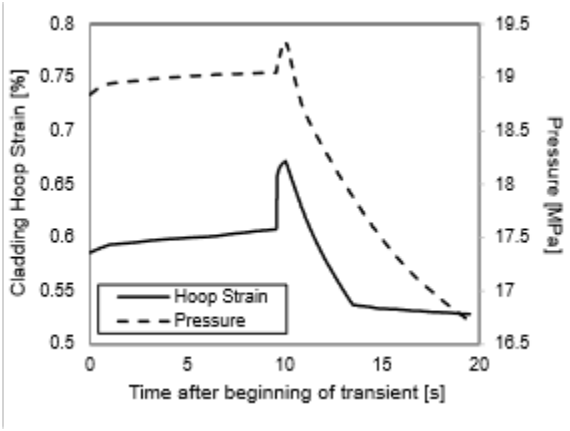


Figure 2: Cladding hoop strain and pressure for the IFBA core peak burnup rod during a control rod ejection accident.

B.65 MARVEL Project Primary Coolant System Pressure Vessel Analysis

Report Participants

Francis, Kyle B[1]
1 Walsh Engineering Services

Scientific Achievement

This project utilizes ABAQUS Standard to calculate stress intensities of the MARVEL pressure vessel for use in elevated temperature code calculations for ASME BPVC Section III Division 5 vessels. Stress intensities are generated for Service Level A, B, C, and D operating classifications using finite-element analyses. HPC was leveraged to run multiple models simultaneously and meet demanding project needs.

Significance

MARVEL's primary boundary is shown to pass all time-dependent and time-independent operating and off-normal allowables from the provided stress intensity contours. This endorses the project with a secure primary boundary designed in accordance with ASME BPVC Section III Division 5.

Key Publications

Francis, K. (2023). ECAR-6564, MARVEL Project Primary Coolant System Pressure Vessel Stress Documentation. (In Process, not for external publication)

Sponsor/Program

MARVEL Project

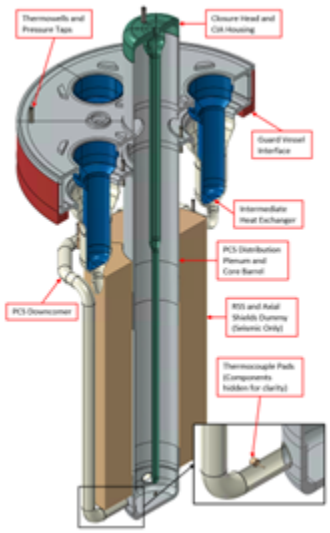


Figure 1: ABAQUS parts for the MARVEL primary boundary.

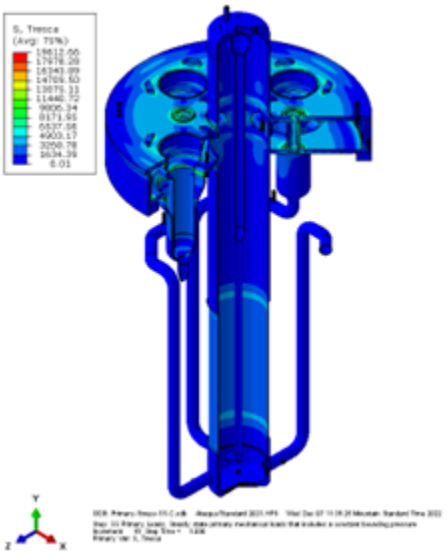


Figure 2: Primary stress intensity for normal operating conditions.

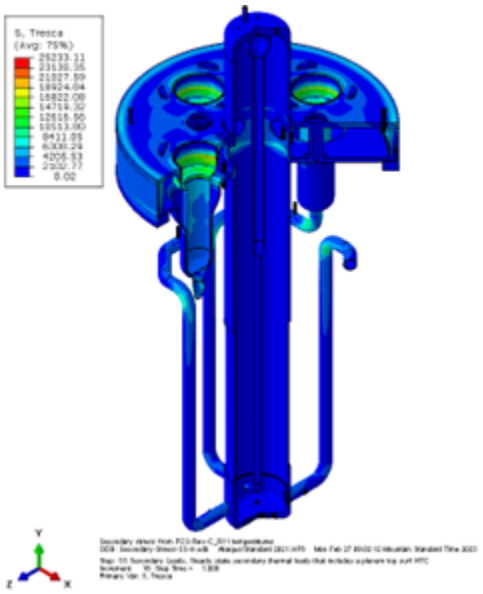


Figure 3: Secondary stress intensity for normal operating conditions.

B.66 System Thermal-Hydraulic Modeling of the EU DEMO Helium-Cooled Pebble-Bed Breeding Blanket

Report Participants

Froio, Antonio [1]
1 Dipartimento Energia, Politecnico di Torino

Scientific Achievement

The project, part of the activities carried out by the EUROfusion Consortium for the conceptual design of the Europran Union (EU) DEMO, a tokamak fusion reactor, aims at developing a transient model of the helium-cooled pebble bed (HCPB) breeding blanket (BB) using RELAP5-3D, including the primary heat transfer system up to the helium and molten salt intermediate heat exchanger. The work started in October 2022 when the RELAP5-3D license was issued. As the molten salt used for the intermediate heat exchanger is HITEC, which is not included in the standard RELAP5-3D fluids, the work is currently focused on implementing HITEC properties in RELAP5-3D.

Significance

The thermal-hydraulic modeling of the BB is of paramount importance to support the design of the BB and its related auxiliary systems, to investigate the consequences of possible accidental scenarios (e.g., LOFA), and to support future licensing. The work is ongoing, having started in October 2022, as the HITEC molten salt thermophysical properties needed to be implemented as a RELAP5-3D fluid; currently, such properties are being implemented and compiled using INL's HPC to enable modeling the whole HCPB system.

Key Publications

" G. Zhou, F. A. Hernndez, J. Aktaa, F. Arbeiter, L. V. Boccaccini, I. Cristescu, A. Froio, C. Garnier, M. Jetter, X. Z. Jin, M. Kamlah, B. Kiss, C. Klein, C. Koehly, I. Maione, L. Maqueda, C. Moreno, I. Moscato, I. Palermo, J. H. Park, V. Pasler, D. Passafiume, P. Pereslavtsev, A. Retheesh. 2022 Status of design activities of the Helium Cooled Pebble Bed breeding blanket in Europe, presented at the 25th Topical Meeting on the Technology of Fusion Energy (TOFE2022), 12 16 June 2022, Anaheim, CA, USA

Sponsor/Program

NCRC

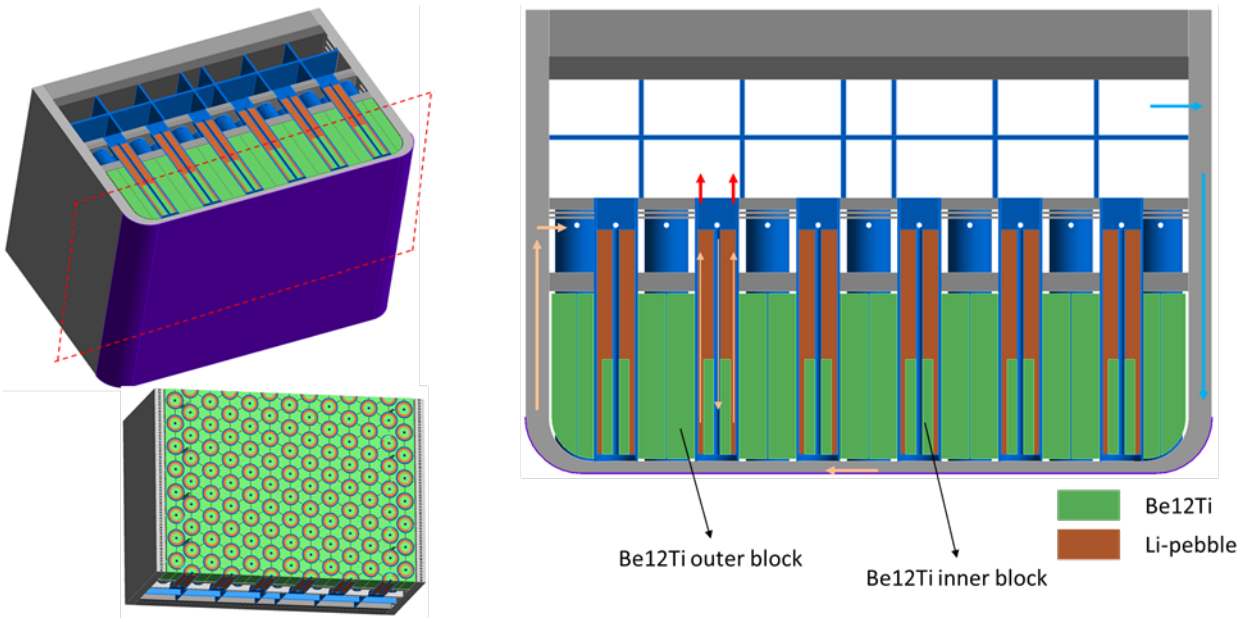


Figure 1: Flow path of the 2022 EU DEMO HCPB.

B.67 Framatome Evaluation of NEAMS for Advanced Reactors

Report Participants

Thomas, Justin E[1], Hobson, Gregory H[1]
1 Framatome

Scientific Achievement

This work evaluated Griffin for an HTGR prismatic fuel and advanced reactor analysis.

Significance

The work is currently in progress. Level 1 access was acquired for the Griffin code (on INL HPC resources). Initial calculations of fuel blocks and an HTGR core were run in 2022. The goal of this work is to learn to use Griffin and assess its capabilities through comparison to existing MCNP calculations for a helium gas-cooled reactor with prismatic TRISO fuel. Calculations range from fuel particles to fuel blocks to a 2D core layer, and finally, to a 3D core. Knowledge of Griffin will allow Framatome to assist advanced reactor companies with design and analysis tasks.

Key Publications

Previous year document: Framatome internal document FD-21-02199, Hobson, G. (2021). NEAMS Neutronics Codes 2021 Report, Griffin and VERA Document on current work on Griffin is in progress.

Sponsor/Program

NEAMS
Industry (Framatome project)

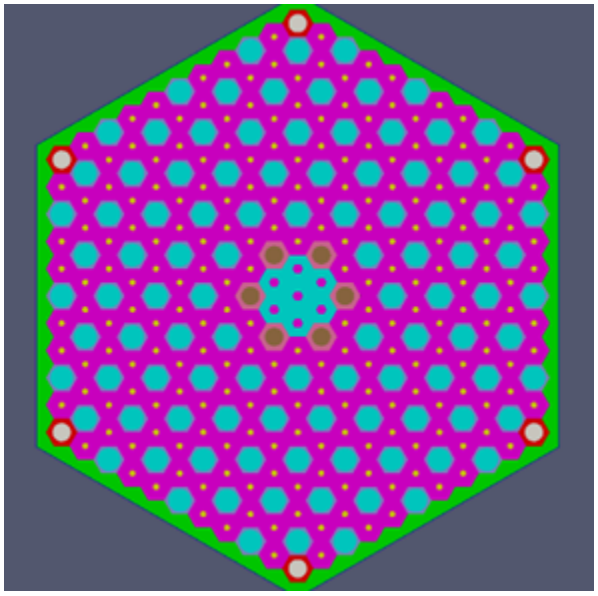


Figure 1: Standard fuel block.

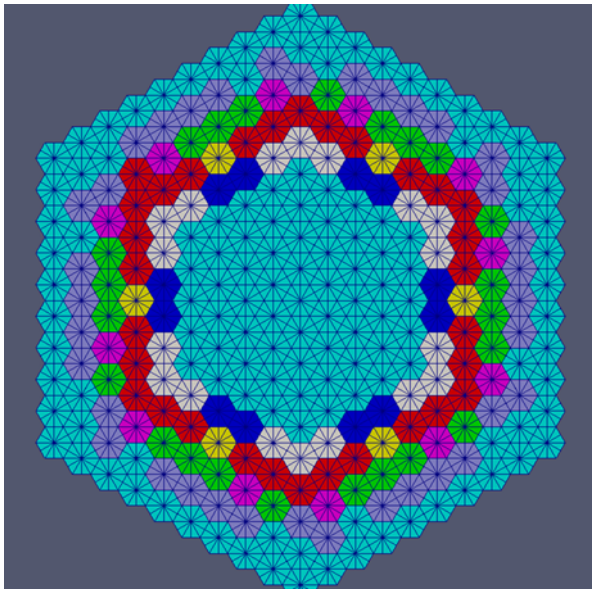


Figure 2: HTGR core design.

B.68 Development of a Creep Model Informed by Lower-Length-Scale Simulations to Simulate Creep in Doped UO2

Report Participants

Galvin, Conor O[1], Andersson, David [1], Cooper, Michael W[1]
1 Los Alamos National Laboratory

Scientific Achievement

Using molecular dynamics via the LAMMPS code, we predicted information at the atomistic scale to develop a mechanistic UO2 creep model for use in higher-length-scale fuel performance codes, such as BISON. We have performed segregation energy calculations at the grain boundary in UO2. These calculations are a key component that allows us to solve the defect concentrations at the grain boundary, which are input into our mechanistic creep model.

Significance

A number of improvements are being addressed to improve the mechanistic UO2 creep model. As this creep model uses point defects, there can be issues predicting unphysical high dopant concentrations at the grain boundary. Previously, to deal with this, a Madelung correction was applied as an energy penalty on the segregation energy models. To properly address this issue, charge neutrality within the grain boundary must be accounted for. A script was developed to apply an electron potential solver to the grain boundary that gives charge neutral combinations of defects. The segregation energies for oxygen interstitials, oxygen vacancies, electrons, and holes have been calculated using molecular dynamics. This information was put into the electron potential solver (along with the uranium vacancy and uranium interstitial segregation energy models) and used to calculate physical concentrations of the defects at the grain boundary. These concentrations will then be used to update the creep model and compare against experiment data.

Key Publications

A talk at TMS 2023 will include the segregation energy calculation results.

Sponsor/Program

NEAMS

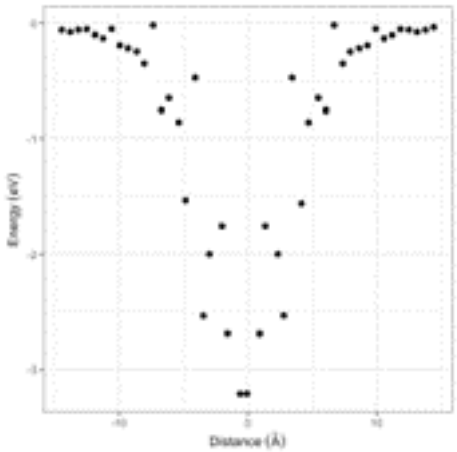


Figure 1: Segregation energy as a function of distance for uranium vacancies at the grain boundary.

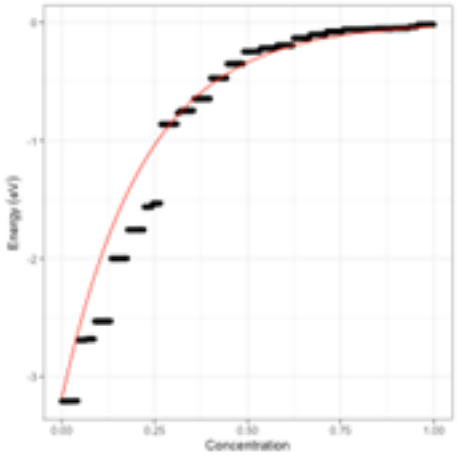


Figure 2: Segregation energy as a function of concentration for uranium vacancies at the grain boundary.

B.69 Systems of Nuclear Auxiliary Power (SNAP)

Report Participants

Garcia, Samuel [1], Naupa, Aguirre I[2], Lindley, Benjamin A[1], Kotlyar, Dan [2]
1 University of Wisconsin-Madison
2 Georgia Institute of Technology

Scientific Achievement

Neutronics and multiphysics modeling of the Systems of Nuclear Auxiliary Power (SNAP) 8 experiments using Serpent and NEAMS tools. At this point, a benchmark model of the SNAP 8 Experimental Reactor (S8ER) dry experiments (no coolant, low power) has been completed and submitted for publication and is currently under review. Additionally, progress has been made on Serpent-Griffin modeling workflow, wherein the Griffin model is within 100 pcm of Serpent results for the dry critical configuration experiment. Publications detailing these results, along with work leading up to the dry experiment publication, are available through the American Nuclear Society (ANS).

Significance

The significance of the benchmark model were three-fold: outlining and encountering errors with original SNAP documentation, creating neutronics models with great agreement to study microreactor features (solid moderator, hardened spectrum, hydrogen sensitivity, etc.), and creating a reference solution for multiphysics modeling. The progress on the multiphysics modeling is significant as it showcases preliminary results to validate Griffin against the reference solution for critical configurations. Continuing this work will enable multiphysics studies that are unique and of interest to current microreactor research problems (hydrogen permeation behavior, reactivity effects due to hydrogen permeation, burnup characteristics for solid moderators, etc.). With the dry experiment benchmark models created, it composes the first half of what will become a full dry and wet benchmark publication under the International Handbook of Evaluated Reactor Physics Benchmark Experiments (IRPhE).

Key Publications

Garcia, S., Naupa, I., Boyd, A., Paleen, O., Kotlyar, D., & Lindley, B. (2023). Detailed Reflector and Drum Modeling of the SNAP8 Criticality Configuration Experiments using Serpent with ENDF/B-VII.1 and ENDF/B-VIII.0 Libraries. Transactions of the American Nuclear Society, 128, 744–747. https://doi.org/10.13182/T128-42063

Garcia, S., Naupa, I., Boyd, A., Paleen, O., Kotlyar, D., & Lindley, B. (2022). Validation of SNAP8 Criticality Configuration Experiments Using SERPENT. Transactions of the American Nuclear Society, 127, 1158–1161. https://doi.org/10.13182/T127-39586

Garcia, S., Naupa, I., Paleen, O., Fowler, E., Boyd, A., Kotlyar, D., & Lindley, B. (n.d.). Reproducible Benchmark for the SNAP 8 Experimental Reactor at Dry Conditions. Annals of Nuclear Energy. (In Progress)

Naupa, I., Garcia, S., Lindley, B., & Kotlyar, D. (n.d.). Methods and Tools for SNAP Multiphysics Benchmark Evaluation. ANS 2023 Student Conference, Knoxville, TN. Naupa, I., Garcia, S., Terlizzi, S., Abou-Jaoude, A., Lindley, B., & Kotlyar, D. (August 13-17). Verification of the

Serpent-Griffin Workflow using the SNAP 8 Experimental Reactor. The International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering, Niagara Falls, Ontario, Canada.

Sponsor/Program

the DOE Office of Nuclear Energy NEUP under Contract No. DE-NE0009217
Office of Nuclear Energy of the U.S. Department of Energy and the Nuclear Science User Facilities under Contract No. DE-AC07-05ID14517.

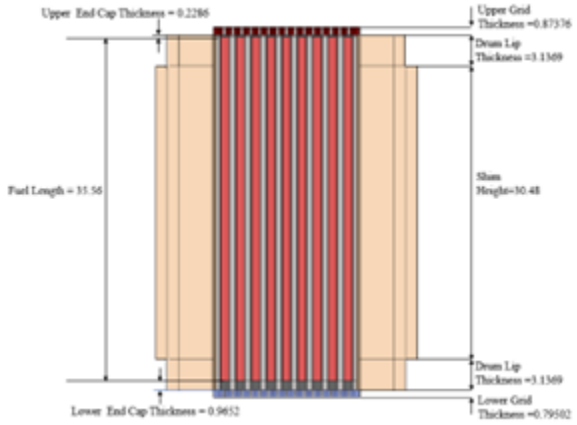


Figure 1: Dimensioned axial view of the S8ER.

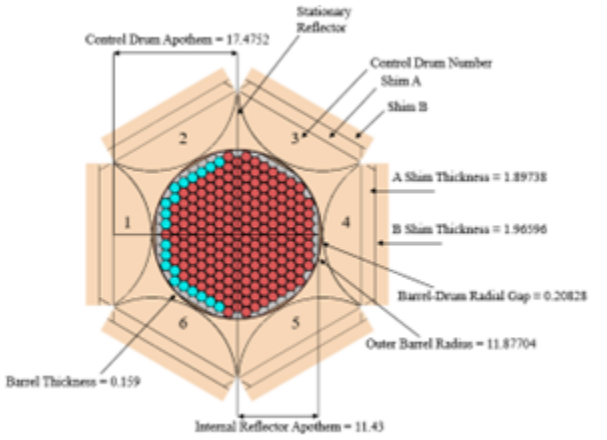


Figure 2: Dimensioned radial view of the S8ER.

B.70 Simultaneous Fuel Cracking and Pellet-Cladding Mechanical Interaction using Multiphysics Phase-Field Modeling

Report Participants

Gauthier, Vincent [1], Shirvan, Koroush [1]
1 Massachusetts Institute of Technology

Scientific Achievement

My work aims at implementing PCMI in a BISON simulation with the fragmentation of the pellet modeled with a phase-field damage model. The work was split in two parts. The first part proposed a benchmark for mechanical contact conditions under MOOSE framework. To that end, a numerical simulation of an SFCT beam that features an interface between a ceramic (concrete) and metal (steel) was proposed. The simulations showed that the mortar contact method is the more suitable to reproduce an experimental crack pattern at a lower computational cost. The second part of this work consists of leveraging the settings determined during the benchmark study to implement PCMI in BISON by picking up the work carried out in [1].

Significance

Implementing PCMI enables more accurate simulations of the stress state within the cladding during nominal and incidental conditions. As a result, the predictability of nuclear codes is enhanced by implementing PCMI, which increases nuclear safety.

Key Publications

M&C conference (13-17 August 2023, Niagara Falls).

Sponsor/Program

Office of Nuclear Energy of the U.S. Department of Energy and the Nuclear Science User Facilities under Contract No. DE-AC07-05ID14517
US Department of Energy under award DE-NE0009212

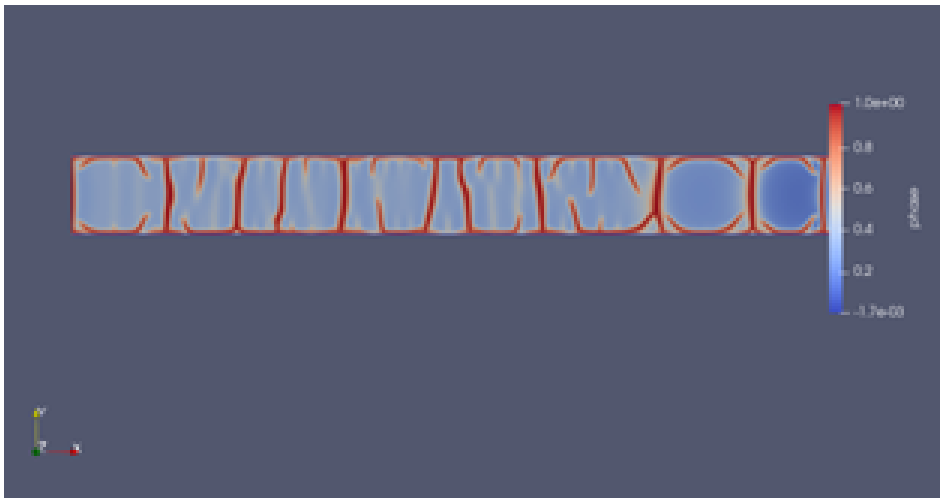


Figure 1: Crack pattern obtained for a tensile on a SFCT beam.

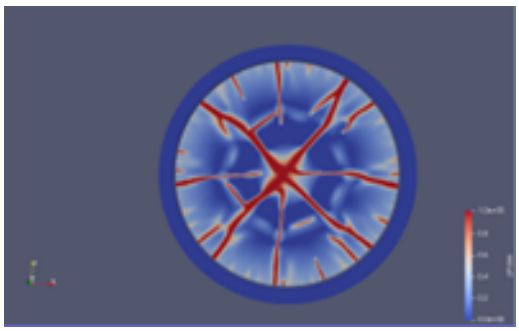


Figure 2: Crack pattern obtained in [1].

B.71 Microstructure and Irradiation Effects on UO2 Fracture Via Phase-Field Approach

Report Participants

Gencturk, Merve [1], Ahmed, Karim [1]
1 Texas A&M University

Scientific Achievement

The introduction of this new approach enhances the fundamental comprehension of nuclear fuel performance during normal and transient conditions. It also provides a predictive modeling tool for deriving physics-based criteria for the fracture behavior of the current and new nuclear fuel designs.

Significance

We developed a new mesoscale model using multiphysics that utilizes phase-field fracture modeling to forecast fracture occurrences in various nuclear fuels under different circumstances.

Key Publications

The proposed manuscript is under preparation for submission/publication.

Sponsor/Program

NEUP-DE-NE0009134, Project # is 21-24460, Package ID NU-21-TX-TAMU-020104-04

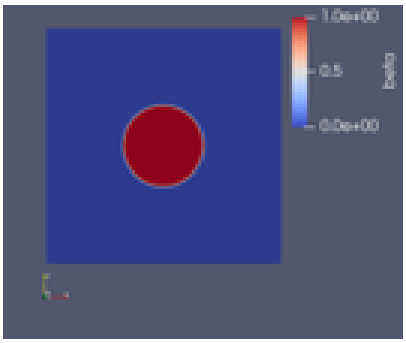


Figure 1: A void in the microstructure.

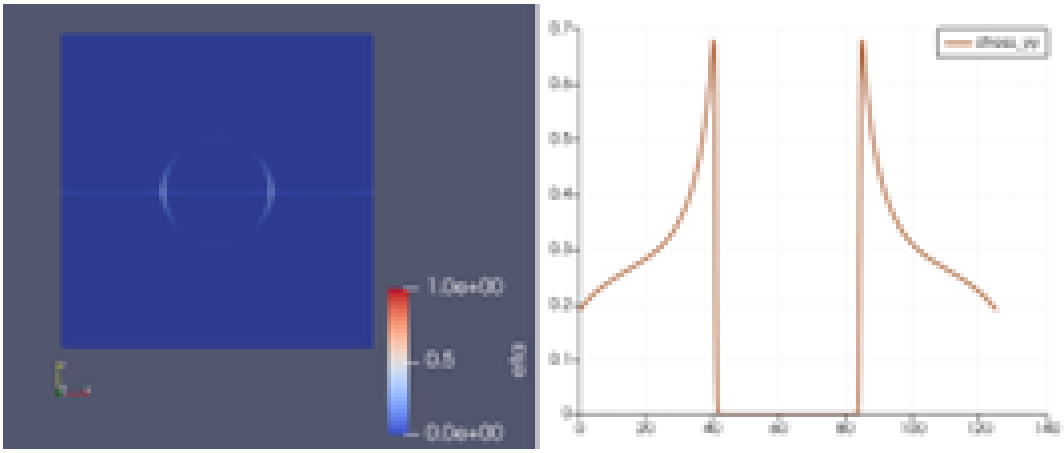


Figure 2: Voids in the microstructure indicate the accumulation of stress.

B.72 Design and Analysis of Kaleidos Shielding Systems

Report Participants

Giuggio, Morgan A[1]
1 Radiant Industries Incorporated

Scientific Achievement

This work examined understanding the effects of radiation on the environment in deep shielding problems relevant to the design and implementation of Radiant's portable micro-HTGR. I utilized HPC resources to perform analyses that inform the design decisions for the reactor under development at Radiant.

Significance

The work is still in progress but thus far has included activation projections of the ground and shielding materials as well as dose predictions to ensure the safety of the public and radiation workers. Since Kaleidos will be conducting fueled testing at INL, this work has also contributed to creating requirements for the EBR-II testing dome. Future work will include an analysis of neutron shielding attenuation and optimization, activation of the shipping container, and the effects of high-flux environments on silica materials. The resources at INL have been invaluable for my shielding design and analysis work. Since shielding calculations are computationally expensive, I utilize Sawtooth or Lemhi every day. These resources are critical to my work, both for shielding analysis and the development of our in-house software. Additionally, the ease of use of the systems and staff assistance when issues arise has been exceptional.

Key Publications

None

Sponsor/Program

Industry

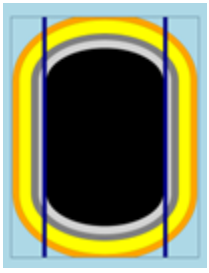


Figure 1: Cross section of preliminary shielding design.

B.73 CLOWE Fuel Element Conceptual Design

Report Participants

Gluntz, Andrew J[1], Cichocki, Eric R[1], Mervis, Alec I[1]
1 MPR Associates

Scientific Achievement

The objective of this work is to design an LEU fuel element to be used in ATRC as part of the LEU conversion effort. This LEU fuel element for ATRC will be called CLOWE. During the design process, the performance of several conceptual design iterations in ATRC is evaluated, considering previously defined functional and operational requirements. Several of the CLOWE conceptual design iterations are created by making minor changes to the LOWE fuel element designed for use in ATR. These changes include decreasing the fuel foil arc length, decreasing the fuel enrichment, decreasing the fuel foil thickness, and defueling one of the fuel plates. Other designs are considered that use the LOWE fuel element and adjust the ATRC core to accommodate this element, including adding boron and other poisons to the core to decrease reactivity.

Significance

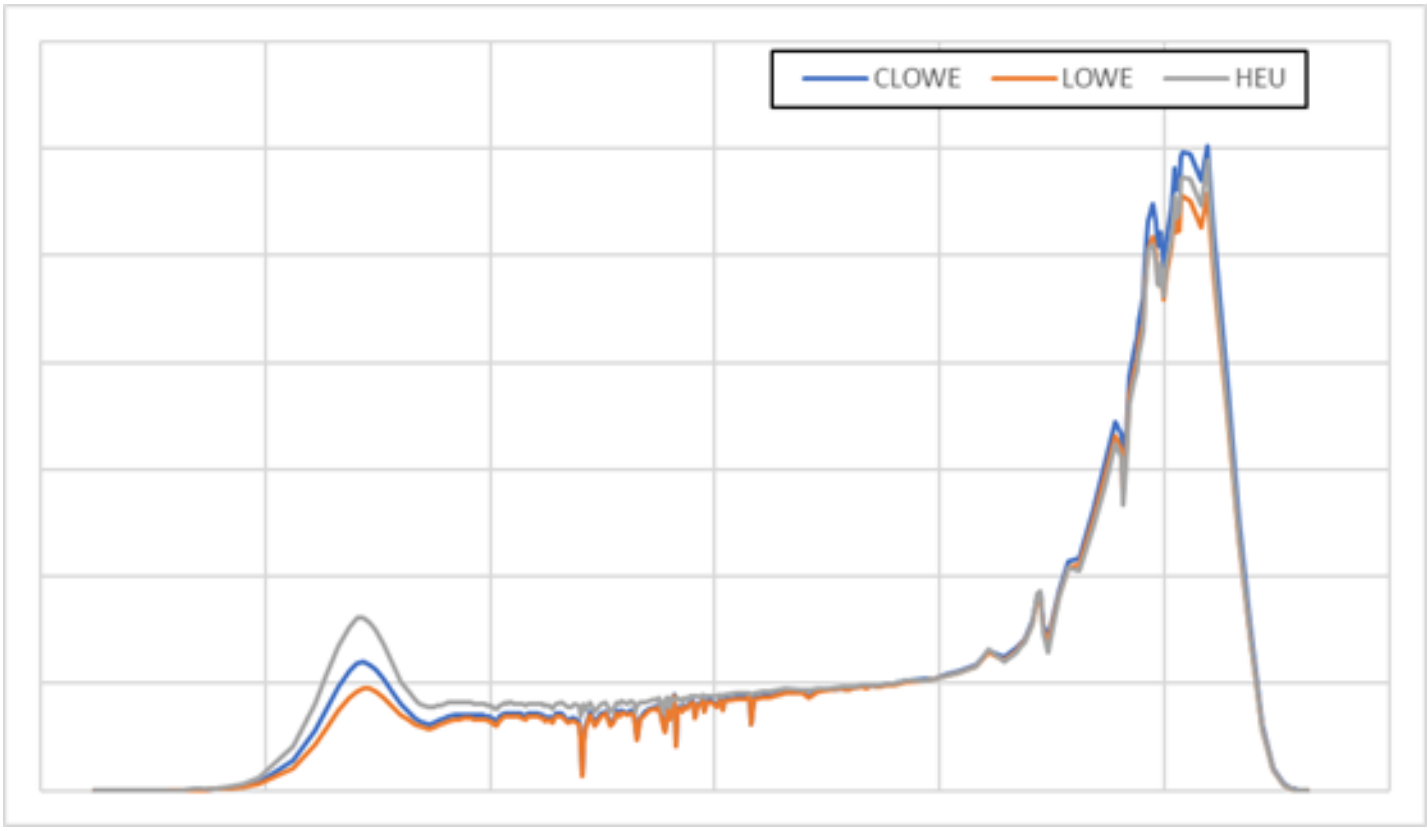
Following the initial conceptual design analysis, the CLOWE arc length reduction conceptual design was selected for further analysis. Additional analysis performed on this design includes spectrum analysis, steady-state kinetics analysis, and transient physics analysis. The results from the spectrum analysis show a difference between the CLOWE element neutron spectrum and the LOWE element neutron spectrum. This may impact the ability of ATRC to act as a mock-up for ATR in the future. It is not anticipated that the CLOWE element will be able to meet all of the functional and operational requirements, but consideration must be given on how to mitigate the effects of the requirements the element does not meet in order to satisfy the objective of using the CLOWE element in ATRC.

Key Publications

" Cichocki, E. & Mervis, A., 2022. CLOWE Conceptual Design Analysis. MPR Calculation 1129-0241-CALC-001, MPR Associates. " Cichocki, E., 2022. CLOWE Conceptual Design Spectrum and Experiment Reactivity Worth Analysis. MPR Calculation 1129-0241-CALC-002, MPR Associates. " Gluntz, A, 2023. CLOWE Conceptual Design Energy Deposition Analysis. MPR Calculation 1129-0241-CALC-005, MPR Associates. " Johnson, A., 2022. CLOWE Conceptual Design Core Kinetics Analysis. MPR Calculation 1129-0241-CALC-003, MPR Associates. " Johnson, A., 2022. ATRC CLOWE Transient Physics Analysis. MPR Calculation 1129-0241-CALC-004, MPR Associates.

Sponsor/Program

ATR, ATRC


CLOWE
LOWE
HEU

B.74 Full-Core Multiphysics LWR Simulations for High-Burnup Fuels

Report Participants

Capps, Nathan A[1], Greenquist, Ian T[1], Wysocki, Aaron J[1], Hirschhorn, Jake [2], Graham, Aaron M[1]
1 Oak Ridge National Laboratory
2 Idaho National Laboratory

Scientific Achievement

Researchers at ORNL have been coupling the LWR codes VERA, SCALE, and BISON to perform multiphysics full-core simulations of very high burnup (>65 GWd MTU-1) fuel in steady-state and transient conditions.

Significance

This work attempts to identify the operating conditions that lead to susceptibility to FFRD, a scenario where very-high-burnup fuel is released into the core after a LOCA leads to cladding rupture. The fuel conditions and susceptibility to rupture are calculated by BISON using operating conditions supplied by VERA and TRACE.

Key Publications

" Greenquist, Ian, et al. "Multiphysics analysis of fuel fragmentation, relocation, and dispersal susceptibility Part 1: Overview and code coupling strategies." Annals of Nuclear Energy 191 (2023): 109913. " Hirschhorn, Jake, et al. "Multiphysics analysis of fuel Fragmentation, Relocation, and dispersal Susceptibility Part 2: High-Burnup Steady-State operating and fuel performance conditions." Annals of Nuclear Energy 192 (2023): 109952. " Wysocki, Aaron, et al. "Multiphysics analysis of fuel fragmentation, relocation, and dispersal susceptibility Part 3: Thermal hydraulic evaluation of large break LOCA under high-burnup conditions." Annals of Nuclear Energy 192 (2023): 109951.

Sponsor/Program

NEAMS

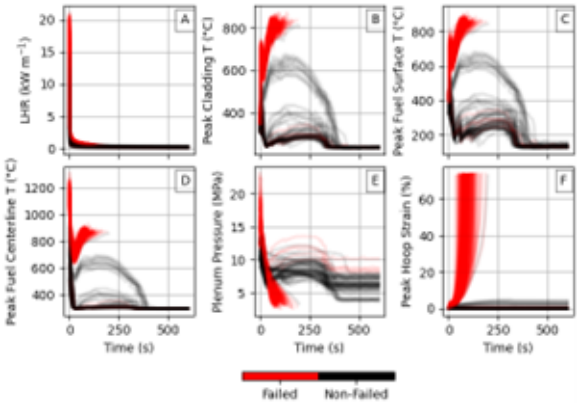


Figure 1: Flow chart of the passing of data between codes used in this work. Blue boxes represent codes, and white ovals represent data passed between codes. The green box represents the calculation of FFRD susceptibility. The steady-state steps are all in the gray region.

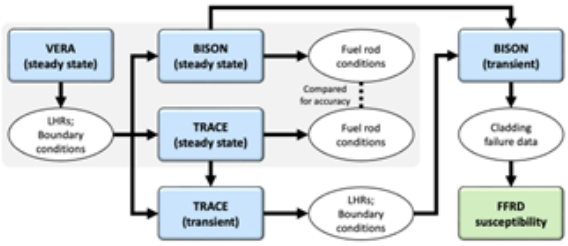


Figure 2: BISON predictions of fuel and cladding performance of 242 high-burnup rods during the large-break loss-of-coolant accident (LBLOCA) transient. Lines are colored based on whether the Chapman correlation predicted cladding burst.

B.75 Using Physics-Informed Artificial Neural Networks (ANNs) to Characterize Phase-Field Microstructures

Report Participants

Hafen, Joseph [1], Rhoads, Benjamin M[1], Choudhury, Samrat [1]
1 University of Mississippi

Scientific Achievement

Artificial neural networks (ANNs) are a data-processing method used to characterize complex datasets of images and other types of data. Over the previous year, I trained ANNs to characterize 2D phase-field-generated ferroelectric microstructures. My research focuses on improving the neural network's ability to characterize and reproduce microstructural data with an accuracy comparable to phase-field. I achieved this goal by implementing three phase-field equations into the ANN as loss functions.

Significance

The present research helps expedite the materials design process by increasing the accuracy of expedited phase-field-generated microstructural data with physics-based learning constraints in the form of loss functions. This research serves as preliminary research on uranium-based nuclear fuel for fellow researchers at the University of Mississippi. Given that ANNs are commonly used to characterize materials data, this research will likely be used and cited by other research groups.

Key Publications

This research will be presented in the upcoming The Minerals, Metals, & Materials Society' conference in Orlando, FL. Once results are finalized, they will be submitted to a journal for publication at the end of this year or early next year. The publishing company still has not yet been determined.

Sponsor/Program

University of Mississippi

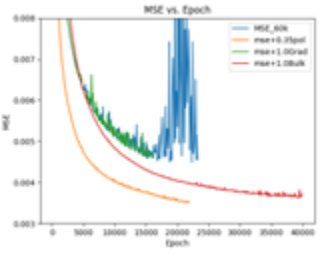


Figure 1: Decreased MSE loss with phase-field-based loss functions.

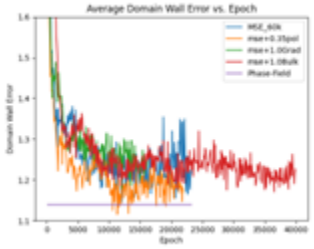


Figure 2: Achieving metrics closer to phase-field accuracy with phase-field-based loss functions.

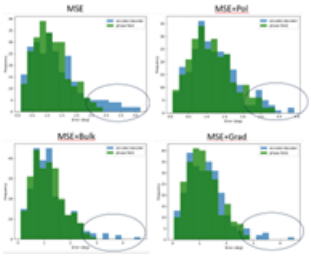


Figure 3: Decrease of domain wall error (frequency) with phase-field-based loss functions.

B.76 Full-Core Fuel Performance of High-Burnup Fuel in LWRs

Report Participants

Halimi, Assil A[1], Shirvan, Koroush [1]
1 Massachusetts Institute of Technology

Scientific Achievement

Pursuing better nuclear fuel utilization through higher burnups has been an effective approach to improve the fuel cost of nuclear power plants, reduce the waste volumes, and achieve better conversion ratios. To allow higher than current standards of burnup operation (i.e., >62 MWd/kgHM average pin), the technical feasibility of new limits (e.g., 68 or 75 MWd/kgHM) has to be investigated. For such reason, core design, fuel performance, and safety analyses are performed to analyze the implications of these potential new limits and underline the practical challenges in adopting high-burnup fuels. Core design and reactorwide safety features are evaluated using the STUDSVIK package (CASMO4e/SIMULATE3), and fuel performance is evaluated using the auditing tool FRAPCON4.0 as the low fidelity simulation code in addition to BISON as the high-fidelity modeling code. ATF's capability to enable high-burnup operation is assessed using BISON. For a more realistic assessment, the fuel performance analysis (with both FRAPCON and BISON codes) is carried out with a full-core approach (i.e., all pins in the core are analyzed). In BISON, a scaling approach is adopted to reduce the computational cost. An example of full-core fuel performance results is illustrated in Figure 1. The INL HPC capability is used to run BISON fuel performance simulations.

Significance

Two approaches to achieve high-burnup operation in a PWR have been identified. The first relies on longer cycle operation (i.e., 24 months), improving the capacity factor of the reactor and hence its O&M cost (assuming limited impact on outage durations). The second reduces the fuel reload fraction and consequently improves the fuel cost. After achieving core design and optimization in neutronics codes (CASMO/SIMULATE), the fuel design is altered based on outputs from fuel performance tools, such as BISON, to comply with the current NRC regulatory limits. While this work focuses on steady-state and transient power operation, accidental scenarios are evaluated separately by the University of Tennessee as part of the same NEUP project. Satisfactory core performance has been obtained for both fuel management approaches. A full-core fuel performance assessment using FRAPCON has been finalized. A high-fidelity fuel performance evaluation using BISON is currently under implementation as single pin modeling discrepancies between FRAPCON and BISON had to be fully characterized before running the full-core evaluation. The satisfactory performance of high-burnup fuel and core designs in neutronics and fuel performance tools with respect to NRC limits as well as industry best practices is the main objective of this effort. It is a first step before testing, licensing, and commercializing higher burnups in LWRs.

Key Publications

Halimi, A., Shirvan, K., 2022. Investigation of Achievable Peak Rod Average Burnup with Full Core Fuel Performance for 4-Loop PWRs, TopFuel Conference, Rayleigh, NC.

Sponsor/Program

NEUP U.S. Department of Energy Project 21-23984, Safety Implications of High Burnup Fuel for a 2-Year PWR Fuel Cycle.

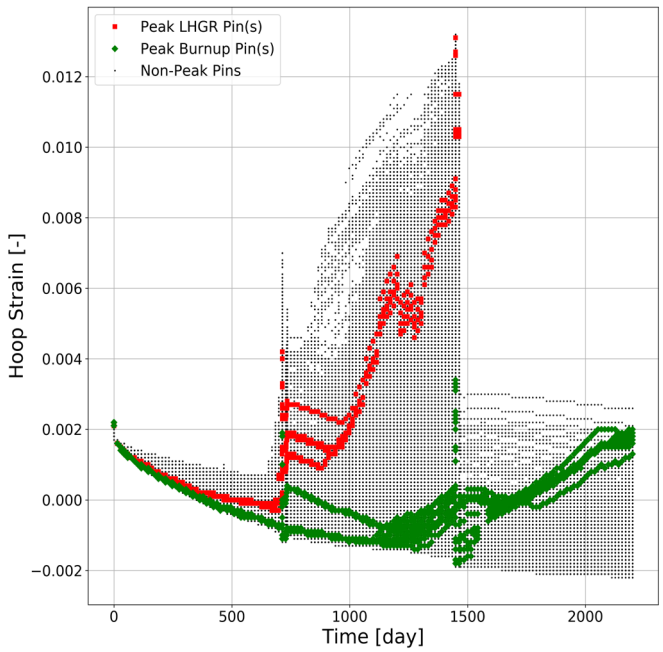


Figure 1: Example of parameters of interest (cladding hoop strain and rod plenum pressure) in full-core fuel performance modeling of a high-burnup PWR core.

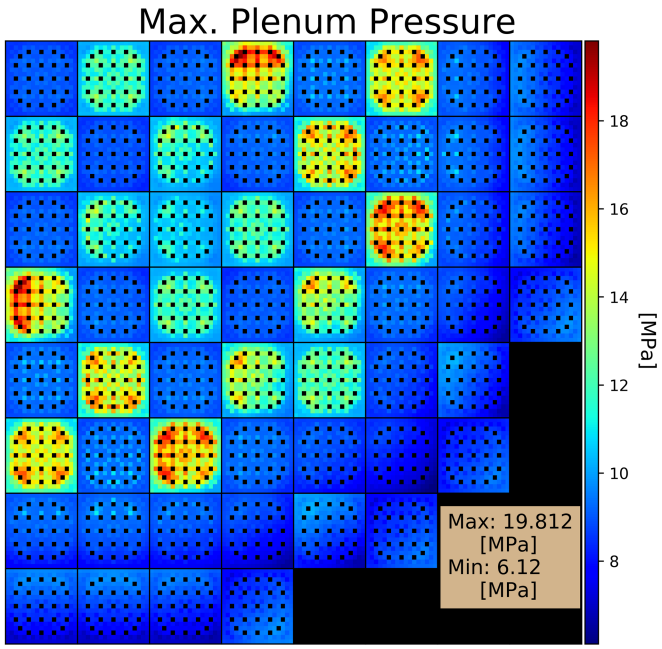


Figure 2: Max plenum pressure.

B.77 Design of Plausible ATR Cycles to Perform Element Test (ET) 3 Under the ATR LEU Fuel Project

Report Participants

Harron, Marc A[1], Tortorello, John C[1], Brown, Curtis A[1], Hardtmayer, Douglas E[1]
1 MPR Associates

Scientific Achievement

This work demonstrates that an experiment which supports the qualification of an LEU fuel element designed for ATR, referred to as the LOWE element, is achievable in plausible ATR cycles. This experiment, referred to as ET-3, is one in a series of experiments under the ATR LEU Fuel Project. The set of ATR cycles that meet the needs of ET-3 are developed as part of this effort. The work consists of a radiation transport analysis, material depletion analysis, and extensive data analysis with Python.

Significance

This work informs the design of the actual ATR cycles that will contain this high-powered experiment. This experiment is a significant contribution to the ATR LEU Fuel Project at INL, and to other reactors nationwide as part of the USHPRR Conversion Program, that will reduce the use of HEU in research reactors. A database of plausible hypothetical cycles containing LOWE fuel is produced as part of this work. This database provides several other LOWE-related efforts with models of representative ATR cycles containing LOWE fuel, further supporting progress in the abovementioned projects.

Key Publications

MPR Associates. 2021. MPR Calculation 1129-0279-CALC-001, Rev. 0 (In progress).

Sponsor/Program

ATR

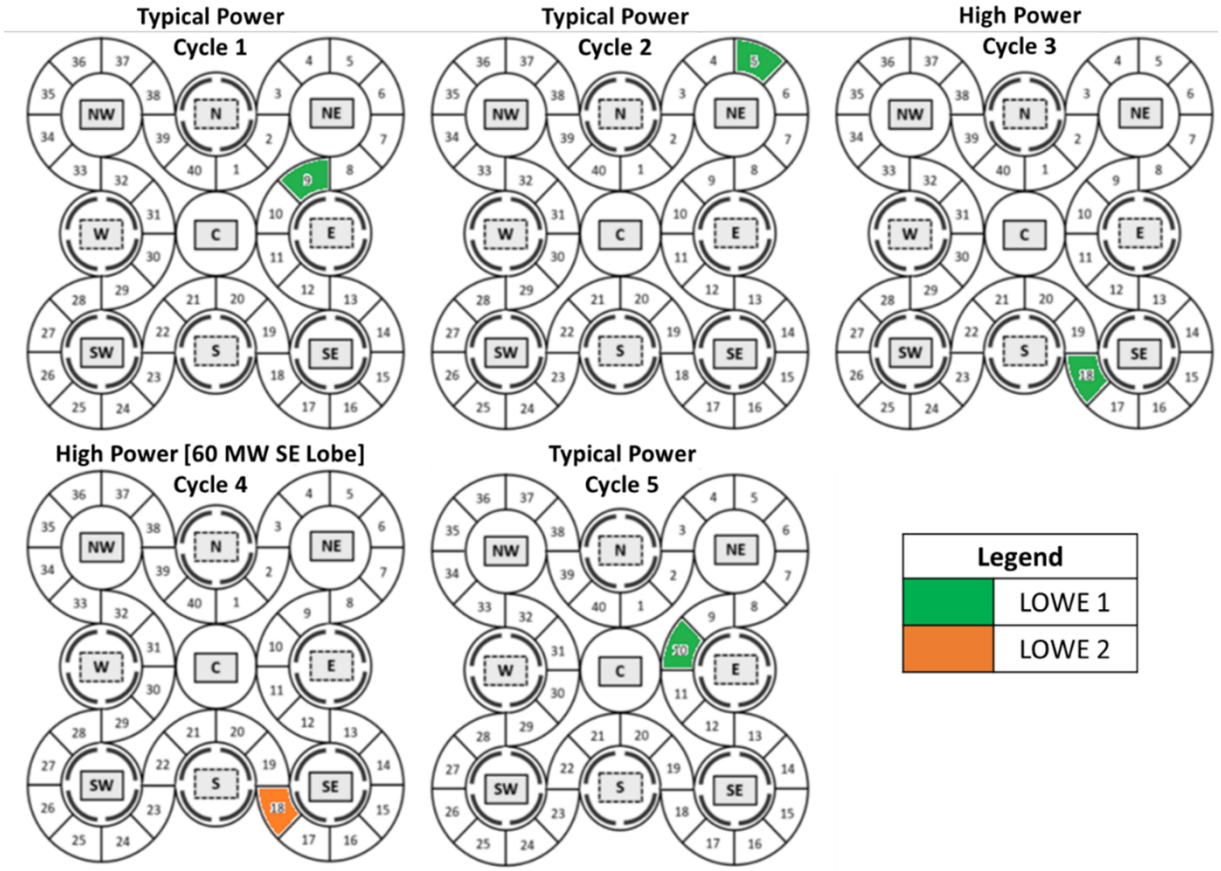


Figure 1: Plausible ATR cycles containing the ET-3 experiment.

B.78 Re-solution of Xe Gas Bubbles in the U-10Mo Fuel

Report Participants

Hasan, ATM-Jahid [1], Malakkai, Linu [2], Swischer, Matthew [2], Beeler, Bejamin [2]
1 North Carolina State University
2 Idaho National Laboratory

Scientific Achievement

To understand the U-10Mo fuel evolution under irradiation, mesoscale, and engineering-level fuel performance models require knowledge of the fundamental mechanistic behavior of fission products in the fuel. As such, knowledge of the progression of Xe gas bubbles in the fuel is crucial. The Xe gas bubbles act as a sink for individual Xe atoms (trapping Xe) and subsequently grow in size after absorption. Under irradiation, the Xe atoms in the gas bubble are re-solved back into the fuel matrix, and this process reduces the bubble size. In this work, we investigate the re-solution of xenon gas bubbles in U-Mo fuel with MD simulations. The efficiency of both the homogeneous and heterogeneous resolution mechanisms is investigated via the primary knock-on atom and thermal spike methods, respectively.

Using the data obtained from MD simulations and the electronic stopping power of fission products in U-10Mo fuel, the Xe re-solution rate is calculated. The re-solution rate found in this work is comparable to the re-solution rate used in the Dispersion Analysis Research Tool.

Significance

Molecular dynamics simulations are used in this study to provide a re-solution rate of Xe gas bubbles in U-10Mo fuel. Both homogeneous and heterogeneous re-solution have been simulated using the primary knock-on atom and thermal spike methods. Homogeneous re-solution is found to be negligible in describing the overall re-solution behavior. The fraction of re-solved Xe gas bubble atoms seems to be invariant with respect to bubble pressure and Xe density. This fraction is then used to model the re-solution fraction as a function of effective imparted energy into the lattice. Afterward, the electronic stopping power of Xe fission products in U-10Mo is used to provide a re-solution rate of Xe gas bubbles.

Key Publications

In Progress

Sponsor/Program

USHPRR

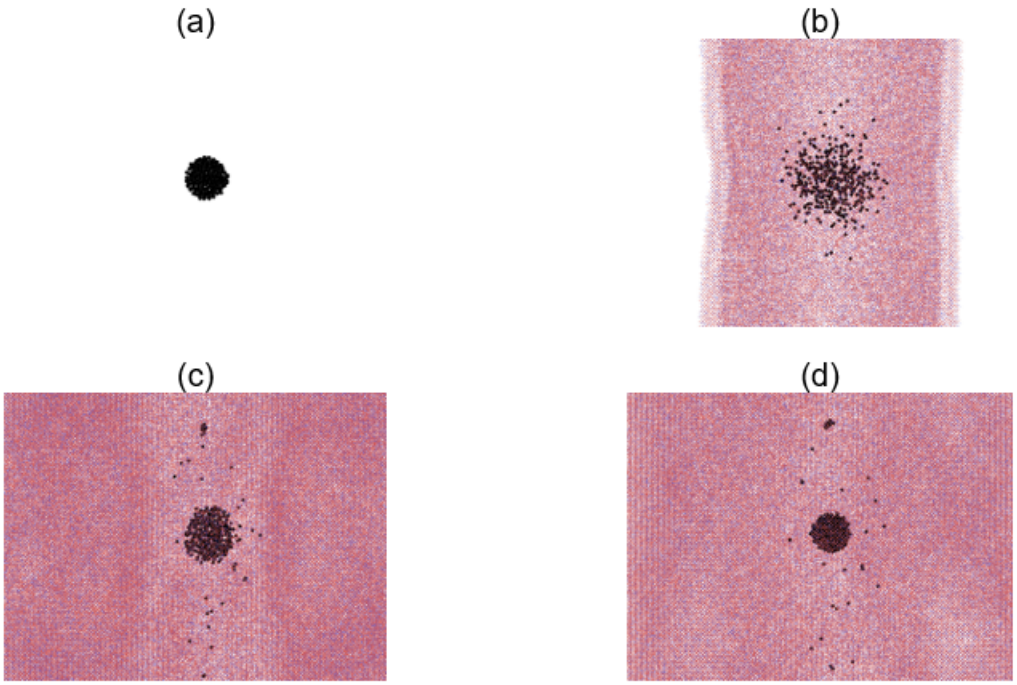


Figure 1: Snapshots of a thermal spike (3.5 MeV) simulation at (a) 0, (b) 1.5, (c) 44.5, and (d) 114.5 ps. Xe atoms are shown in black along with U (red) and Mo (blue) point defects.

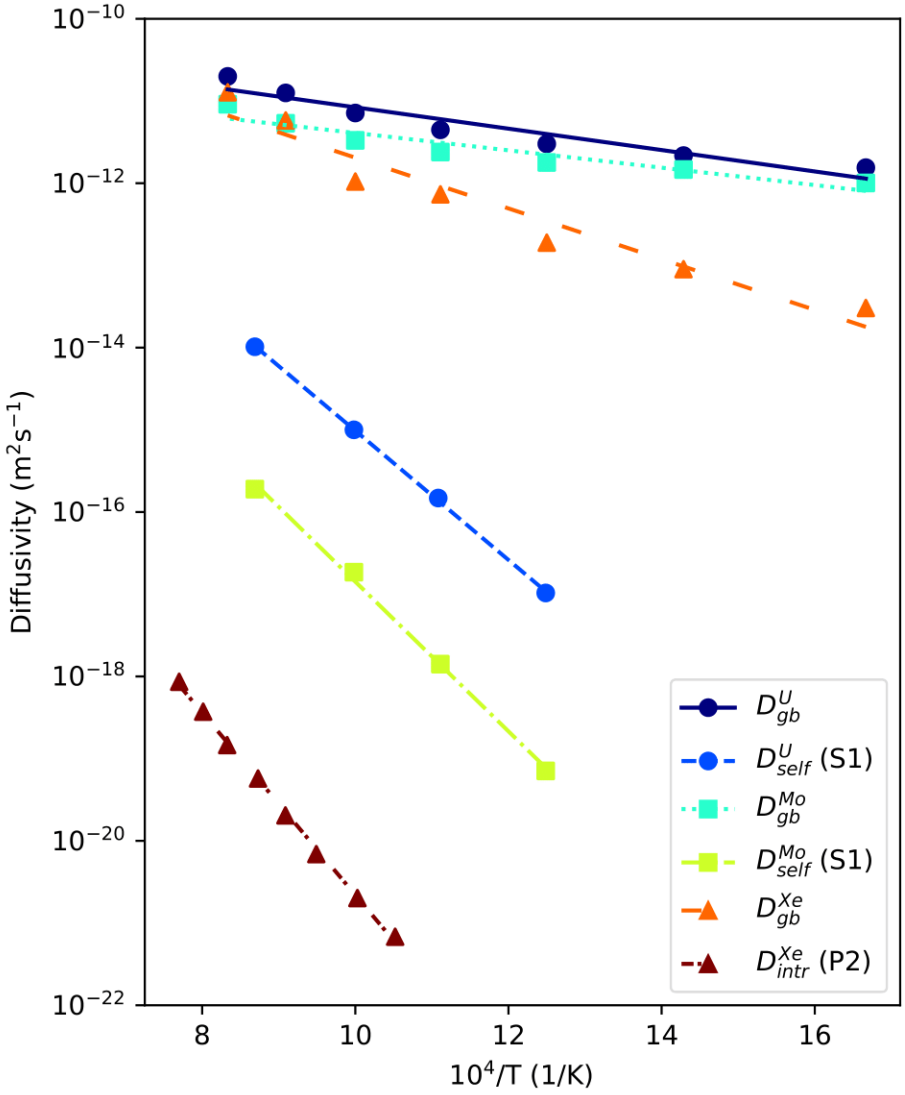


Figure 2: Comparison of the re-solution rate calculated in this work with the rate used in the Dispersion Analysis Research Tool model.

B.79 Multiscale Multiphysics Modeling and Simulations of Advanced Nuclear Reactors

Report Participants

Hu, Rui [1], Zou, Ling [1], Yang, Gang [1], Ooi, Zhiee J[1], Mui, Travis [1], O'Grady, Daniel J[1]
1 Argonne National Laboratory

Scientific Achievement

The primary goal of this work was to develop a multiscale multiphysics modeling capability for analyzing advanced nuclear reactors. Simulating advanced nuclear reactors requires capturing the phenomena of several fields of physics (e.g., reactor kinetics, thermal hydraulics, thermomechanics, fuel performance). The models are simulated using BlueCRAB and its submodules such as GRIFFIN, SAM, Pronghorn, BISON, etc. The GRIFFIN module is used to simulate the reactor kinetics behavior, the SAM and Pronghorn module are used to simulate the heat transport in the reactor core and heat removal through the primary loop and decay heat removal systems, and the BISON module is used to simulate the fuel performance and thermal mechanics of the reactor cores. The different submodels are coupled together using the MultiApp system in MOOSE. The BlueCRAB multiphysics modeling was demonstrated by performing steady-state analyses and transient simulations of typical reactor design basis events.

Significance

For plant systems analyses and assessing the adequacy of the emergency core cooling features of a design, the NRC is developing a suite of codes called BlueCRAB. BlueCRAB is the coupled combination of NRC codes and codes developed by the DOE NEAMS Program and can simulate a broad range of conventional and advanced reactor designs. To prepare for independent analysis as part of the review and to demonstrate the capabilities of BlueCRAB, this work supported the NRC to develop reference plant models for various advanced reactor types. The purpose of a reference plant is to provides both a test bench for the BlueCRAB system and a means to identify potential modeling and simulation challenges before a design review is underway.

Key Publications

Gang Yang, Ling Zou, Joseph Kelly, and Rui Hu, Updated SAM Model of a Reference Fluoride-Salt-Cooled High-Temperature Reactor for Multi-Physics Simulations, ANL-NSE-23/17, March 2023. Gang Yang, Ling Zou, and Rui Hu, Updated SAM Model for the Molten Salt Reactor Experiment (MSRE), ANL-NSE-23/8, Feburary 2023 Hu, R; J. Fang, D. Nunez, M. Tano, G. Giudicelli, R. Salko, Development of Integrated Thermal Fluids Modeling Capability for MSRs, ANL/NSE-22/56, August 2022.

Sponsor/Program

NRC, DOE NEAMS

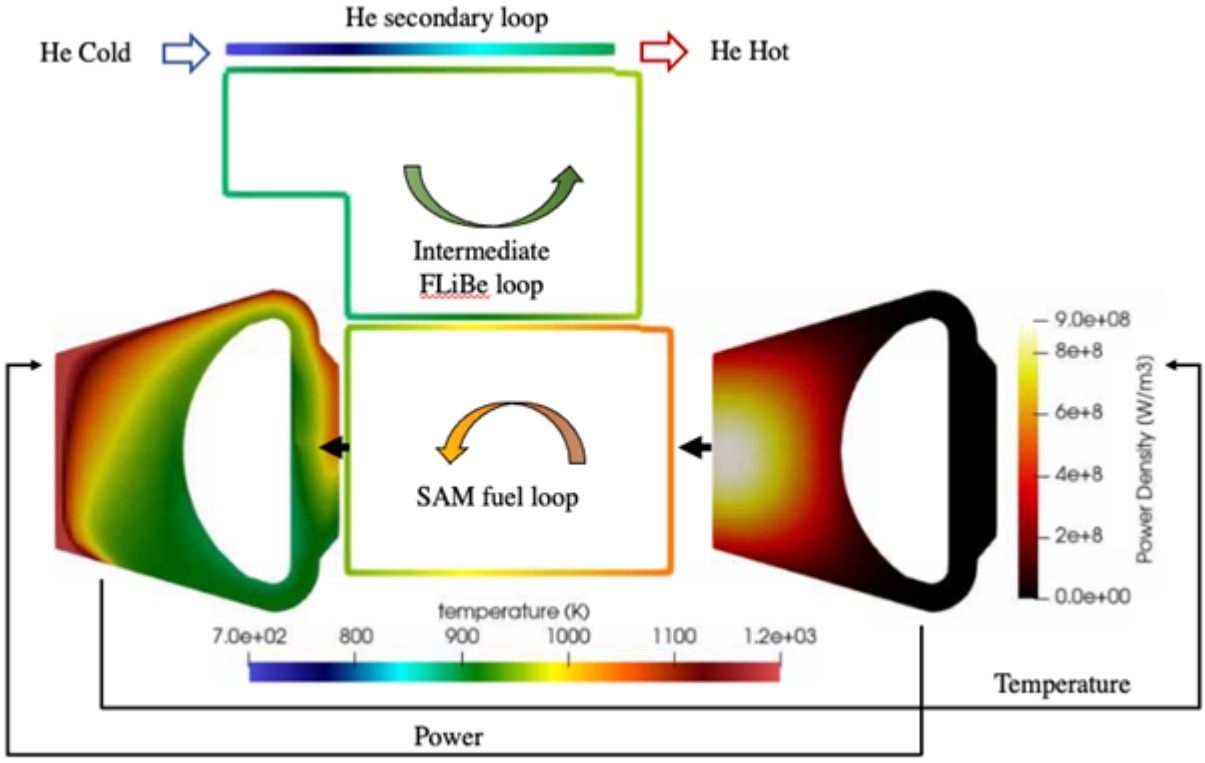


Figure 1: Steady-state results of coupled SAM-Pronghorn-Griffin of an MSR.

B.80 Advanced Test Reactor LEU Fuel Conversion Support

Report Participants

Jaber, Jad R[1], Wolanski, Drew M[1], Cowles, David [1], Rashid, Raheem [1]
1 MPR Associates

Scientific Achievement

The DOE NNSA M3 mission is to convert, remove, and dispose of vulnerable nuclear material located at civilian sites worldwide. As part of its mission, M3's Office of Conversion works around the world to convert research reactors and isotope production facilities to non-weapon-usable nuclear material both domestically and abroad. In support of this effort, the Office of Conversion's USHPRR Conversion Program is working with INL to develop and qualify new LEU fuels and technologies for use in ATR.

In support of this task, MPR is performing thermal hydraulics modeling of safety basis transient events to support LEU ETs in ATR. This ongoing effort involves simulating reactor flow conditions using RELAP5 and performing a Monte Carlo simulation of a single plate using SASQUATCH/ ATR-SINDA to assess conformance to required safety criteria.

Significance

MPR is currently preparing safety analyses to support ET-ATR, a planned ET featuring high-power cycles to stress the LEU fuel. Additionally, ongoing work is being performed to establish a bounding operational envelope for LEU fuel in the ATR core.

Key Publications

None

Sponsor/Program

ATR

B.81 Modeling of Equi-Atomic Refractory High-Entropy Alloys for Use in Gen IV Reactors

Report Participants

Karimpilakkal, Anilas [1], Newkirk, Joseph [1], Schulthess, Jason [2]
1 Missouri University of Science and Technology
2 Idaho National Laboratory

Scientific Achievement

Modeling high-entropy alloys (HEAs) for the particular application is critical as HEAs provide vast compositional freedom. Identifying the weaker atoms in a unit or super cell of a substance and calculating the formation and migration energies of Frenkel pairs are critical to qualitatively predict the microstructure and mechanical property of the substance. This will eventually enable the high-throughput screening of systems for irradiation application in Gen IV reactors. In this project, we have performed ab initio calculations using the Vienna Ab initio Simulation Package (VASP) to calculate the weaker atoms in NbMoTi and NbMoTiZr systems. The next steps will be to determine vacancy and interstitial formation and migration energies thereby enabling to confirm their candidature for the intended application. The strategy will be extended to nine other compositions that are yet to be analyzed.

Significance

HEAs are a new class of materials proven to have special irradiation resistance due to their superior resistance to defect formation and void swelling, higher microstructural stability under irradiation, and limited irradiation hardening over conventional reactor materials. HEA systems consisting of low neutron absorption cross section refractory elements are promising candidates for use in irradiation environments, especially, Gen IV reactors. The hypothesis of the high entropy of the alloys stabilizing the solid solution phases that they form and suppress any deleterious phases are motivating in terms of sophisticated applications like nuclear. The successful demonstration of these alloys in terms of irradiation resistance as well as mechanical properties would see the replacement of conventional alloys in the reactors contributing to building next generation reactors, like Gen IV, which are expected to have higher burnups, higher efficiency, improved safety, and better reliability and sustainability.

Key Publications

" Anilas Karimpilakkal, Joseph W Newkirk, Jason Schulthess 2023 Empirical and CALPHAD based modelling of equi-atomic high entropy alloys composed of low thermal neutron cross section elements for use in irradiation environments Submitted to Journal of Nuclear Materials.

Sponsor/Program

This work was supported through the U.S. Department of Energy under DOE Idaho Operations Office Contract DE-AC07-05ID14517.

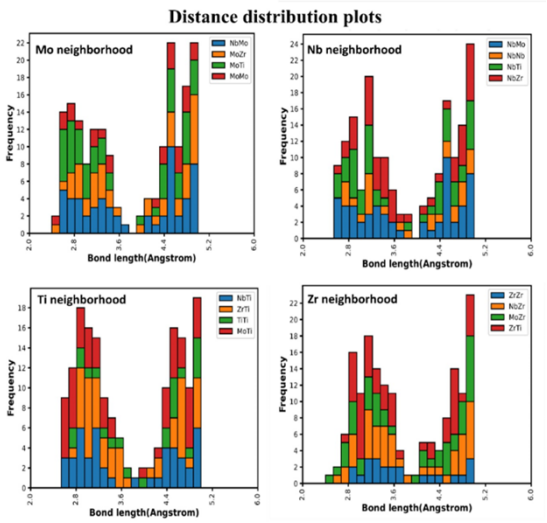


Figure 1: Energy and density optimization calculation for the NbMoTiZr system.

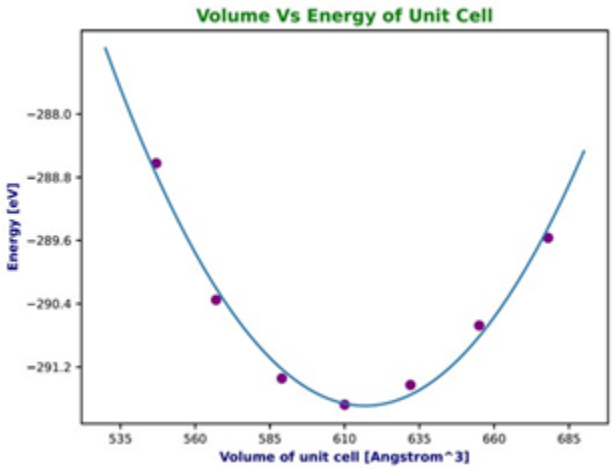


Figure 2: Distance distribution plots to identify weaker atoms in a super cell.

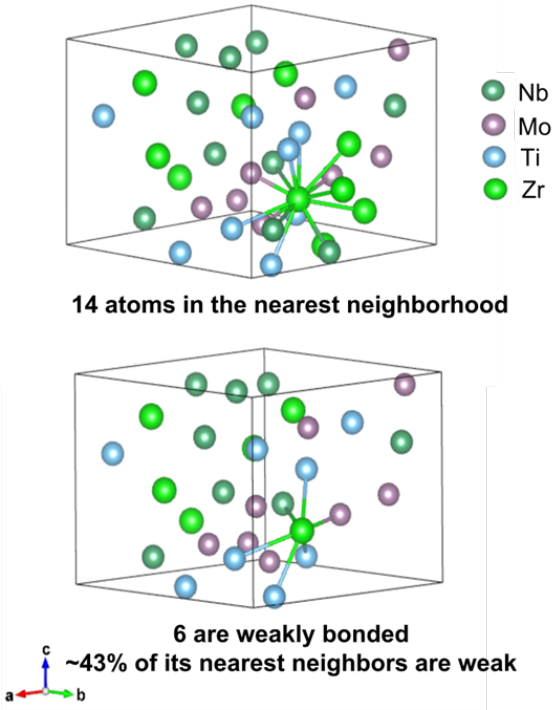


Figure 3: Weaker atom visualization Zr#26.

B.82 RELAP5-3D Modeling of the High-Temperature Test Facility in Support of Benchmark Development Efforts

Report Participants

Kile, Robert F[1], Epiney, Aaron S[1], Brown, Nicholas [2]
1 Idaho National Laboratory
2 University of Tennessee Knoxville

Scientific Achievement

This project aims to develop a benchmark to validate gas-cooled reactor modeling and simulation tools. The project uses experimental data from the HTTF as the basis for assessing code validation. This work used RELAP5-3D and RAVEN to perform sensitivity and calibration studies to assess RELAP5-3D's capability to model HTTF experiments. One such experiment is referred to as PG-26 and represents a depressurized conduction cooldown. We found that RELAP5-3D struggled to match results from PG-26, as shown in Figure 1. We found, though, that RELAP5-3D could model a similar experiment, known as PG-29, with reasonable agreement. These modeling efforts supported the decision to alter the benchmark to use PG-29 rather than PG-26 as the experimental basis for depressurized conduction cooldown modeling. This work was recently accepted for publication in Nuclear Engineering and Design.

Significance

This work supports the development of a gas-cooled reactor thermal hydraulics benchmark for code validation. The development of this benchmark is supported by the ART GCR Program. By providing an opportunity for code validation, this work supports the deployment of block-type gas-cooled reactors by providing vendors developing these reactors an opportunity to demonstrate to their regulator that their codes can match experimental results. A significant outcome of this work has been the decision for the benchmark to pursue PG-29 rather than PG-26 as the benchmark experiment. Benchmark specifications have been drafted and are under review by the OECD.

Key Publications

Kile, R. F., Epiney, A. S., Brown, N. R. (2022). Assessing the impact of effective thermal conductivity on gas-cooled reactor transients in RELAP5-3D. Transactions of the American Nuclear Society, 127, 747-750. Kile, R., Epiney, A., Brown, N. R. (2023). High Temperature Test Facility sensitivity and calibration studies to inform OECD-NEA benchmark calculations. Nuclear Engineering and Design, 2023.

Sponsor/Program

DOE Office of Nuclear Energy, ART GCR Program

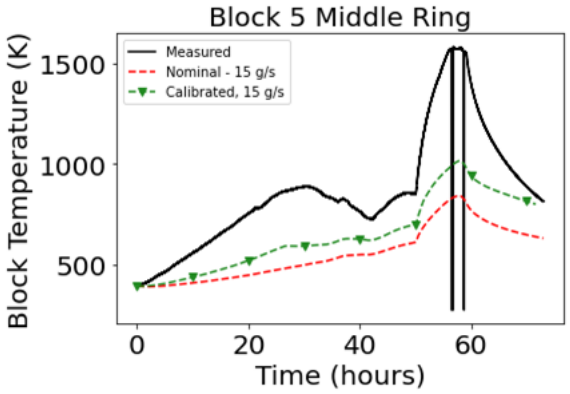


Figure 1: Comparison of RELAP5-3D (nominal and calibrated) results compared to measured data for HTTF experiment PG-26.

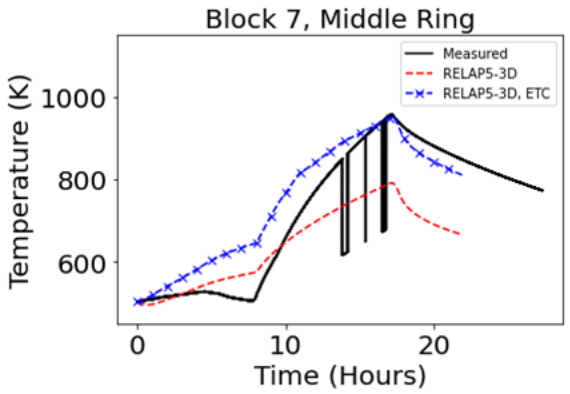


Figure 2: Comparison of RELAP5-3D (nominal and calibrated) results compared to measured data for HTTF experiment PG-29.

B.83 Separate and Multiphysics Effects IRPhEP Benchmark Evaluation Using SNAP Experiments

Report Participants

Kotlyar, Dan [1], Petrovic, Bojan [1], Lindley, Benjamin A[2], Stimpson, Shane G[3], DeHart, Mark D[4]
1 Georgia Institute of Technology
2 University of Wisconsin-Madison
3 BWX Technologies, Inc
4 Idaho National Laboratory

Scientific Achievement

The proposed project will develop an International Reactor Physics Experiment Evaluation Project (IRPhEP) multiphysics microreactor benchmark evaluation based on data from the SNAP program. The proposed work will leverage the extensive experimental measurements accumulated over 15 years. Utilizing the SNAP program experience is a cost-effective way to advance the technology of future microreactors, such as those being proposed for lunar surface power missions (e.g., KRUSTY) or terrestrial deployment (e.g., eVinci). The SNAP program shares many characteristics with today's microreactors, including comparable power output, compact core design, representative physics phenomena (e.g. strong reflector effect), alkali metal heat removal working fluid, and high-temperature solid moderators that are prone to hydrogen migration. While SNAP did not use heat pipes like many of today's concepts, the neutronic characteristics, of primary importance for the IRPhE benchmark evaluation, are well matched and particularly valuable given the paucity of critical and at-power experiments for such systems.

Significance

The SNAP program used a design-build-test-iterate approach for reactor development. This program yielded a considerable amount of documented experimental data. This includes but is not limited to detailed measurements of profiles, fuel density analyses, hydrogen permeation testing, element categorization, failure mode analysis, high-temperature moderating elements (e.g., ZrHx), stress analysis, and mechanical design and assembly. The two main objectives pursued here are to perform systematic assessments of the experimental data with meticulous compilation and documentation, with the end objective of creating an evaluation compliant with the IRPhE evaluation guide, and validate the performance of specific NEAMS tools to model effects that are unique to microreactors technologies. Although the benchmark should be code agnostic, validating NEAMS tools will help to qualify them as a design and potentially licensing tools in the context of microreactors, as defined by the U.S. NRC BlueCRAB program for advanced reactor analyses. A series of dry and wet critical experiments were conducted during the SNAP program, which are the main pillars for this proposal. Dry critical experiments, among others, include critical loadings, critical drum-reflectors configurations, and measurements of kinetic parameters. Wet experiments include an operational history with documented power and temperature profiles. An effort will be made to separate and benchmark each code and physics against a set of representative measurements, including using Griffin for cold critical assembly benchmarks (i.e., no temperature feedback). The proposed evaluation benchmark and validation efforts will aid the developing and licensing of microreactors by demonstrating the accuracy and quantifying the error or bias uncertainty of reactor physics calculations. This proposal will focus on reactivity feedback effects and control element

worth as these aspects are most relevant to today's microreactor concepts and directly address current modeling challenges. Additionally, thermal hydraulics (T/H) data and models will also be incorporated as this is important for developing and validating coupled solutions. In a future phase, the benchmark could also be extended to cover more complicated multiphysics analyses, such as the permeation or loss of hydrogen, which represents a critical design challenge for single-batch hydride-moderated nuclear reactors.

Key Publications

S. Garcia, I.E. Naupa Aguirre, A. Boyd, O. Paleen, D. Kotlyar, B. Lindley. Validation of SNAP8 Criticality Configuration Experiments using SERPENT, Proc. ANS2022, Phoenix, AZ, USA, November 13-17, 2022. I. Naupa, S. Garcia, S. Terlizzi, A. Abou-Jaoude, B. Lindley, D. Kotlyar. Verification of the Serpent-Griffin Workflow using the SNAP 8 Experimental Reactor, Proc. M&C 2023. An online repository was establishedL https://github.com/CORE-GATECH-GROUP/SNAP-REACTORS

Sponsor/Program

NEUP (MS-NE-1 program)
Federal Grant / Cooperative Agreement Number (CID): DE-NE0009218

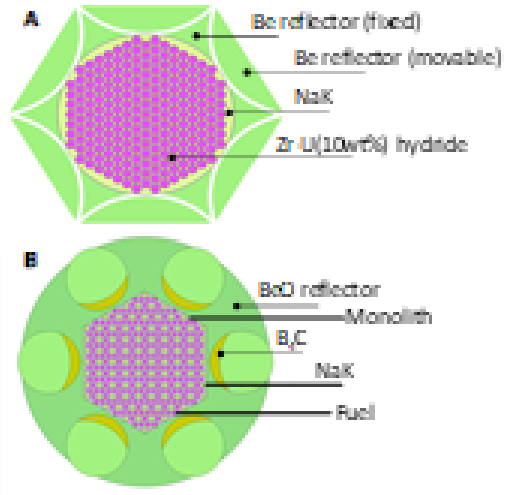


Figure 1: Configuration of the (a) SNAP-8 core and (B) LANL microreactor.

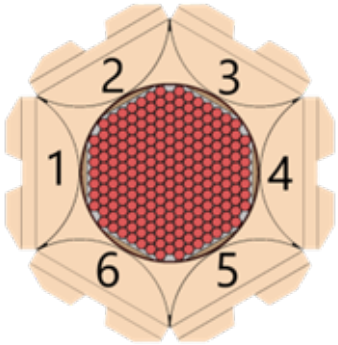


Figure 2: Radial view of the SNAP8 model.

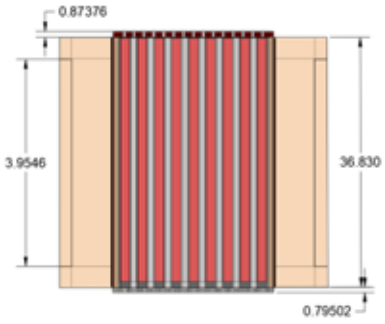


Figure 3: Axial view of the SNAP8 model.

B.84 Validation of the VERA for the NPP Krako Calculations

Report Participants

Kromar, Marjan [1]
1 Jozef Stefan Institute

Scientific Achievement

The VERA code will be used for the scientific studies of the neutron transport inside PWR cores and ex-core regions. Specifically, VERA will be validated by performing a detailed pin-by-pin depletion of all completed 32 NPP Krako fuel cycles. NPP Krako is a two-loop Westinghouse PWR plant located in Slovenia. Results will be compared to the in-house CORD-2 system and in-core measurements performed periodically on the plant. VERA will be used to study the sensitivity of calculation models applied to the typical PWR core calculation. A sensitivity analysis of the grid and energy mesh could significantly speed up the calculations. With validated core models, ex-core calculations will be performed. Results will be compared to the ADVANTG/MCNP calculations with sources determined from the CORD-2 calculations. For validation purposes, a comparison to the dosimetry data from the NPP Krako Ex-Vessel Neutron Dosimetry system will be performed. So far only preliminary calculations have been done. Initial calculations performed on the fuel assembly level have been completed. During the comparison phase, some deficiencies of the CTF code application were discovered and reported. VERA coding was corrected in VERA Version 4.3.

Significance

Initial calculations performed on the fuel assembly level have been completed. Comparison with the Serpent-Finix calculations has indicated some deficiencies of the CTF code application. This was corrected in VERA Version 4.3. A possibility to replace CTF fuel temperatures with temperature tables generated by BISON and tables from CORD-2 is currently being investigated. The impact of different temperature model approaches on the neutron transport and burnup calculation results on the reactor core level will be valuable information regarding the way the VERA simulator should be assembled for the complete VERA validation on all 32 NPP Krako fuel cycles. VERA core simulator capabilities to predict NPP Krako fuel characteristics has been explored (Figure 1). Comparison of the nuclide isotopic vector, multiplication factor and decay heat with the Serpent2 and NEWT/TRITON sequence from the SCALE package, performed on the NPP Krako fuel test cases, has enabled the validation of the VERA calculation sequence. Since VERA is a 3D core simulator, the focus was on investigating the 3D effects and nonlinearity of the soluble boron concentration averaging process, which are difficult to assess with majority of available calculation tools. A difference in the isotopic vector, multiplication factor, and decay heat prediction between the 3D and 2D model approaches has been analyzed. In addition, the impact of the Inconel grids on the fuel characteristics was determined. Demonstration on the Watts Bar Unit 1 Cycle 1 depletion test case (Figure 2) has shown formidable VERA capabilities to accurately predict spent fuel decay heat during the fuel cooling. Published paper of this work was the first published paper demonstrating VERA capabilities for the spent fuel decay heat determination.

Key Publications

Kromar, M., & Godfrey, A. T. (2022, December 5). Determination of the spent fuel decay heat with the VERA core simulator. Frontiers in energy research, Volume 10, 2022, ISSN 2296-598X. https://doi.org/10.3389/fenrg.2022.1046506

Sponsor/Program

CASL, VERA Users Group (VUG)

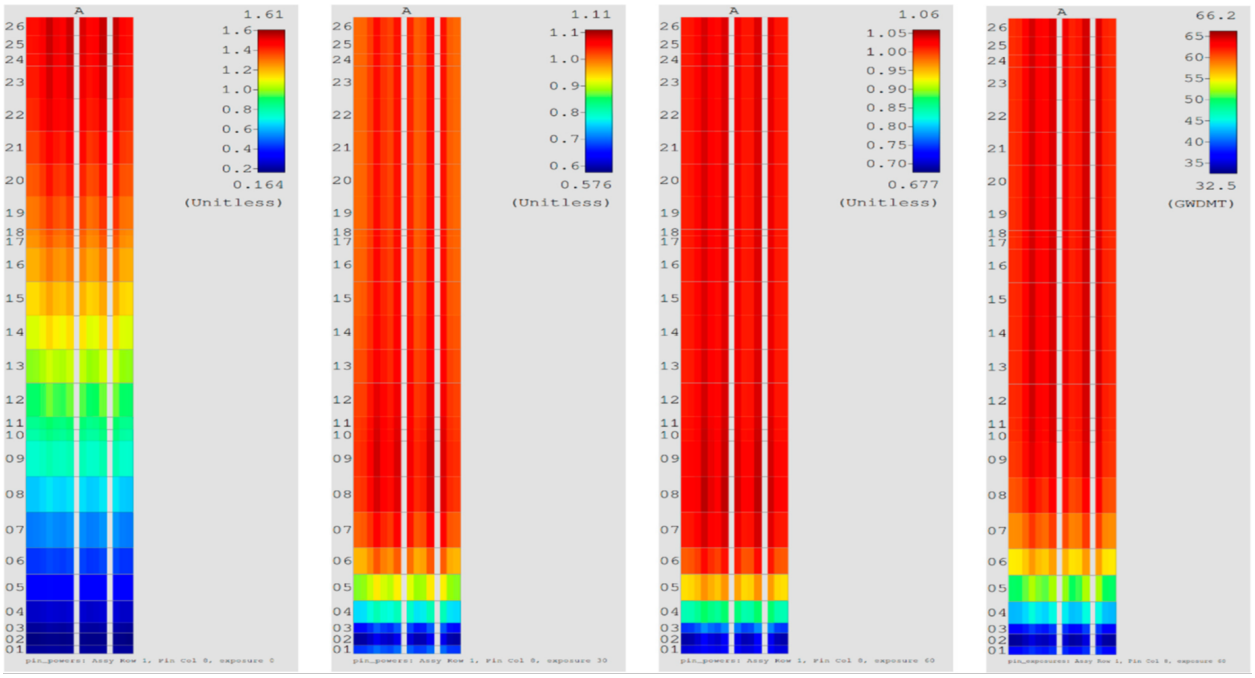


Figure 1: Axial relative power distribution at 0, 30,000, and 60,000 MWD/MTU and burnup distribution at 60,000 MWD/MTU of the NPP Krako 16 × 16 fuel.

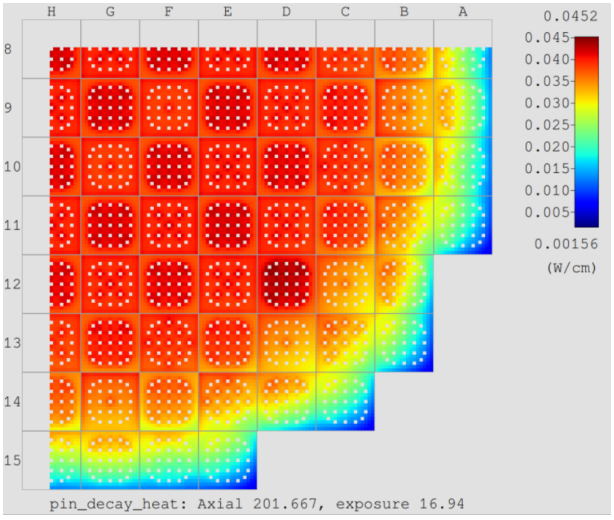


Figure 2: Radial and axial decay heat distribution after 1 year of cooling—Watts Bar Unit 1 Cycle 1.

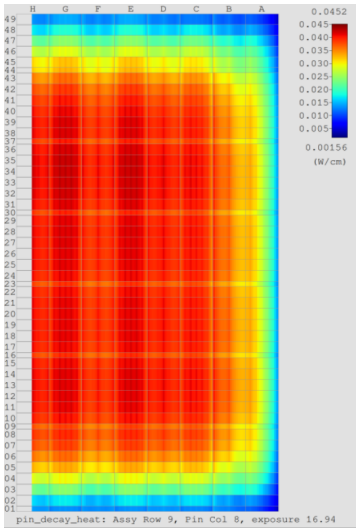


Figure 3: Radial and axial decay heat distribution after 1 year of cooling—Watts Bar Unit 1 Cycle 1.

B.85 Steady-State and Transient Multiphysics Modeling and Analysis of a Microreactor Using the DireWolf Code Suite

Report Participants

Kucukboyaci, Vefa N[1], Cao, Liping [1], Boychenko, Mykola [1], Shockling, Michael A[1], Laboure, Vincent M[2]
1 Westinghouse Electric Company
2 Idaho National Laboratory

Scientific Achievement

We demonstrated the successful use of INL's MOOSE-based DireWolf code suite to model the steady-state and transient behavior of a heat-pipe-cooled microreactor. A detailed model of a TRISO fueled, graphite moderated, and heat-pipe-cooled microreactor reactor was developed, including neutronic and thermal mesh and nuclear cross sections. DireWolf was used to determine the critical drum position at beginning of life, and a coupled thermal-neutronic solution, including fast and thermal flux, power distributions, and temperature distributions was obtained. DBA transients, such as loss of coolant, heat pipe failure, overcooling, and reactivity insertion transients, such as an inadvertent rotation of control drums, were performed. The evolution of the total core power and reactivity and component temperatures was demonstrated, and 3D flux, power, and temperature distributions were predicted to help guide the design process.

Significance

Westinghouse is designing a TRISO-fueled, heat-pipe-cooled, graphite-moderated microreactor, which is a tightly coupled system, requiring multiphysics tools to accurately model both steady-state and transient behavior. INL's MOOSE-based DireWolf code suite is tailor-built to model heat-pipe reactors, and its ability to model the coupled steady-state and transient behavior in a limiting accident condition needed to be demonstrated. A microreactor, specifically one cooled with heat pipes, is intrinsically a tightly coupled system. Traditional loosely coupled, single-physics models are not sufficient to accurately predict the system behavior; a true multiphysics approach is required. To this extent, INL has taken existing MOOSE-based, finite-element computational tools and packaged them into a code suite specifically tailored for heat-pipe reactors, called DireWolf, which includes Griffin for neutronics modeling, BISON for thermal-mechanical analysis, and Sockeye for heat-pipe modeling. Those tools are being used in transient analyses to demonstrate the safe operation of the design and help Westinghouse in the licensing process.

Key Publications

" Roskoff, et al., Modeling and Analysis of a Micro-reactor using the DireWolf Code Suite, Proceedings of PHYSOR 2022, May 15-20, Pittsburgh, PA " Roskoff, et al., Transient Analysis of a Micro-reactor using the DireWolf Code Suite, Proceedings of PHYSOR 2022, May 15-20, Pittsburgh, PA

Sponsor/Program

Industry, DOE

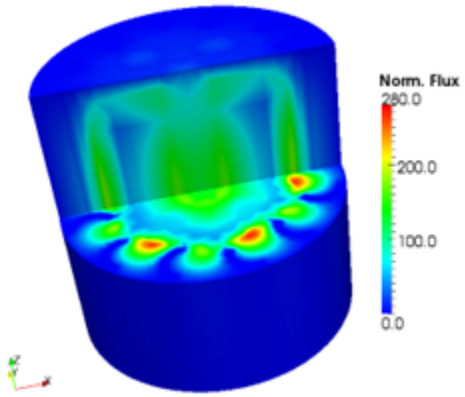


Figure 1: Thermal flux distribution at time of maximum power (2.12 seconds) during an inadvertent drum rotation accident.

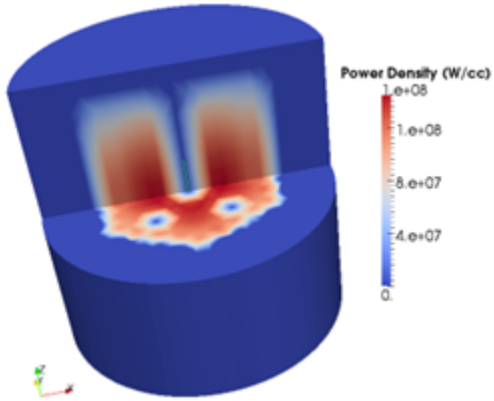


Figure 2: Power density distribution at time of maximum power (2.012 seconds) during an inadvertent drum rotation accident.

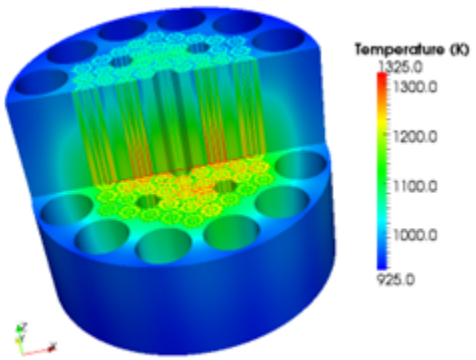


Figure 3: Temperature distribution at time of maximum fuel temperature (3.66 seconds) during an inadvertent drum rotation accident.

B.86 Adding Pin Power Reconstruction Capabilities to Griffin Reactor Physics Code

Report Participants

Kumar, Shikhar [1], Lee, Changho [1], Wang, Yaqi [2], Ortensi, Javier [2]
1 Argonne National Laboratory
2 Idaho National Laboratory

Scientific Achievement

As part of NEAMS project, ANL and INL have been collaborating on the Griffin reactor physics code. In order to introduce added functionality to the diffusion solvers within Griffin, pin power reconstruction capabilities are currently being added to the code for simplified analysis of reconstructed pin powers from solution fluxes. The base functionality is in place and now we are working on implementing transfers to incorporate multiphysics feedback.

Significance

Pin power reconstruction uses the reconstructed flux from Griffin to compute pin-by-pin powers, and heterogeneous flux information from external Monte Carlo solvers, such as Serpent, can be leveraged as well. This functionality is requested by key stakeholders in the Griffin reactor physics code. Focus of this year is to implement a workflow for simplifying calculation of full-core form functions to reproduce pin powers with Monte Carlo reference solutions.

Key Publications

Prince, Z. M., Wang, Y., Hanophy, J. T., Laboure, V. M., Kumar, S., Jung, Y. S., & Lee, C. (2022). Improvements to the Griffin Transport Solvers (No. INL/RPT-22-69391-Rev000). Idaho National Lab.(INL), Idaho Falls, ID (United States). Kumar, S., Lee, C., Jung, Y.S.., & Wang, Y. Pin Power Reconstruction Capabilities for the Griffin Reactor Physics Code, ANS Winter Meeting (2022).

Sponsor/Program

NEAMS

Pin Power Reconstruction Implementation

- Pin power reconstruction functionality implementation in progress
  - Leverages HFEM-PN solver to reconstruct pin-by-pin powers on a homogeneous mesh grid
  - Support definition of *form function data* from ISOXML to super-impose single-assembly heterogeneous flux distributions onto homogeneous flux calculations
  - Generalized to support on various mesh types
    - Cartesian, hexagonal, unstructured grids
  - Pin powers are outputted by assembly in a user-readable format

```
[UserObjects]
  [pin_power_userobject]
    type = PinReconstruction

    assembly_id_name = assembly_id     # element integer for indicating coarse
                                       # mesh assembly IDs

    assembly_types = '1 1;             # map assembly ID to assembly type ID
                      2 1
                      3 1'
    form_function_file = 'ff.xml'      # the XML storing the form functions
                                       # i.e. the pin powers indexed with assembly type
                                       # The specification of pins can be either regular
                                       # or with an unstructured assembly mesh.
  []
[]
```

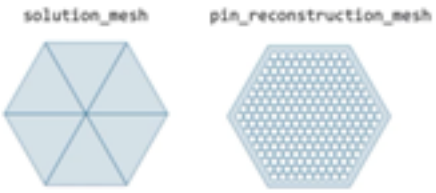


Figure 1: Pin power reconstruction implementation in Griffin reactor physics code.

B.87 Improvement and Verification of Griffin Performance

Report Participants

Lee, Changho [1], Park, Hansol [1], Jung, Yeon S[1]
1 Argonne National Laboratory

Scientific Achievement

High-fidelity deterministic steady-state simulations of the Empire microreactor problem were performed using the DFEM-SN solver of Griffin augmented by the online cross-section self-shielding API. The 68-group cross-section libraries for the self-shielding API were generated using a suite of Python scripts and Serpent2/NJOY/MC2-3 with ENDF/B-VII.0, VII.1, and VIII.0 data. The calculation results demonstrate that Griffin achieves accurate simulation of the 2D and 3D Empire microreactor benchmark problems under steady-state conditions, considering different control drum locations, when compared to corresponding Monte Carlo solutions.

Significance

The high-fidelity deterministic steady-state simulation capability of Griffin has been demonstrated using the Empire microreactor problem. This allows us to accurately simulate a complex reactor problem, providing detailed high-resolution neutron flux and power solutions of a reactor problem in various steady-state and transient conditions.

Key Publications

C. H. Lee, H. Park, and Y. S. Jung, High-fidelity Simulation pf the Empire Micro Reactor Benchmark Problem Using Griffin with Online Cross Section Generation, M&C 2023, Niagara Falls, ON, Canada, 8/12-17

Sponsor/Program

NEAMS

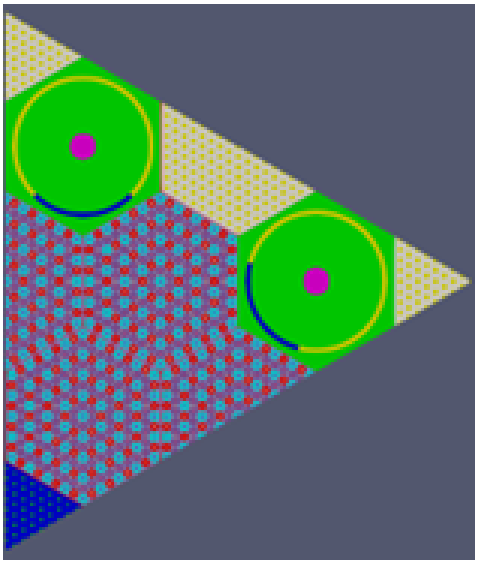


Figure 1: 1/6 model of Empire.

B.88 Role of Fluid and Temperature in Fracture Mechanics and Coupled THMC Processes for Enhanced Geothermal Systems

Report Participants

Yoon, Hongkyu [1], Lee, Jonghyun [2], Bao, Jichao [2]
1 Sandia National Laboratories
2 University of Hawaii at Manoa

Scientific Achievement

One of the main objectives of this project is to address key controllable parameters that have the most significant impact on optimal heat extraction by advancing the capabilities of EGS simulator, FALCON. Synthetic data set (e.g., temperature and pressure data) created from the FORGE site model was used to infer the hydrogeological and geomechanical properties. The effective permeability and thermal conductivity values were identified as our initial efforts. FALCON was used for thermo-hydro-mechanical (THM) simulations, and a Gauss-Newton solver was applied to estimate the effective permeability and thermal conductivity. The results showed good agreement of the effective parameters and great data fitting.

Significance

Key parameters, such as reservoir permeability and thermal conductivity, have a great influence on the THM process. The Gauss-Newton solver is an inversion approach that calibrates key parameters to better predict the THM process. It is beneficial for reservoir management and heat extraction with a better understanding of the THM process. We have performed permeability and thermal conductivity inversions for a 3D homogeneous case and a 2D heterogeneous case. The homogeneous case showed great parameter estimation and temperature and pressure data fitting results. The heterogeneous case is still ongoing, but the preliminary results showed reasonable temperature and pressure data fitting. A 3D inversion model will be developed in the future to characterize the FORGE site to provide a better prediction of the THM process.

Key Publications

Bao, J., Lee, J., Yoon, H., & Pyrak-Nolte, L. (2023). Subsurface Characterization using Bayesian Deep Generative Prior-based Inverse Modeling for Utah FORGE Enhance Geothermal System, In 57th U.S. Rock Mechanics/Geomechanics Symposium, Atlanta, Georgia, USA, June 2023

Sponsor/Program

Other

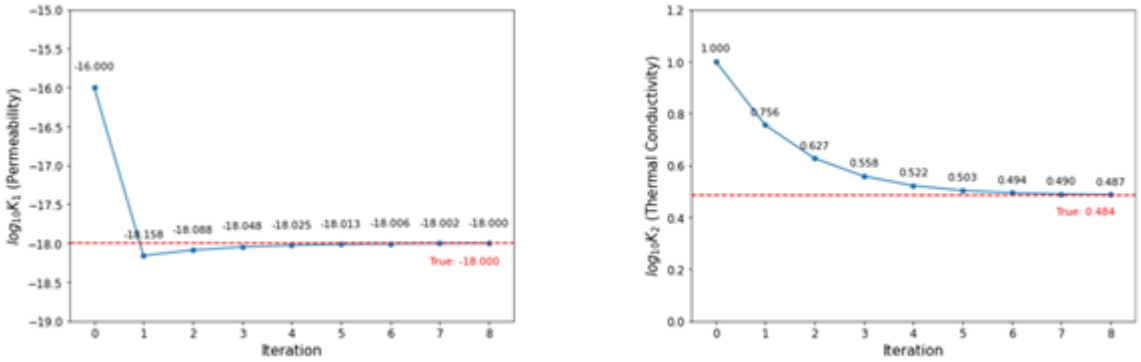


Figure 1: Estimation of permeability and thermal conductivity of the granitoid layer, assuming that the permeability and thermal conductivity are homogeneous and isotropic.

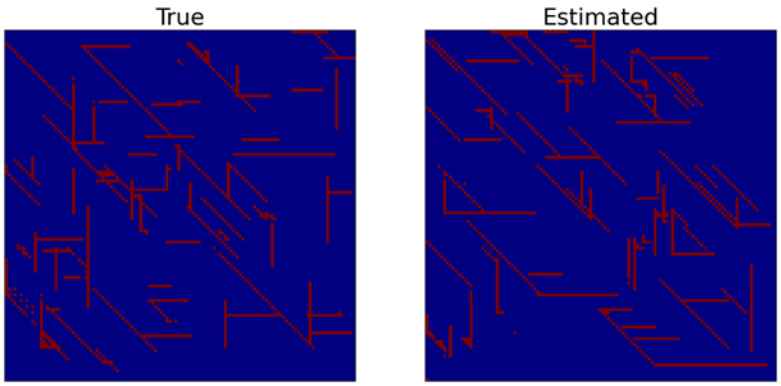


Figure 2: Estimation of heterogeneous permeability of the granitoid layer, where the true permeability field is shown on the left and the estimation result is shown on the right. The red lines represent fractures with a permeability of 1e-14 m^2, and the permeability of the blue area is 1e-16 m^2.

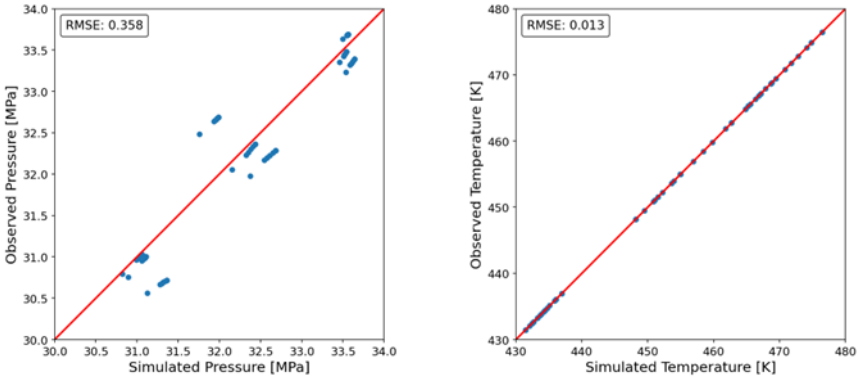


Figure 3: Pressure and temperature data fitting of the heterogeneous case. The fitting error is shown as the root mean square error.

B.89 Heat Pipe Experimental Facility Design for a Microreactor Using Sockeye Code

Report Participants

Lee, Saya [1], Hisahara, Erik [1], Balbier, Christopher T[1]
1 Pennsylvania State University

Scientific Achievement

The objective of this project is to design, construct, and operate a heat-pipe experimental facility to provide validation data and insight into closure models for the INL Sockeye code development. Erik Hisahara and Christopher Balbier as graduate students are learning the code. Erik attended the Sockeye code workshop during his 2023 summer internship at INL. Based on the test case developed by the INL Sockeye code developer, Joshua Hansel, and some inputs for a heat pipe experimental facility design, Christopher built an experimental facility, and some preliminary results will be presented at the ANS 2023 Winter Meeting. Once the experimental facility starts generating reliable data later in 2023, the team will run Sockeye simulations and compare the results from early 2024.

Significance

The present work aims to develop a Sockeye model to design an experimental facility at Penn State. This facility will provide optimized experimental conditions and will be constructed accordingly. The initial phase involved replicating and testing a SAFE-30 model, which was accomplished successfully. For the heat-pipe design, a simplified heat pipe with a five-layer screen wick (mesh #100) demonstrated excellent performance, exceeding 20 kW at the target temperature of 1073 K. A limit calculation was performed as shown in Figure 1. Based on the simulation, an experimental facility was built as shown in Figure 2 and preliminary data were obtained as shown in Figures 3 and 4. Supported by the Sockeye code developer, the participants will work on various operating conditions for the simplified heat pipes and some convergence issues will be fixed.

Key Publications

The team is an experimental group and is running the Sockeye code in parallel with the experimental progress. This year, the team is generating experimental data to support the Sockeye code development, and a preliminary experimental result will be presented at the ANS 2023 Winter Meeting. More simulation and experiment comparison publications will be available from 2024.

Balbier, C., Smith, N., Kim, H., & Lee, S. (2023). Feasibility Test of Fiber Optic Temperature Sensors in Sodium Heat Pipes. American Nuclear Society (ANS) Winter Meeting and Technology Expo 2023, November 12-15, 2023, Washington D.C.

Sponsor/Program

The team is generating preliminary test data and additional simulation results to apply for research grants and industrial sponsors

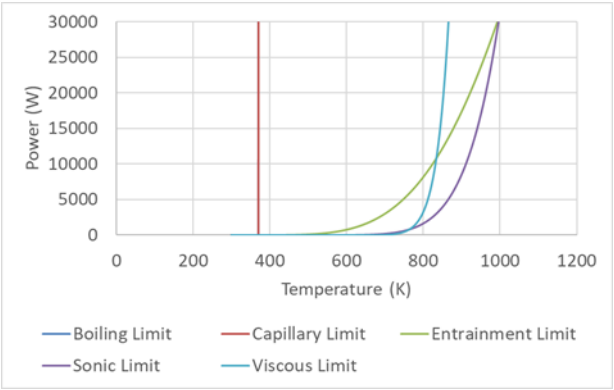


Figure 1: Operational limit of 6 ft heat pipe with mesh #100.

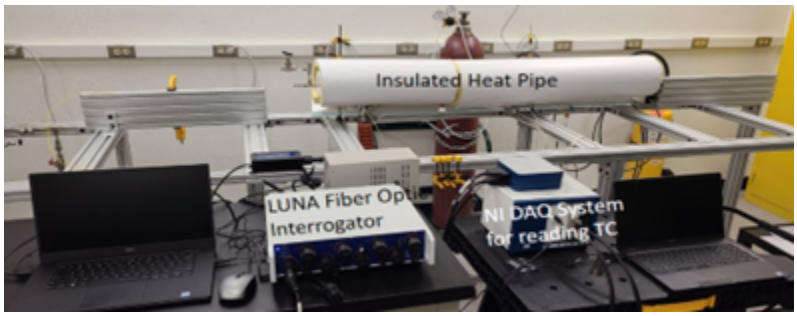


Figure 2: Heat-pipe design and experimental facility based on the Sockeye code simulations and current status.

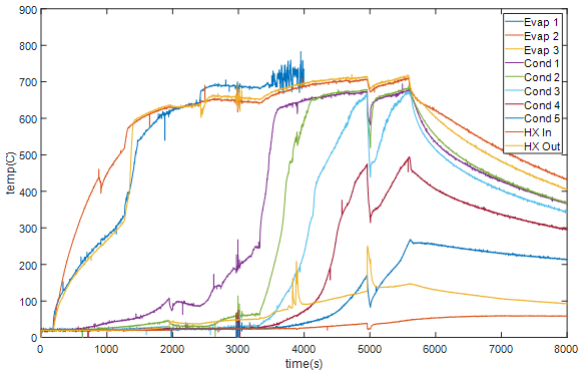


Figure 3: Thermocouple data readings.

B.90 BISON Analysis of FeCrAl and Zircaloy Cladding Deformation During Simulated BWR Cyclic Dryout Conditions

Report Participants

Lee, Soon K[1], Capps, Nathan A[2], Brown, Nicholas [2]
1 Argonne National Laboratory
2 Oak Ridge National Laboratory

Scientific Achievement

The BISON fuel performance analysis code has been used to study FeCrAl and Zircaloy cladding performance to better understanding cladding deformation behavior in BWRs during conditions caused by anticipated operational occurrences (AOOs) or by anticipated transient without scram (ATWS).

Significance

BISON models of novel separate effects tests simulating ATWS events predicted mechanical responses to extreme thermal cycling boundary conditions, where assessments were made to determine which mechanical models were best suited for cyclic dryout event analyses for both FeCrAl and Zircaloy claddings. BISON's modeling capability for BWR AOO or ATWS events looks very promising.

Key Publications

Lee, S. K., Capps, N. A., & Brown, N. R. (2023). BISON analysis of FeCrAl and Zircaloy cladding deformation during simulated BWR cyclic dryout conditions. Journal of Nuclear Materials, 154243.

Sponsor/Program

Advanced Fuels Campaign Program.

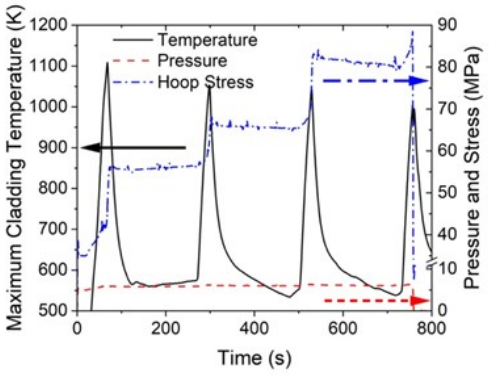


Figure 1: Applied boundary conditions and BISON-calculated hoop stress during the cyclic dryout test.

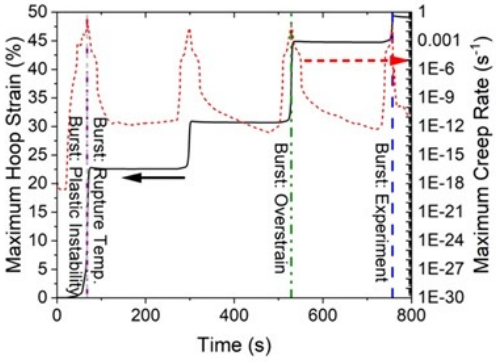


Figure 2: Zircaloy-2 cladding hoop strain and creep strain during the cyclic dryout test.

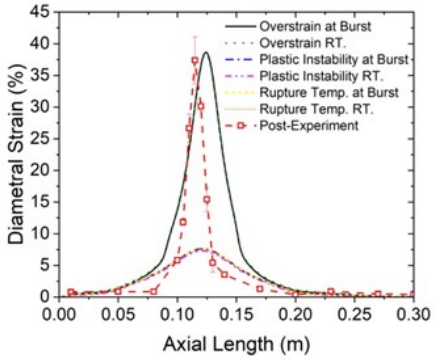


Figure 3: BISON-calculated and measured strain profiles for Zircaloy-2.

B.91 Reactor Physics Modeling in Support of Advanced Reactors

Report Participants

Lemke, Christopher A[1], Tsvetkov, Pavel [1]
1 Texas A&M University

Scientific Achievement

A conceptual model for a prismatic HTGR utilizing annular TRISO fuel compacts was developed for use in a parametric performance study. Using this model, design parameters will be systematically modulated. The effect of the design perturbations will be analyzed through the comparison of various computational simulations, including shielding evaluations, criticality calculations, and fuel cycle studies. The use of the SCALE code system on the INL HPC resources will be a key tool and driver in the ability to conduct said high-fidelity simulations.

Significance

We are still in the beginning stages and literature review process looking into specific design parameters that will be analyzed.

Key Publications

Nothing to report yet.

Sponsor/Program

No formal proposal has been written yet but the project is expected to fall under the DOE/NNSA umbrella.

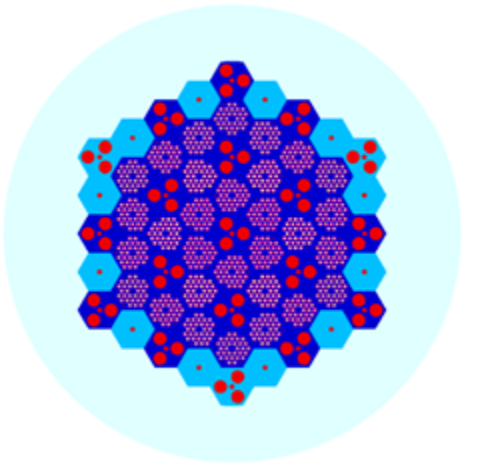
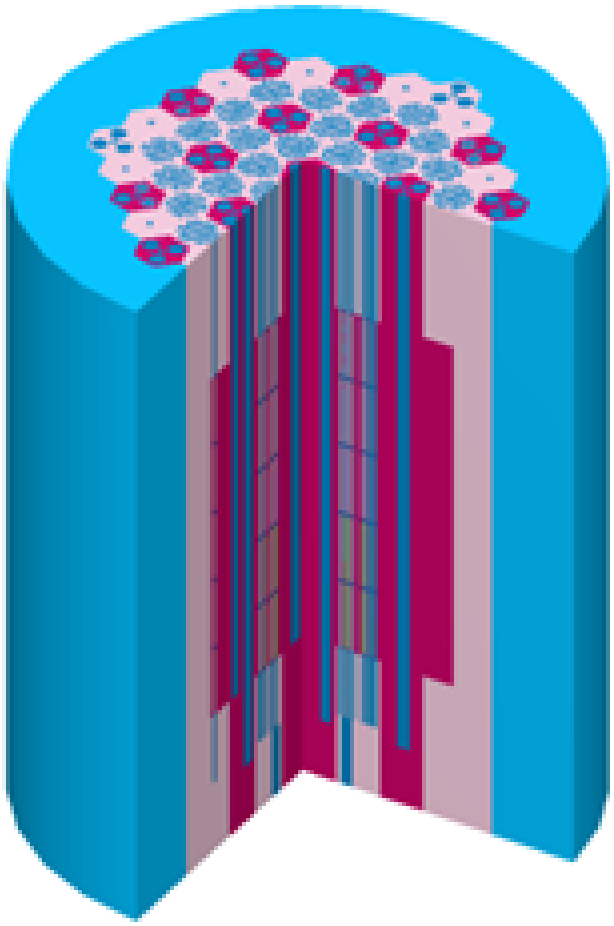


Figure 1: HTGR concept for reactor physics modeling and performance studies.



B.92 An Integrated Statistical-Thermodynamic Model for Fission Gas Swelling and Release in Nuclear Fuels

Report Participants

C Lieou, Charles K[1]
1 University of Tennessee Knoxville

Scientific Achievement

We propose a new model for burst fission gas release induced by microcracking in ceramic nuclear fuels, such as uranium dioxide. The model stipulates that the densities of defects in the fuel material, such as microcracks and fission gas bubbles on grain boundaries, evolve in accordance with the second law of thermodynamics. Central to the model is the notion of an effective temperature, conjugate to the configurational entropy of the fuel material, and is directly linked to the burnup. We simulated a series of fuel rod irradiation experiments using the proposed model in BISON. The model predicts that microcracking, driven by the internal stress state of the fuel material, reduces the bubble storage capacity of grain boundaries, and accounts for burst fission gas release during rapid temperature transients that simulate power transients, reactor startup, and LOCA conditions.

Significance

Within the framework of our model, termed SIFGRSX to represent the improved physical ingredients versus the original SIFGRS model currently implemented in BISON, burst fission gas release is dominated by grain refinement. The physical interpretation is that we need a large density of grain faces to store fission gas that can be released via grain-face cracking during burst release. Our results shed important light on the interplay between microstructural evolution, thermomechanical behavior, and fission gas release in nuclear fuels. As such, our work provides an important bridge between experiments and atomistic modeling in the quest to develop accurate and predictive models for fuel performance. Simulations of fuel pellet behavior based on our current work will constitute an integral part of ongoing and future work that will benefit both the DOE NEAMS and SciDAC Programs.

Key Publications

C. K. C. Lieou, N. A. Capps, M. W. D. Cooper, P. C. A. Simon, B. D. Wirth. 2023. An Integrated Statistical-Thermodynamic Model for Fission Gas Swelling and Release in Nuclear Fuels. Journal of Nuclear Materials, to be submitted. C. K. C. Lieou, N. A. Capps, M. W. D. Cooper, P. C. A. Simon, B. D. Wirth. 2023. An Integrated Statistical-Thermodynamic Model for Fission Gas Swelling and Release in Nuclear Fuels. Poster presentation at the Gordon Research Conference on Physical Metallurgy, Easton, MA, July 9-14, 2023.

Sponsor/Program

DOE Office of Nuclear Energy and Office of Advanced Scientific Computing Research, Fission Gas SciDAC project DE-SC00018359 at the University of Tennessee, in collaboration with Los Alamos National Laboratory, Idaho National Laboratory, Sandia National Laboratories, and Ar-

gonne National Laboratory.

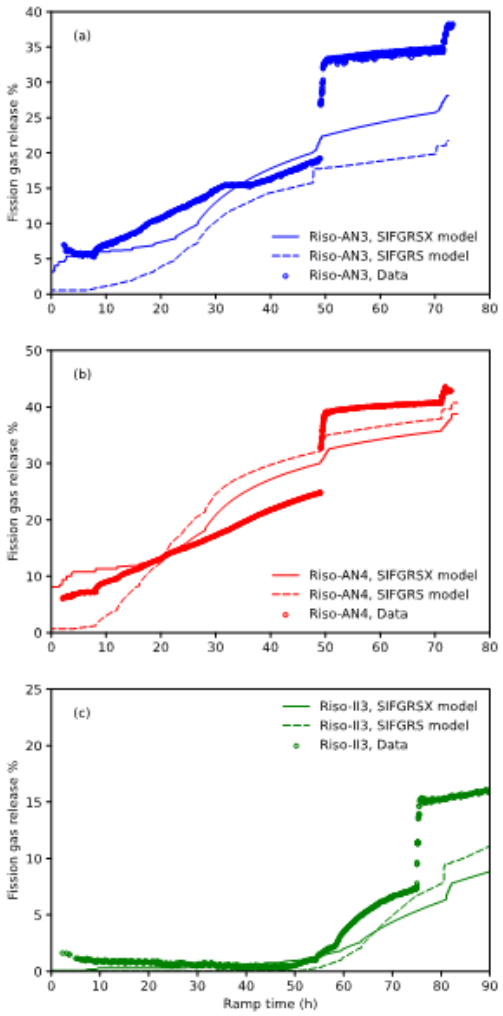


Figure 1: Fission gas release percentage, as a function of time, during the (a) Riso-AN3, (b) Riso-AN4, and (c) Riso-II3 ramp tests. Open circles represent experimental measurements and solid lines represent SIFGRSX model predictions. Original SIFGRS model results are shown in dashed lines for comparison.

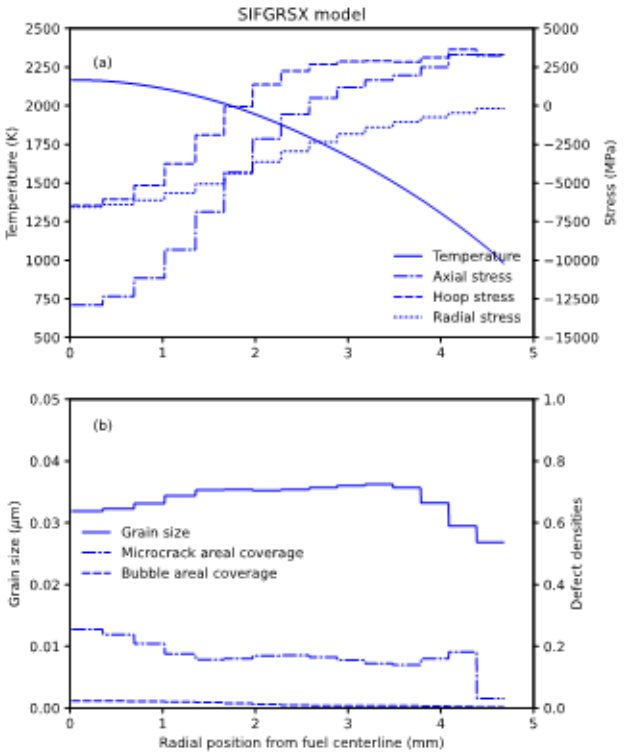


Figure 2: SIFGRSX model results for the variation of (a) temperature, axial stress, hoop stress, and radial stress and of (b) grain size, microcrack areal coverage, and bubble areal coverage, with the radial position from the centerline of the fuel rod, immediately after the temperature transient 48 hours after the start of the Riso-AN3 ramp test.

B.93 NEAMS, Shift and Griffin Development for LWR and Advanced Reactors

Report Participants

Pandya, Tara M[1], Bostelmann, Friederike [1], Ghaddar, T [1], Britt, Philip S[1], Johnson, S [1], Jessee, Matthew A[1]
1 Oak Ridge National Laboratory

Scientific Achievement

We have developed several TRISO-fueled reactor models for the Shift Monte Carlo code. Using these models, we performed thorough runtime and memory performance assessments that eventually led to the addition of capabilities that enable user-friendly modeling options and dramatically improve runtime for such double-heterogeneous models. This effort was conducted in preparation of generating multigroup cross sections for these types of reactors with Shift for Griffin.

Significance

This work will benefit NEAMS by expanding the capabilities of the NEAMS software suite, Shift and Griffin, as applied to LWR and advanced reactor multiphysics analysis. Comparisons of results from Griffin using Shift-generated cross sections and Serpent-generated cross sections serve as verification and validation.

Key Publications

Pandya, T., Bostelmann, F., Jessee, M., Ghaddar, T., Britt, P., Johnson, S. Modeling, Performance Assessment, and Nodal Data Analysis of TRISO-Fueled Systems with Shift. Oak Ridge National Laboratory Report ORNL/TM-2022/2601. https://info.ornl.gov/sites/publications/Files/Pub183158.pdf

Sponsor/Program

NEAMS

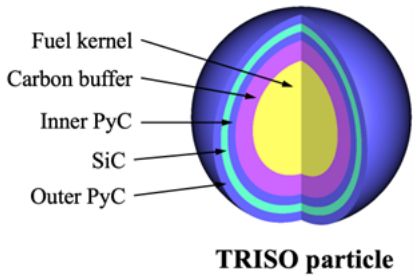


Figure 1: TRISO fuel particle.

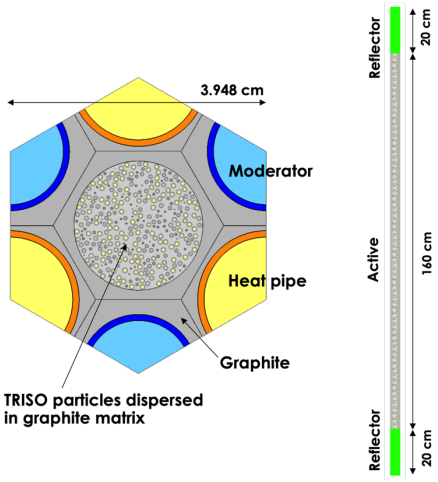


Figure 2: Heat-pipe reactor unit cell.

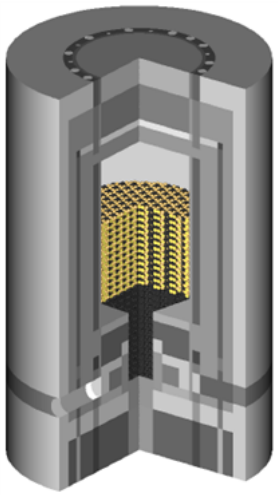


Figure 3: HTR-10.

B.94 A Temperature-Dynamic CALPHAD-Based Phase-Field Model for the Fe-Cr-Ni System

Report Participants

Lin, Albert C[1], Zhang, Yongfeng [1]
1 University of Wisconsin-Madison

Scientific Achievement

A quantitative phase-field model is developed in MOOSE to model steels using the Fe-Cr-Ni system. CALPHAD-based free energies are used to provide a physical thermodynamic basis for the model. The free energies are modified to provide temperature-dynamic capabilities and to alleviate numerical challenges associated with CALPHAD free energy expressions. The model can model interdiffusion as well as secondary nucleation behavior. The thermodynamic basis and kinetic parameterization of the model has been validated against experimental phase diagrams and EPMA results from diffusion couple experiments

Significance

Powder metallurgy hot isostatic pressing (PM-HIP) is a novel manufacturing and an alternative to traditional manufacturing techniques, such as forging, rolling, and casting. PM-HIP relies on the compaction and sintering of powder to fuse metal particles together to form near-net shape components. However, the microstructural evolution during the process has yet to be fully quantified. This phase-field model attempts to capture the interdiffusion and secondary nucleation behavior during the process. In order to replicate the thermal history during the PM-HIP cycles, temperature-dynamic capabilities were implemented into the phase-field model with polynomial-fitted free energy functions. Utilizing temperature-dependent atomic mobilities, the model was able to recreate experimental phase diagrams (Figure 1) and experimental diffusion couple results with various thermal histories (Figure 2). Secondary nucleation is also a concern in PM-HIP as the formation of carbides near the interface can decrease the mechanic strength of the final component. Nucleation physics were implemented into the phase-field model using classical nucleation theory in conjunction with the Discrete Nucleation module in MOOSE. This can be expanded later with the proper thermodynamic model to simulate the carbide formation at grain boundaries.

Key Publications

Lin, Albert C, and Yongfeng Zhang. Temperature-Dynamic CALPHAD-Based Phase-Field Modeling of the Fe-Cr-Ni System. In Progress. A Lin, Y Zhang. Phase-field Modeling of Hot Isostatic Pressing for Joining Dissimilar Metals (2022). Conference talk at MS&T 2022. REFERENCES: [1] Xiong, W. (2012). Thermodynamic and kinetic investigation of the Fe-Cr-Ni system driven by engineering applications (Doctoral dissertation, Kungliga Tekniska Hogskolan Royal Institute of Technology). [2] Hillert, M., & Qiu, C. (1990). A reassessment of the Cr-Fe-Ni system. Metallurgical Transactions A, 21(6), 1673-1680

Sponsor/Program

This work is part of the NEET/Advanced Materials and Manufacturing Technologies NEUP

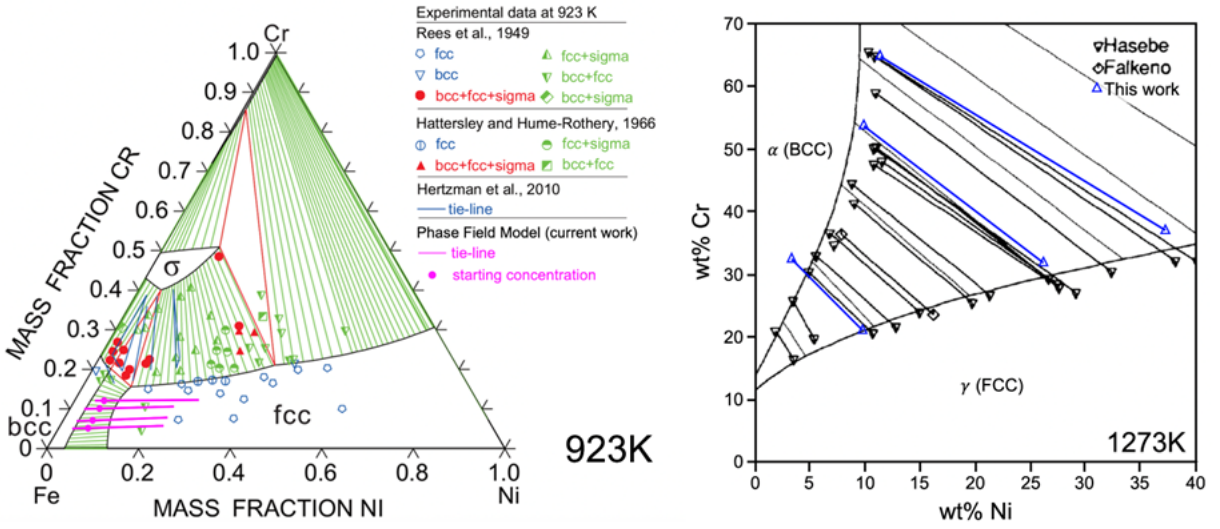


Figure 1: Experimental phase diagrams adapted from Xiong, W. [1] and Hillert, M., & Qiu, C. [2] with phase-field results overlaid.

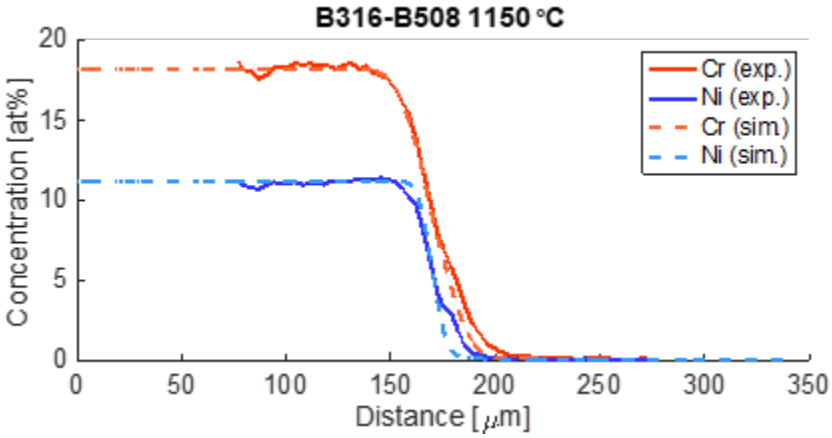


Figure 2: Concentration profiles EPMA (exp.) and phase-field simulation (sim.) of a 316L-A508 1150°C temperature cycle diffusion couple.

B.95 Component-Based Cost Functions for NuScale SMR

Report Participants

Lindley, Benjamin A[1], Baker, Una [1]
1 University of Wisconsin-Madison

Scientific Achievement

With a growing share of renewables in energy markets, there is increased interest in flexible power operation for nuclear reactors. For multiunit SMRs, particularly the NuScale SMR, there are opportunities to optimize flexible power operation across multiple units to limit the degradation of structural and control components. In our project, we focus on the degradation of in-core components, specifically the control rods and reactor pressure vessel. Performing these studies requires a high-fidelity, multicycle representation of the NuScale SMR, with a detailed representation of the structural and control components. To this end, the NuScale SMR has been modeled using the VERA software. The entire transition to equilibrium is simulated, from Cycle 1 through to the equilibrium cycle. The equilibrium cycle model shows a good agreement with the NuScale design certification application results, with differences attributable to a combination of using public domain data for the present study and methodological differences. K-effective, power distributions, reactivity coefficients, and boron letdown curves are compared and closely match. This shows that the VERA model is suitable for further studies. We have since progressed onto calculating cost functions for the degradation of in-core components, which is in progress.

Significance

The key finding to date is that a multicycle model of NuScale's SMR can successfully be developed in VERA that is suitable for derivation of cost functions. Vessel fluences and in-core flux distribution are consistent with previously reported values. This provides an excellent platform for continuing work.

Key Publications

[1] Baker U, Garrouste M, Choi S, Soto G J, Lindley B, Kochunas B. Development of a High-fidelity Multi-cycle Model of the NuScale Small Modular Reactor using VERA. PHYSOR 2022. May 15-20, 2022. Pittsburgh, PA

Sponsor/Program

NEUP DE-NE0008975

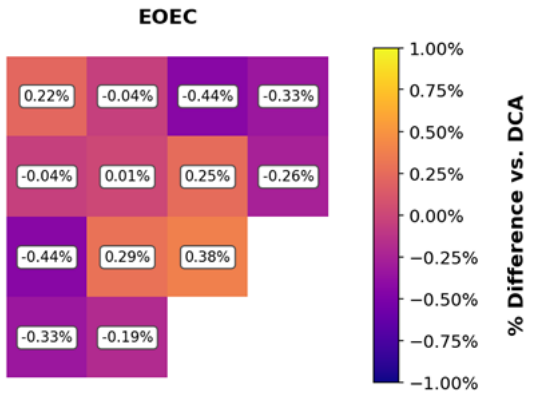


Figure 1: Difference in assembly powers for equilibrium cycle between VERA and NuScale reported values.

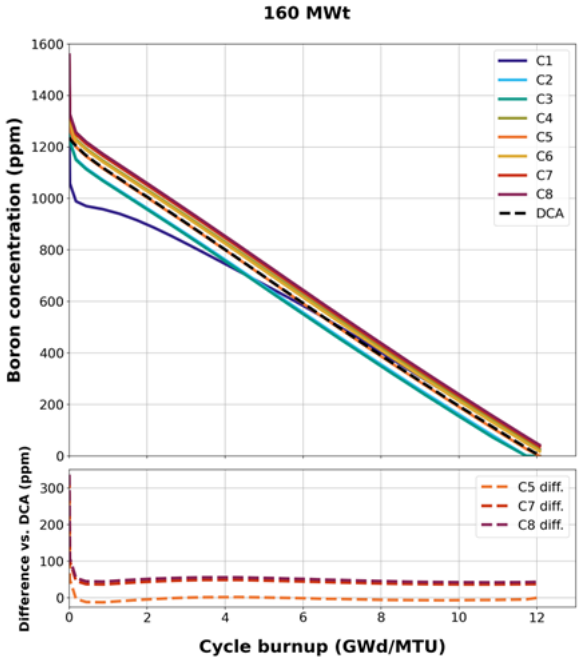


Figure 2: Boron concentration predicted by VERA compared to NuScale reported values.

B.96 Safety Implications of High-Burnup Fuel for a 2 Year PWR Cycle

Report Participants

Lindsay, Isabelle O[1], Brown, Nicholas [1]
1 University of Tennessee Knoxville

Scientific Achievement

This work performed a safety analysis of two high-burnup fuel designs for a Westinghouse PWR. The goal is to identify potential opportunities and gaps for high-burnup fuel by evaluating fuel performance, reactor physics, thermal-hydraulics, and plant system-level responses. The fuel performance aspect will be accomplished using BISON. Using BISON, selected AOOs and DBAs were simulated for individual fuel pins of interest. The first fuel type is the Westinghouse IFBA design, while the second is a proposed design by the Massachusetts Institute of Technology (MIT). The two designs were compared against current NRC guidance.

Significance

We performed a fuel safety analysis of two fuel design candidates for high-burnup fuel and fuel cycle extension. This analysis utilized boundary conditions developed in RELAP5-3D and PARCS. Between the two designs, the MIT annular design demonstrated greater safety performance due to a greater margin of safety. The MIT annular design experienced less extreme temperature rises in the cladding and fuel regions during a hot zero power control rod ejection. In normal operation and control rod withdrawal, it is not expected that the cladding will fail in either design. However, during a hot zero power control rod ejection, the IFBA design experienced an enthalpy rise consistent with a cladding failure prediction.

Key Publications

Lindsay, I., Fox, M., Seo, S., Sweet, R. T., Brown, N. R. (2023, June 11-15). ANS Annual Meeting: Failure Is Not An Option. Pressurized Water Reactor Contorl Rod Ejection Analysis Using PARCS, RELAP5-3D, and BISON for High Burnup Fuel.

Lindsay, I., Fox, M., Capps, N., Brown, N. R. (2023, August 20-25). 20th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-20). Evaluation of High-Burnup Fuel Coolability during a Control Rod Withdrawal.

Sponsor/Program

NEUP program, grant DE-NE0009212

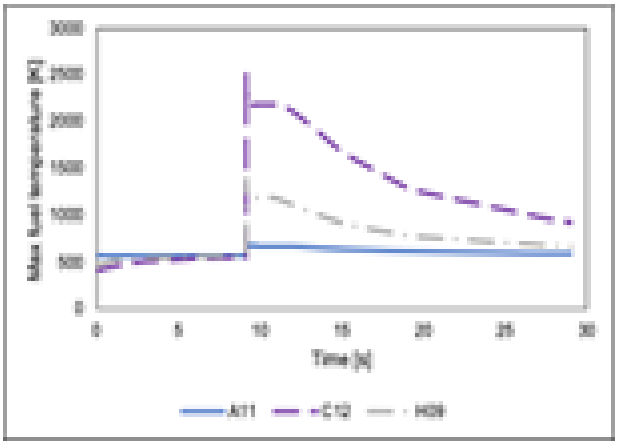


Figure 1: Maximum fuel temperature experienced by IFBA pins of interest.

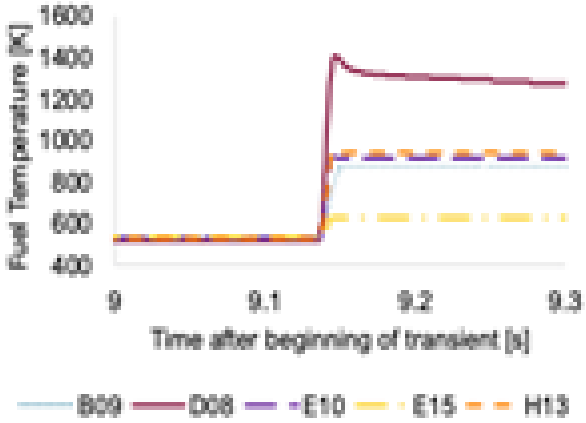


Figure 2: Maximum fuel temperature experienced by MIT annular pins of interest.

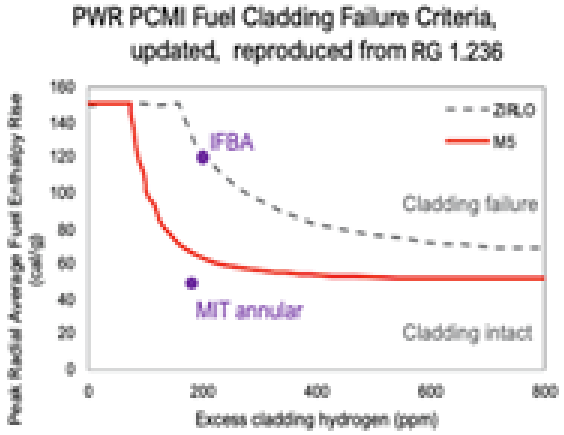


Figure 3: Comparison of most extreme enthalpy rise from each fuel design with respect to regulatory guidance.

B.97 Computation Investigation of U/UN Interface

Report Participants

Lu, Yizhou [1], Choudhury, Samrat [1], Jerred, Nathan [2]
1 University of Mississippi
2 Idaho National Laboratory

Scientific Achievement

In this project, the team investigated the atomic structure and segregation tendency of elements and in particular fission products to the (U-Mo)/UN interface to support the experimental investigation of the nanostructured U-Mo alloys. The U-Mo/UN interface is comprised of two surfaces, namely U-Mo alloy and UN ceramic. For our calculations, we considered a (100)-UN surface with an orientation relationship of [001] U|| [001] UN and (100) U|| (110) UN due to charge neutrality with an equal number of positive (U) and negative (N) atoms in ionic crystal UN. As the size of the nanoparticles grow, the interface between the metal and nitride phase transitions from being coherent (Figure 1a) to a semicoherent (Figure 1b) with the formation of misfit dislocation resulting in a relaxation of interfacial strain. For example, the strains in U in the coherent interface are 24.64% and 18.08% along the x and y directions, respectively, while the corresponding strains in the semicoherent interface are -0.29% and 3.32%. In the case of the semicoherent interface, along the y direction, eight columns of U atoms corresponding to seven columns of N atoms led to the formation of misfit dislocation. We calculated the segregation energy for some solid and gaseous fission products (Ce, Kr, La, Xe) at the U/UN interface with and without interfacial Mo. All the computational work is performed by electronic structure calculation using VASP. Additionally, in this research, we leveraged modern ML tools installed in Python to predict the solute segregation energies at the U/UN interface with a fraction of computational cost compared to first-principles calculations. Twenty-eight commonly substitutional solutes were considered to segregate to the semicoherent U/UN interface: Ti, Sc, Y, Mg, Zr, Hf, Zn, Cd, Co, Os, Sr, Al, Ni, Cu, Rh, Ir, Pd, Pt, Ag, Ba, V, Nb, Na, Ta, K, Rb, W, and Mo.

Significance

The work is still in progress. In this scheme, a negative segregation energy indicates the solute prefers to segregate to the interface, while a positive segregation energy means the solute prefers to reside in the bulk U matrix. For the semicoherent interface, two atomic sites at the interface were chosen, namely the coherent and misfit region of the interface. It is interesting to observe that the solute segregation tendencies change significantly as the interface transition from coherent and semicoherent natures (Figure 2). Further, the segregation tendencies at the semicoherent U/UN interface are dependent on the local chemistry at the segregation site (with and without Mo). A distribution of segregation tendencies was also observed between the coherent terrace and at the misfit region of the interface (Figures 2(b) and (c)). In the ML-guided investigation, we used ML tools such as feature selection to identify the key solute parameters or features that govern the solute segregation energy at the U/UN interface (Figure 3(a)). Chemical features of the solute and features linked to strain energy (such as the bulk modulus of the solute) play a vital role in governing the segregation tendency of a solute, while geometric features (linked to the local atomic environment, such as solute-U distance, U-N distance, solute-N distance) play a relatively minor role in determining solute segregation behavior. In Figure 3(b), the ML-predicted segregation energy is plotted against the segregation energy obtained from first-principles calculations in a semicoherent U/UN

interface. The results show it is possible to predict the solute segregation behavior at (U-Mo)/UN interface with the help of ML tools, such as kernel ridge regression, providing an alternative pathway to obtain the segregation energy of elements at a semicoherent interface with orders of magnitude reduced computational cost compared to first-principles calculations.

Key Publications

Publication is prepared in progress. " Y. Lu, J. Akins, B. Uberuaga and S. Choudhury. "Prediction of solute segregation at metal/ceramic interfaces using machine learning approach . Adv. Mater. Interfaces. 2023 (UNDER PREPARATION)

Sponsor/Program

LDRD Project 21A1050-128FP: Nanostructuring of Uranium Based Metallic Fuels via Spark Plasma Sintering

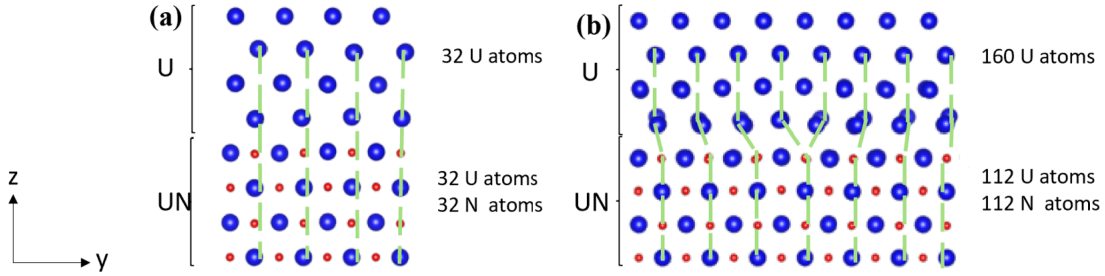


Figure 1: The relaxed U/UN interfaces: (a) coherent interface and (b) semicoherent interface. Orientation relationship: [001] U|| [001] UN and (100) U|| (110) UN.

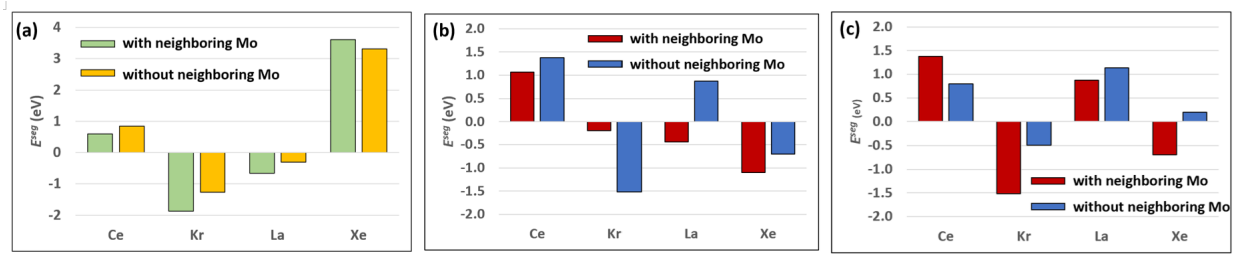


Figure 2: Segregation energy of fission products (Ce, Kr, La, Xe) at the (a) coherent interface, (b) misfit region in the semicoherent interface, and (c) coherent region in the semicoherent interface.

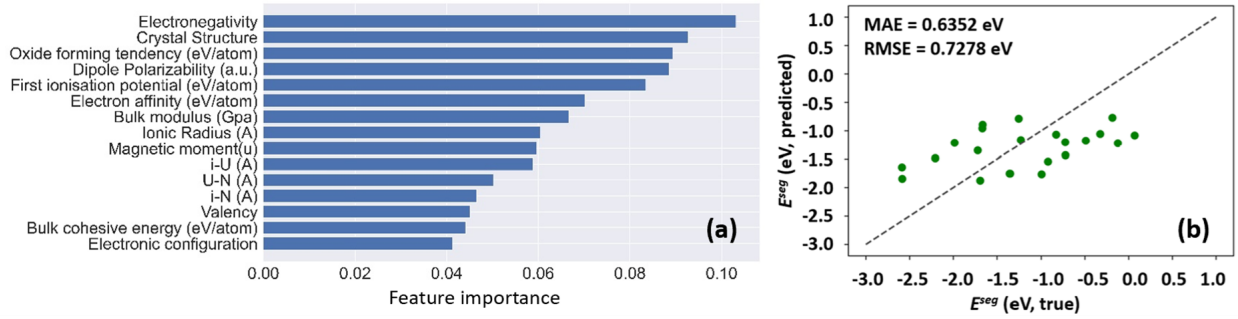


Figure 3: ML results: (a) feature importance analysis (i: solute) and (b) predicted segregation energy (Eseg) vs. computational Eseg from the optimized kernel ridge regression model.

B.98 Improving Autoencoder Performance with Physics Information

Report Participants

Rhoads, Benjamin M[1], Hafen, Joseph [1], Choudhury, Samrat [1], Xian, Min [2]
1 University of Mississippi
2 University of Idaho

Scientific Achievement

This work involves an autoencoder trained on a large dataset of simulated ferromagnetic microstructures under different offset angles and grain boundary transition temperatures. By implementing additional energetic components (bulk and interfacial) into the loss function of the neural network, the model is able to achieve a lower error in its predictions. Many ML models were trained using INL HPC Hoodoo clusters to understand how to improve the model performance in this way. The extent to which the physics information can improve the model was also analyzed by training many models using these computational resources.

Significance

This finding adds a new capability for materials scientists to improve the performance of ML models in their applications to various kinds of materials science applications. Additional runs on larger datasets are currently underway, and once completed, the manuscript for these findings will be written.

Key Publications

A paper on these findings is expected to be written during this summer (2023).

Sponsor/Program

NEAMS

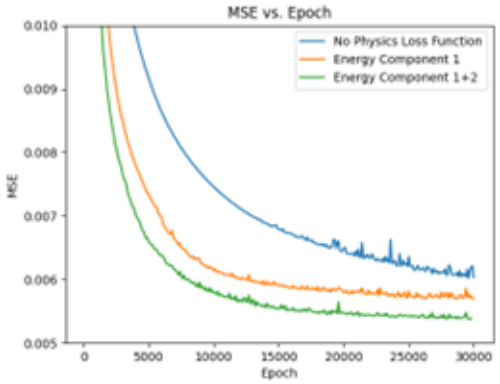


Figure 1: Mean squared error vs. epoch of physics-informed neural network.

Figure 2: Autoencoder-predicted local polarizations in the x-direction.

Figure 3: Example of targeted true polarizations in the x-direction.

B.99 Deimos Experiment Multiphysics Modeling & Simulation with MOOSE and Griffin

Report Participants

Maldonado, Alexis [1]
1 Los Alamos National Laboratory

Scientific Achievement

Utilized the MOOSE Heat Conduction module to simulate transient heat transfer behavior in the experiment. This capability informed experiment designers of a range of electrical powers needed to reach target temperatures, lag time between peak heater temperature and thermocouples, estimated time to reach target temperatures, and more. Additionally, Griffin was used to solve the point kinetics equation with temperature feedback. With Griffin, the experiment approach to critical with a neutron source was simulation with reactivity, kinetic parameters, and temperature reactivity coefficients input from MCNP6. This capability informed experiment designers on the estimated wait time for the neutron population to stabilize during subcritical multiplication, general stability and behavior of the experiment, and more. Deimos is an experiment planned for the National Criticality Experiment Research Center (NCERC). Future work includes estimating the maximum target temperature the experiment can reach while staying within NCERC regulations and validating MOOSE and Griffin with experimental data from Deimos.

Significance

This use of MOOSE and Griffin will test the codes predictive capabilities. Once experimental data is gathered, it will be analyzed with the simulation results to validate the MOOSE and Griffin codes.

Key Publications

Maldonado, Alexis (2022), Design, Simulation, and Analysis of Microreactor Experiments at the National Criticality Experiments Research Center, NCERC Futures Workshop, Los Alamos, NM, Los Alamos National Laboratory, LDRD 20220084DR

Sponsor/Program

LDRD 20220084DR, LA-UR-22-30320

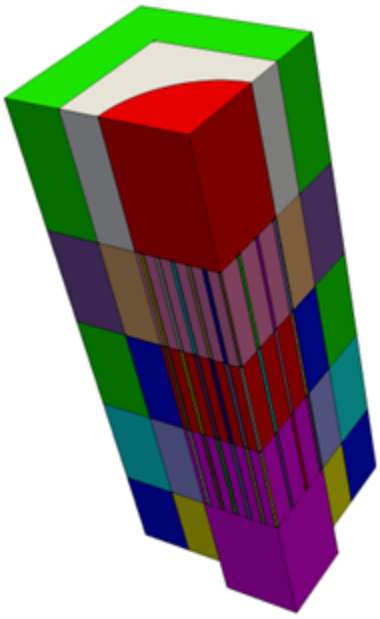


Figure 1: Deimos 1/4th radial, full-axial geometry, and mesh created in Cubit.

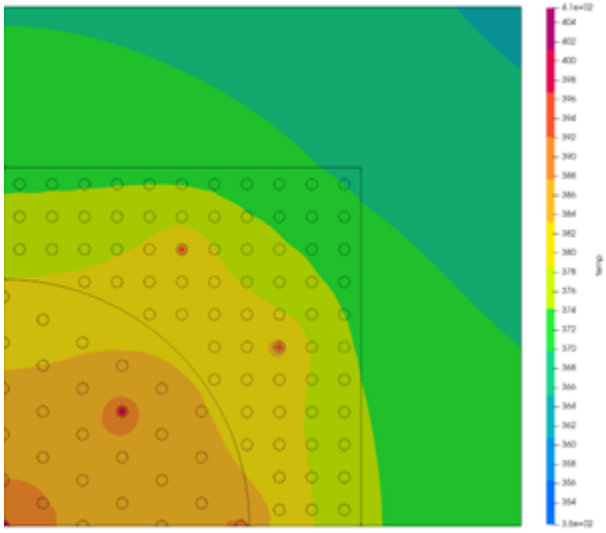
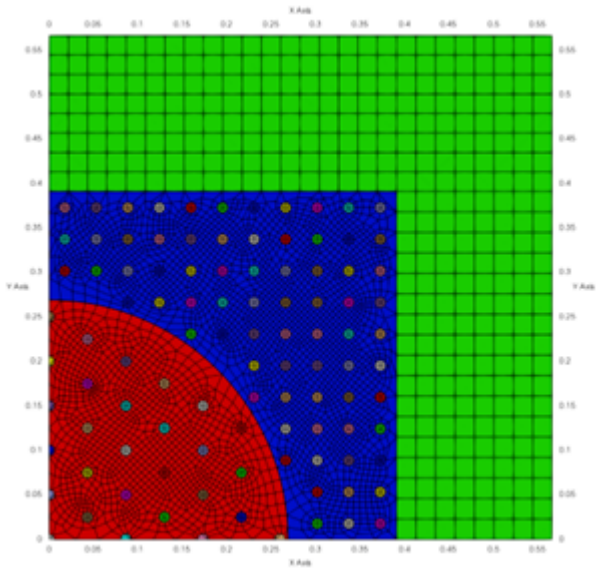


Figure 2: Deimos temperature distribution (MOOSE heat conduction) while heating up (left) and subcritical multiplication behavior (Griffin point kinetics equation) while reactivity is inserted (right).


X Axis
Y Axis
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5
0.55

B.100 FPoliSolutions Risk-Informed System Engineering Method Within FPoliAAP Platform Deployed on HPC

Report Participants

Frepoli, Cesare [1], Valeri, Jarrett D[1], Heagy, Steve [1], Gosdin, Christopher A[1], Mankosa, Michael G[1], Johnston, Timothy E[1]
1 FPoliSolutions LLC

Scientific Achievement

FPoli Agile Application Platform (FPoliAAP) is a digital infrastructure from which highly responsive digital solutions can be quickly deployed and customized. Specifically, for risk-informed solutions, the mission has been to develop and commercialize an integrated data and simulation management framework that will enable a rapid introduction of risk-informed system analysis services for NPPs. The solutions target both the operating fleet, as well as advanced reactors under development. Within the FPoliAAP Platform is RISE: Risk-Informed System Engineering. The RISE service has been developed specifically to orchestrate the complexities associated with implementing a risk-informed design process in line with the proposed 10 CFR Part 53 rule as formulated in the NEI-18-04 roadmap. The objective of the new rule is to provide a generic risk-informed and technology-neutral licensing framework. However, its practical implementation is quite complex, and the definition of an economical and effective solution that satisfy the original intent of the LMP is nontrivial. This represents a gap that RISE was specifically built to close. RISE is powered by the FPoliAAP digital framework. The platform uses modern data management and simulation management tactics to orchestrate complex workflows with a generic powerful UI/UX. Several uses cases can be supported from test data management (FPoliDON), document management (FPoliDOX), and simulation management (FPoliSIM). RISE is the new service designed to automate and facilitate the workflow associated with NEI-18-04 and is built within the same FPoliAAP framework. FPoliAAP is being deployed on the INL's HPC for projects including INL Contract No. 254061 associated to SOW-18518.

Significance

The main goal of this project is to address specific concerns relative to the implementation of 10 CFR Part 53. FPoli will use its RISE service to orchestrate the engineering activities toward this goal, including: " Generate event trees " Perform SSC classification " Identify safety-basis events (deterministic assessment using event trees) " Develop a practical evaluation methodology in line with the proposed 10 CFR Part 53 rule as formulated in the NEI-18-04 roadmap. " Determine defense-in-depth adequacy " Implement enhanced automation of workflows for implementing an analysis methodology utilizing FPoliAAP technology " Population of selected data in FPoliAAP platform to support digital documentation " Post-process analysis results

Key Publications

None

Sponsor/Program

Industry

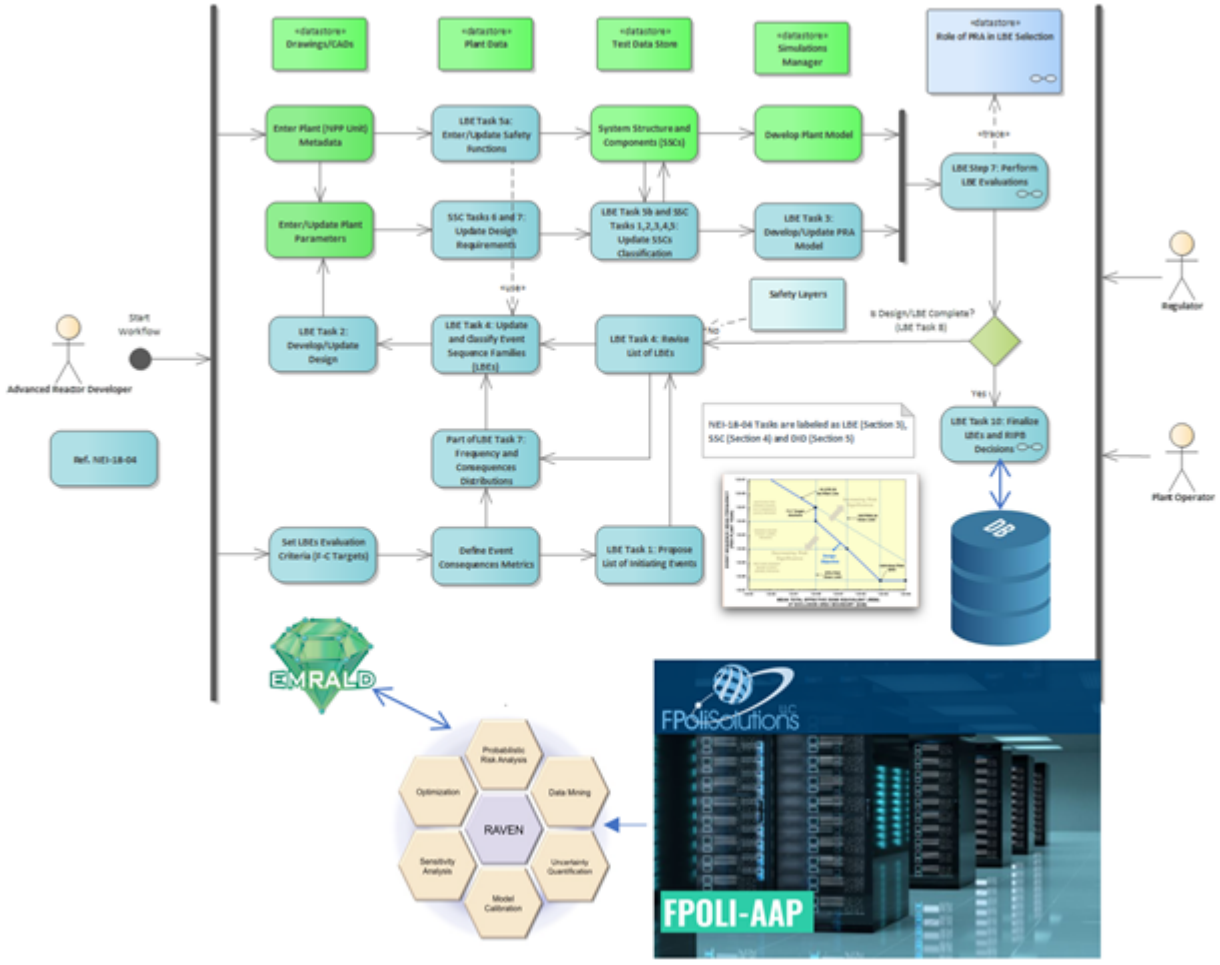


Figure 1: FPoliAAP RISE Platform: A digital solution to orchestrate complexities associated with the implementation of risk-informed design in response to NEI-18-04 (LMP).

B.101 UN/UCO TRISO Particle Fuel Performance Analysis

Report Participants

Masri, Abdullah M[1], Zhang, Yongfeng [2], Rezwan, Aashique [2]
1 University of Wisconsin-Madison
2 University of Wisconsin Madison

Scientific Achievement

Using the INL HPC, we simulated a smeared cracking model of the TRISO particle buffer layer. Using a porosity-dependent fracture strength model, we aimed to see how porosity distribution within the buffer layer affects fracture mode (delamination vs. radial propagation). Currently, we are working with an experimental researcher to analyze the buffer layer pore structure to increase the fidelity of a porosity-dependent fracture strength model.

Significance

Being able to predict how the buffer layer will fail is integral to optimizing TRISO particles. While no fracture is preferred, delamination is significantly better than radial crack propagation, as delamination ensures the buffer layer remains intact. Furthermore, radially propagating cracks can propagate across the IPyC layer and into the SiC layer. If the SiC layer is cracked, the entire TRISO particle is considered failed. Understanding the mechanisms that control fracture modes can allow researchers to study potential solutions for preventing TRISO particle failure.

Key Publications

Study is in progress.

Sponsor/Program

UNLP graduate fellowship

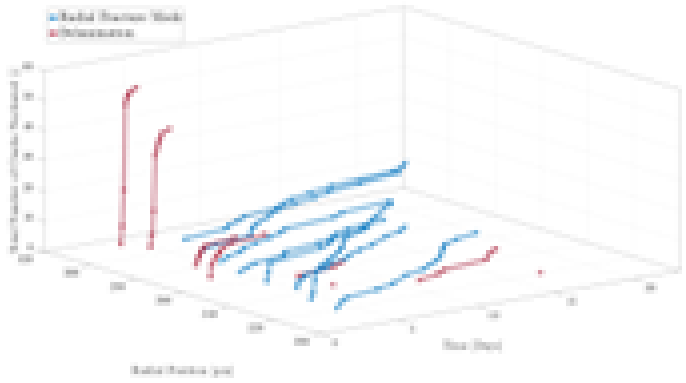


Figure 1: Cracks nucleated over time and distance in the buffer layer, showing how the crack propagation profile differs between different fracture modes.

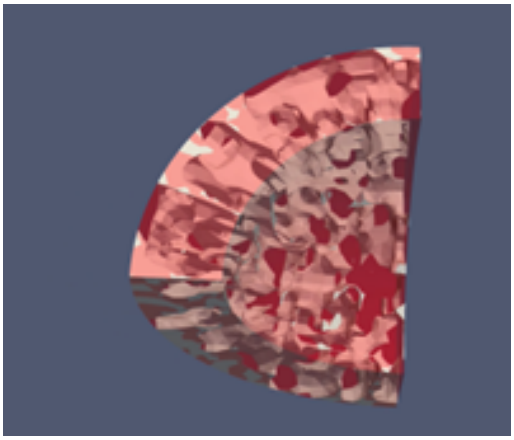


Figure 2: Radial fracture mode.

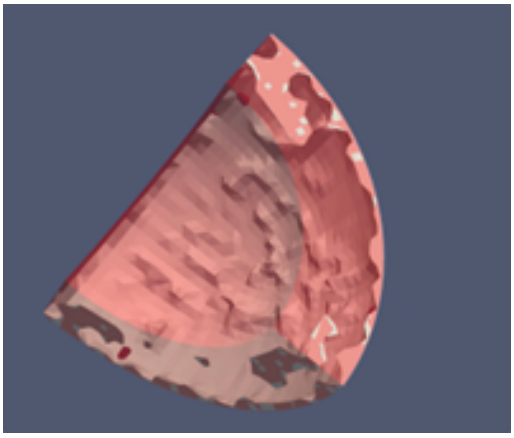


Figure 3: Delamination fracture mode.

B.102 Improvement of NEAMS Fuels Codes

Report Participants

Matthews, Christopher [1], Cooper, Michael W[1], Rizk, Jason T[1], Andersson, David [1]
1 Los Alamos National Laboratory

Scientific Achievement

The team here are heavily involved in the development of NEAMS codes for fuel performance simulations, fundamental nuclear fuel material behavior, and large-scale reactor simulations. This work includes improvements to the BISON fuel performance code, Marmot phase-field code, and the DireWolf reactor tool-suite, either directly or indirectly. In support of these developments, the resources provided by the INL HPC are primarily in the GitLab repository of the MOOSE-based tools. Occasionally, HPC compute nodes are utilized in support of model development.

Significance

The primary significance of the findings here were based in the ability of modeling to play a larger role in improving the understanding of nuclear fuel under irradiation. This helps in both design tasks for which mechanistic models can be used to analyze materials in unique operational space or geometries, but also in the licensing aspects of advanced materials.

Key Publications

Matthews, C., Laboure, V., DeHart, M., Hansel, J., Andrs, D., Wang, Y., et al. (2021). Coupled Multiphysics Simulations of Heat Pipe Microreactors Using DireWolf. Nuclear Technology, 207(7), 1142–1162. http://doi.org/10.1080/00295450.2021.1906474

Cooper, M. W., Pastore, G., Che, Y., Matthews, C., Forslund, A., Stanek, C. R., et al. (2021). Fission gas diffusion and release for CrO-doped UO: From the atomic to the engineering scale. Journal of Nuclear Materials, 545, 152590. http://doi.org/10.1016/j.jnucmat.2020.152590

Andersson, D. A., Matthews, C., Zhang, Y., & Beeler, B. (2021). Density functional theory calculations of the thermodynamic and kinetic properties of point defects in -U. Journal of Nuclear Materials, 557, 153238. http://doi.org/10.1016/j.jnucmat.2021.153238

Sponsor/Program

NEAMS

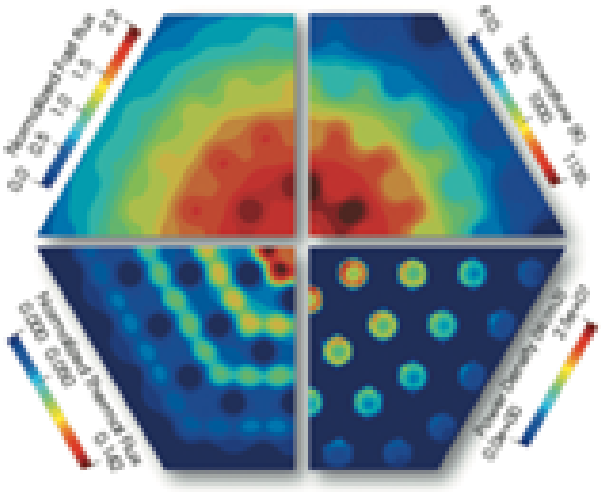


Figure 1: Example of the complex interconnected behavior needed to be captured during microreactor simulations.

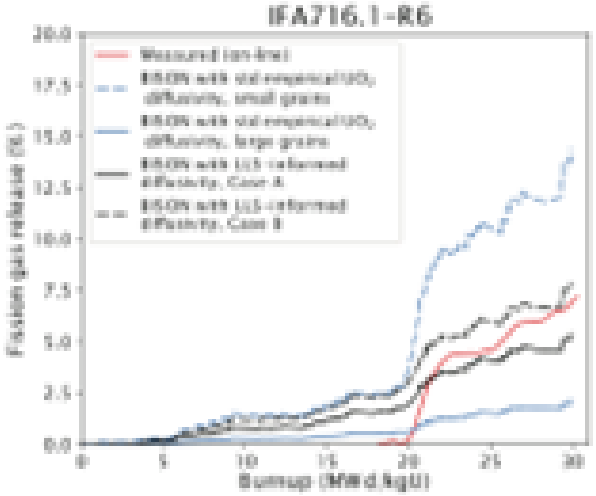


Figure 2: Fission gas release calculated by BISON for a doped-UO2 fuel with and without mechanistic correlations for xenon diffusion.

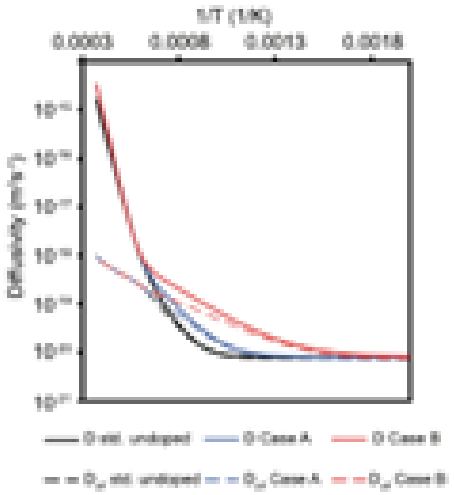


Figure 3: Updated fission gas diffusivity computed via multiscale and mechanistic model development.

B.103 Optimization of Nuclear-Renewable Grids

Report Participants

Richards, James [1], Alfonsi, Andrea [1]
1 Ultra Safe Nuclear Corporation

Scientific Achievement

The RAVEN package is used to optimize a nuclear-renewable grid for cost and size and to manage optimization and sampling strategies.

Significance

This model helps Ultra Safe Nuclear Corporation optimize strategy regarding VRE and microreactor integration. It also helps us develop and produce features for RAVEN, such as the hausdorff similarity measure by aalfonsi Pull Request #2085 idaholab/raven GitHub. This work also supported testing features in RAVEN and led to bug catches and fixes, such as: [DEFECT] Metropolis Sampler likelihood must be an output of the model Issue #2098 idaholab/raven GitHub and [DEFECT] Genetic Algorithm and Simulating Annealing Explicit Constraints initial points Issue #2049 idaholab/raven GitHub.

Key Publications

None

Sponsor/Program

Industry

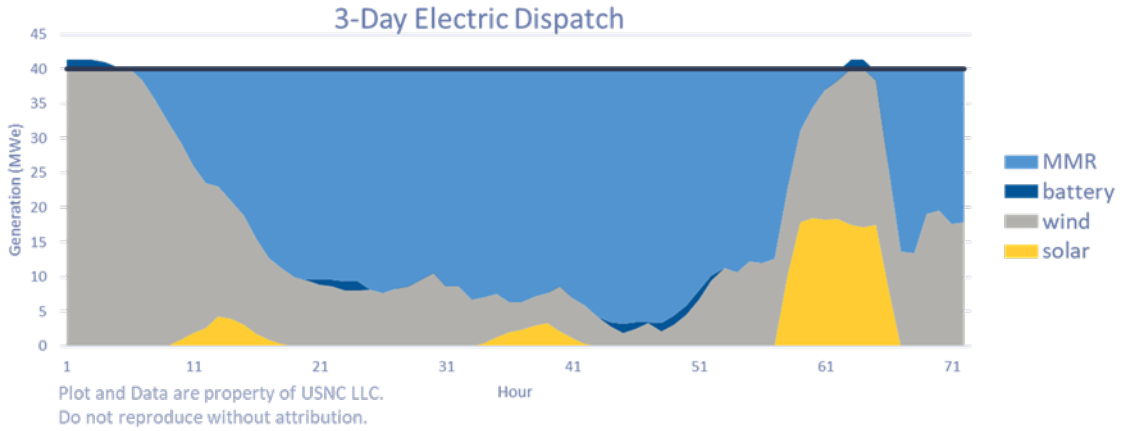


Figure 1: Sample of an optimal dispatch produced by the RAVEN-based optimization model. Because of the high temporal resolution required, the HPC facilitates parallelization for more rapid optimization of RAVEN feature testing. Do not reproduce plot without attribution to Ultra Safe Nuclear Corporation, LLC.

B.104 Validation of Pronghorn-Subchannel Using EBR-II Shutdown Heat Removal Tests

Report Participants

Tano Retamales, Mauricio E[1], Kyriakopoulos, Vasileios [1], McCay, James W[2], Arment, Tyrell W[2]
1 Idaho National Laboratory
2 Oklo Inc

Scientific Achievement

Pronghorn-Subchannel (Pronghorn-SC) is a subchannel code integrated within the MOOSE framework that has been recently extended to simulate liquid metal flows in hexagonal wire-wrapped nuclear fuel assemblies. This collaborative project between NEAMS and Oklo Inc. has validated Pronghorn-SC against steady-state and transient data from EBR-II loss-of-flow Shutdown Heat Removal Tests (SHRT) 17 and 45R. Pronghorn-SC agreed well with experimental data for both transient and steady-state conditions.

Significance

Shutdown heat removal and behavior during LOFAs are important parts of the safety case for a reactor, and validated tools for modeling such events are needed. Subchannel codes allow for detailed estimates of temperatures in the core's fuel assemblies, which are often the limiting factor in a reactor's resilience to a transient. While several other subchannel codes for liquid metal flows exist, they have either limited physics for transients or are difficult to extend and couple with other codes. Pronghorn-SC improves on both issues, as it is a modern code in the versatile MOOSE framework that can model transient flows. This study is a significant step towards validating it for industrial use.

Key Publications

Tano, M., Kyriakopoulos, V., McCay, J., Arment, T., (2023). Validation of Pronghorn's subchannel code using EBR-II shutdown heat removal tests: SHRT-17 and SHRT-45R. Paper in development for submission to Nuclear Engineering & Design.

Sponsor/Program

NEAMS

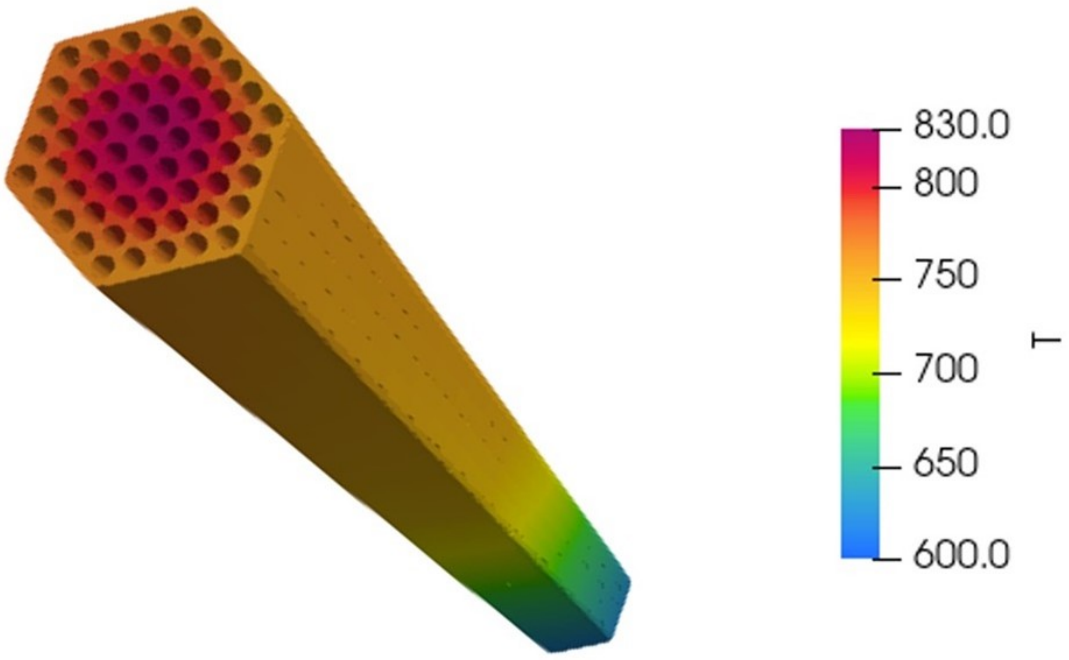


Figure 1: Temperature in an EBR-II assembly predicted by Pronghorn-SC.

B.105 Controlling RELAP5-3D Through Python GEKKO Model Predictive Control

Report Participants

Wallace, Jarron [1], Hill, Daniel [1], Hedengren, John [1], Memmott, Matthew J[1]
1 Brigham Young University

Scientific Achievement

Model predictive control (MPC) has been proposed for use in the nuclear industry to assist with load-following capability. While existing simulators can operate in real time, they do not have any feed-forward ability. MPC can help nuclear power plants coupled to a thermal energy storage (TES) system or other energy storage and consumption unit, such as hydrogen production, will be vital to ensure the reactor is operating most effectively to utilize these systems. The MPC proposals for NPPs have utilized another mathematical model to test the control. This research proposes utilizing a first-principles model coupled to MPC to control RELAP5-3D. By controlling REALP5-3D with MPC, plant designers can incorporate MPC methodology into future licensing requests. For example, to aid in licensing a TES unit on an existing PWR, RELAP5-3D and MPC can be used to model the thermal-hydraulic operation of both the reactor and the TES while it is undergoing feed-forward control based on grid predictions. The results from these simulations, which are performed much faster than real time, can show the operation and stability of the reactor coolant pressure boundary under load-following circumstances. In addition, by coupling to RELAP5-3D, this methodology allows for the rapid prototyping of TES designs while monitoring the thermal-hydraulic operation of the core and TES.

Significance

RELAP5-3D can be interfaced with Python to create, run, and analyze RELAP models. That interface can then be coupled with Python GEKKO to allow for MPC of the created RELAP5-3D model. The REALP5-3D model and first-principles model utilized in the MPC methodology were derived from an experimental apparatus that modeled thermal energy storage in water. The MPC of RELAP5-3D worked and accurately controlled the RELAP5-3D system while minimizing the error between the current temperature and temperature setpoints. This work was performed under DOE NEUP Project no. DE-NE0008866, and this work has been concluded.

Key Publications

J. Wallace, D. Hill, D. Thurston, J. Hedengren, M. Memmott, Controlling RELAP5-3D Through Python Gekko Model Predictive Control , Publication Pending

Sponsor/Program

U.S. DOE-NE NEUP Project no. DE-NE0008866

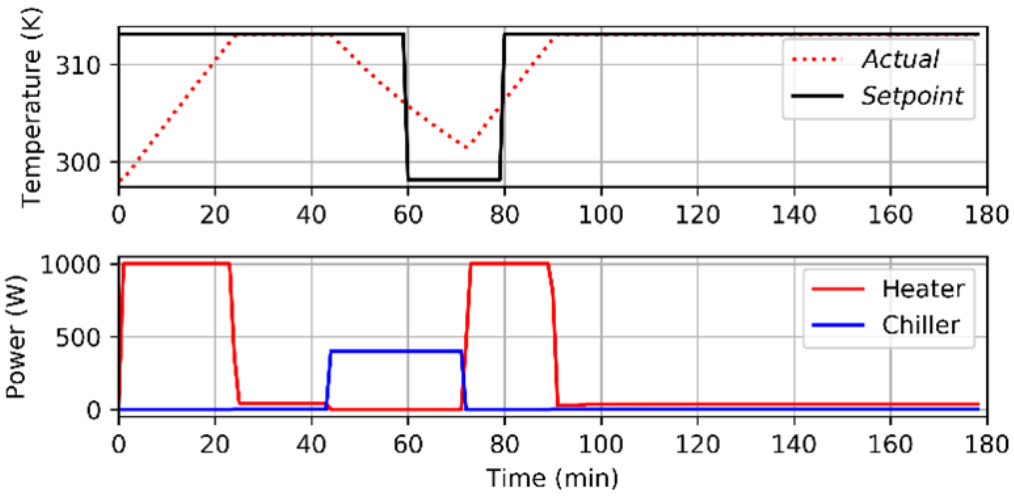


Figure 1: RELAP5-3D MPC with an integer solver and 25 minute time horizon utilizing an absolute difference objective function.

B.106 Evaluation of the BISON Code for Simulating Metallic Fuels

Report Participants

Miao, Yinbin [1]
1 Argonne National Laboratory

Scientific Achievement

Establishing comprehensive fuel performance simulation capabilities for SFR metallic fuel is an important component of the development of the advanced fuel performance code BISON. Legacy irradiation data of these metallic fuels are needed to evaluate, verify, and validate the related models in BISON. In this project, we have been working on integrating the SFR fuels irradiation and physics database (FIPD) with BISON to support the metallic fuel model evaluation and improvement effort of BISON leveraging the U.S. experiences with SFR metallic fuels.

Significance

SFRs are an important type of advanced reactor being developed by multiple industry vendors as well as being investigated by the U.S. government. Metallic fuels (U-10Zr and U-xPu-10Zr) are the mainstream SFR fuel in the United States because of the country's extensive irradiation experience with metallic fuel, a significant fraction of which is organized and maintained in the FIPD database. In this project, FIPD data are used to generate input files for BISON simulations as well as to be compared with the BISON output. All the aforementioned work is automated by implementing corresponding BISON objects that can directly use FIPD data files. In the last year, the cladding-degradation-focused BISON models have been assessed using the data, and the achievements were summarized as BISON Assessment Case X447.

Key Publications

Miao, Yinbin, Oaks, Aaron, Yacout, Abdellatif M., Matthews, Christopher, and Novascone, Stephen. FY22 Progress Report on BISON Metallic Fuel Model Development and V&V Using EBR-II Legacy Data. United States: N. p., 2022. Web. doi:10.2172/1907952.

Sponsor/Program

NEAMS Fuel Performance Technical Area

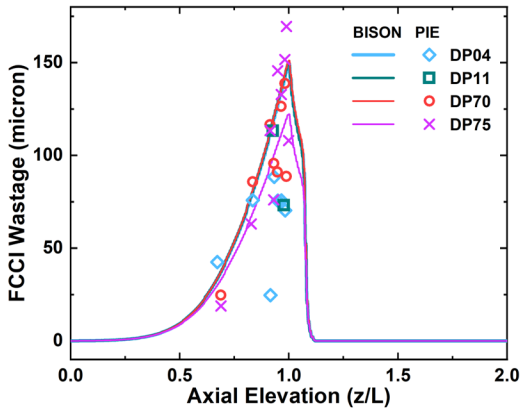


Figure 1: BISON-predicted fuel-cladding chemical interface wastage thickness compared with measured data for four representative U-10Zr/HT9 pins irradiated in X447/A.

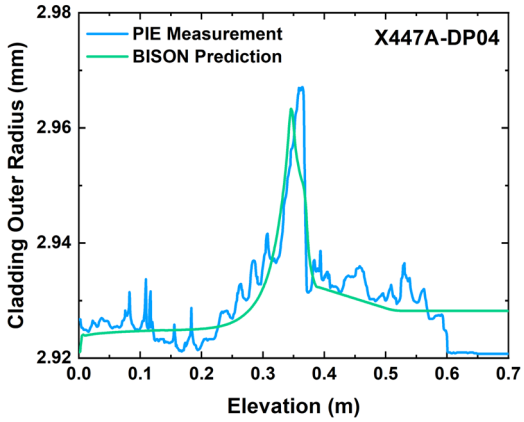


Figure 2: BISON-predicted cladding outer radius in comparison to profilometry measurement for Pin DP04.

B.107 MOOSE Reactor Module Workshop

Report Participants

Shemon, Emily R[1], Miao, Yinbin [1], Mo, Kun [1], Kumar, Shikhar [1], Oaks, Aaron J[1], Jung, Yeon S[1], Lee, Soon K[1], Harbour, Logan H[2], Giudicelli, Guillaume L[2], Stogner, Roy H[2]
1 Argonne National Laboratory
2 Idaho National Laboratory

Scientific Achievement

We are preparing to host a MOOSE Reactor Module Workshop in May 2023 for numerous participants. Access to INL HPC is required to run test cases and access the NEAMS Workbench and MOOSE binary.

Significance

Numerous folks will be trained to perform nuclear reactor mesh generation using MOOSE by the team members as report participants here.

Key Publications

Emily Shemon, Yinbin Miao, Shikhar Kumar, Kun Mo, Yeon Sang Jung, Aaron Oaks, Scott Richards, Guillaume Giudicelli, Logan Harbour & Roy Stogner (2023) MOOSE Reactor Module: An Open-Source Capability for Meshing Nuclear Reactor Geometries, Nuclear Science and Engineering, DOI: 10.1080/00295639.2022.2149231

Sponsor/Program

NEAMS

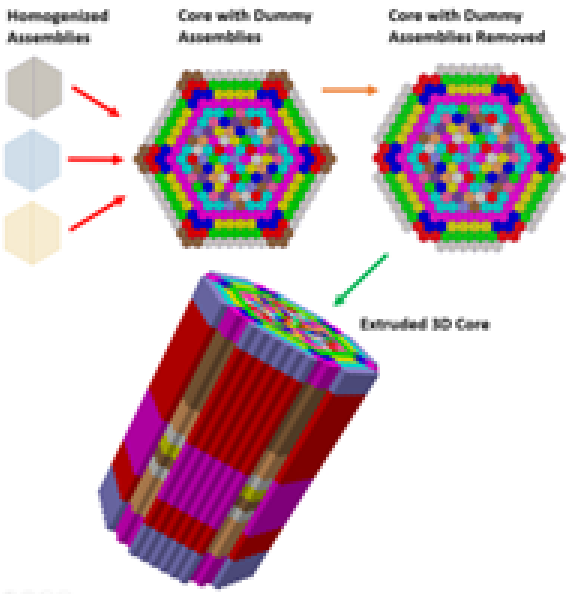


Figure 1: Excerpt from tutorial material on how to build a fast reactor core mesh.

B.108 Assessing Multiphysics Simulations of Microreactors Using MOOSE Applications

Report Participants

Miao, Yinbin [1], Mo, Kun [1], Cao, Yan [1], Nunez, Daniel [1], Abdelhameed, Ahmed A[1], Shemon, Emily R[1], Stauff, Nicolas [1]
1 Argonne National Laboratory

Scientific Achievement

This report summarizes efforts and progress supported by an ongoing NEAMS project on multiphysics simulations of advanced microreactors using a combination of MOOSE applications with focuses on different physics, including Griffin, BISON, Sockeye, SAM, etc. In this project, supported by the NEAMS Microreactor Multiphysics Applications Program, these MOOSE applications are coupled together to simulate the neutronics, thermomechanics, and heat removal performance of advanced microreactors. Both steady-state performance and power transient responses have been simulated to demonstrate the NEAMS tools' capabilities and help direct future improvements. While the light-duty single-physics simulations were mainly performed on ANL's divisional clusters, INL's HPC has been used to perform the multiphysics simulations due to the increasing demands on computational resources.

Significance

The project provides a key demonstration on the powerful capabilities of the MOOSE applications for microreactor-related stakeholders and insightful comments and suggestions for the MOOSE application developers.

Key Publications

1. Stauff, N., Abdelhameed, A., Cao, Y., Kristina,, Miao, Y., Mo, K., and Nunez, D.. Multiphysics Analysis of Load Following and Safety Transients for MicroReactors. United States: N. p., 2022. Web. doi:10.2172/1891258. 2. Nicolas E. Stauff, Ahmed Abdelhameed, Yan Cao, Daniel Nunez, Yinbin Miao, Kun Mo, Changho Lee, Christopher Matthews, Emily Shemon, Justin Thomas, Applications of NEAMS Codes for Multiphysics Modeling of Several Microreactors Problems, Proceedings of the ANS Winter (2022). 3. Ahmed Abdelhameed, Yan Cao, Daniel Nunez, Yinbin Miao, Kun Mo, Changho Lee, Emily Shemon, Nicolas E. Stauff, High-Fidelity Multiphysics Modeling of Load Following for 3-D Gas-Cooled Microreactor Assembly using NEAMS Codes, Proceedings of the ANS Winter (2022).

Sponsor/Program

NEAMS Program, under Multiphysics Applications Technical Area

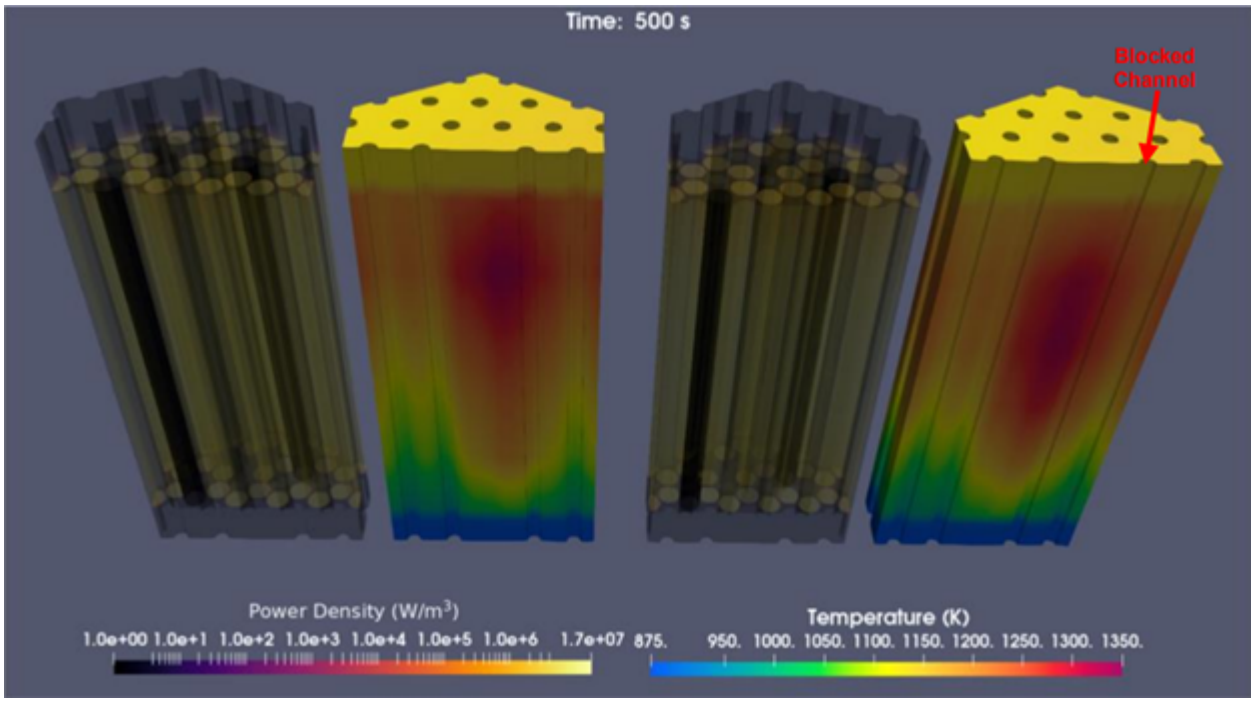


Figure 1: A typical power density and temperature profile of a gas-cooled microreactor assembly after a single channel blockage incident as predicted by multiphyics models using diffusion (left) and CMFD DFEM-SN (right) neutronics approaches.

B.109 Distortion Impact of Geometric Changes to ATR-Style Fuel Elements

Report Participants

Miller, Matthew B[1]
1 Naval Nuclear Laboratory

Scientific Achievement

Understanding the impact that geometric changes have on the distortion behavior of an ATR-style fuel element is important to support any development or improvements in future material test reactor fuel element design. This work created a finite-element model (FEM) to provide the distortion of the complex geometry of an ATR plate-type fuel element. The proven ATR fuel element geometry and variations to that geometry were modeled and distortions calculated. The impact from the geometric variations were determined by comparison to the distortions of the proven ATR fuel element geometry. These studies provide a basis for the preliminary design of future ATR-style fuel elements.

Significance

The comparison of distortions focused on the distance between the fuel plates and overall distortion of the fuel element. The geometric variations evaluated include an increased fuel plate width and reduced number of fuel plates. The geometric variations analyzed showed minimal impact to the distance between fuel plates but had unacceptable overall distortion of the fuel element. The FEM created in this study allows for further geometric variations to be evaluated for feasibility and supports any future fuel element designs for material test reactors.

Key Publications

Miller, M. B., Abdalla Y.G., Beran, M. R., Kurt, E. G. 2022. Thermal Testing Capabilities. Mechanical Studies. INL/RPT-22-69346, Naval Nuclear Laboratory, Idaho National Laboratory

Sponsor/Program

ATR

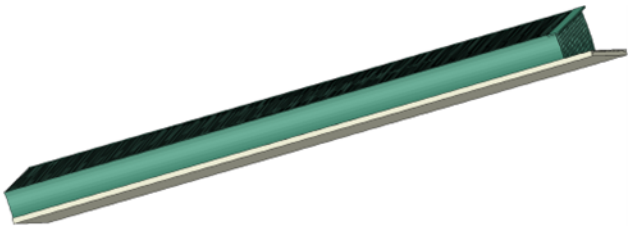


Figure 1: Fuel element quarter symmetry FEM.

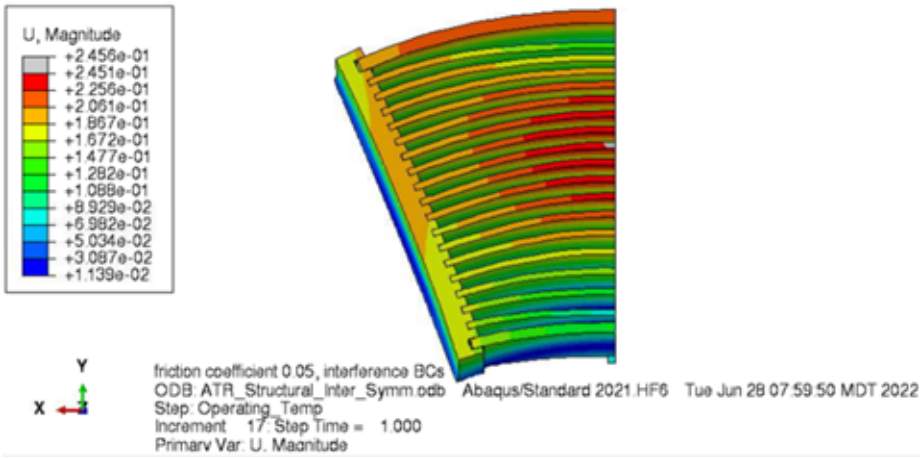


Figure 2: Finite element analysis distortion results.

B.110 Multiphysics Modeling Demonstration of Heat-Pipe-Cooled Reactor Concepts

Report Participants

Mui, Travis [1], Hu, Rui [1]
1 Argonne National Laboratory

Scientific Achievement

The objective of this work is to improve SAM system modeling capabilities for novel heat-pipe-cooled reactor concepts to expand the predictive capability of a coupled multiphysics simulation as part of the BlueCRAB platform. Preliminary work has been performed on heat-pipe modeling improvements in SAM and coupling within the BlueCRAB framework.

Significance

Heat pipes utilize the phase change of a working fluid to transport a large amount of heat from one end to the other with a minimal drop in temperature. These reactor designs make use of hundreds of heat pipes to passively extract thermal power, which has the potential to significantly improve reactor reliability and safety. As such, it is critical to be able to accurately and efficiently capture the physical phenomena of the working fluid that governs the heat transport capacity of a heat pipe. For designs that involve hundreds of heat pipes that need to be simulated, system code efficiency is key for any code to be effective in modeling these designs. Furthermore, the ability to couple SAM's predictive capability with other physics (e.g., neutronics, thermal mechanics) is also needed to simulate systemwide behavior in off-normal transient situations.

Key Publications

(Work in progress)

Sponsor/Program

U.S. Nuclear Regulatory Commission, U.S. DOE Office of Nuclear Energy Nuclear Energy Advanced Modeling & Simulation (NEAMS) program

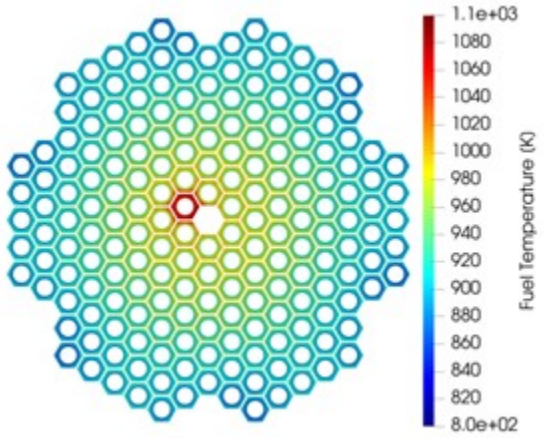


Figure 1: Coupled multiphysics prediction of fuel temperature with a single heat pipe failure in the INL Design A microreactor.

B.111 Cr2O3-Doped UO2 Fuel Rod Irradiation from Halden IFA-677.1 and IFA716.1 & SCIP Ramp Tests

Report Participants

Norman, Jonathan [1], Che, Yifeng [2], Novascone, Stephen R[2], Pastore, Giovanni [1], Wirth, Brian [1]
1 University of Tennessee Knoxville
2 Idaho National Laboratory

Scientific Achievement

This collaborative project was a presentation given at the International Atomic Energy Agency Consultancy Meeting under the CRP for the Testing and Simulation for Advanced Technology & Accident Tolerant Fuels in Vienna, Austria, on December 8, 2022. A comprehensive uncertainty quantification was conducted on Rod 1 from IFA 716, demonstrating a sensitivity to the linear heat rate and contact models used. Additionally, data provided from the SCIP-II program was modeled using BISON to benchmark BISON as a fuel performance code with a focus on PCMI.

Significance

The results of the uncertainty quantification demonstrated that a perturbation in the provided LHR for the given experiment was necessary in order to minimize the error between the measured data and BISON models. Modeling the SCIP-II data demonstrated the impact of impact of chromia-doped fuel on fission gas release and PCMI-related behaviors.

Key Publications

Two untitled publications are presently in progress for the aformentioned topics.

Sponsor/Program

DOE, University of Tennessee, Knoxville

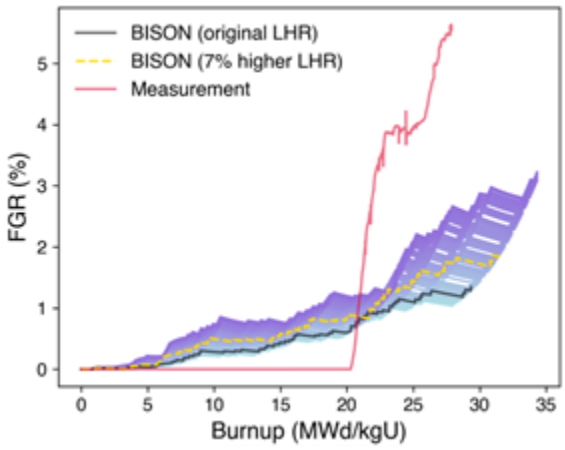


Figure 1: QU for IFA716.1.

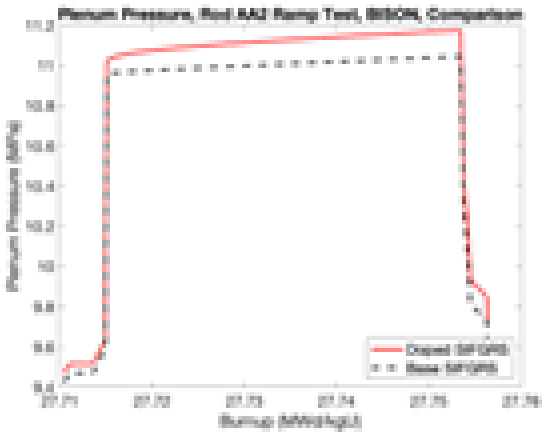


Figure 2: Effect of chromia dopant on SIFGRS.

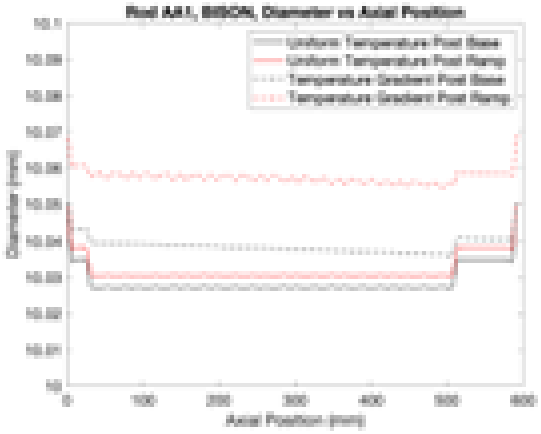


Figure 3: Diametrical change comparisons.

B.112 Machine Learning Guided Prediction of Fe-C Solidification

Report Participants

Rhoads, Benjamin M[1], Choudhury, Samrat [1], Hu, Shenyang [2], Li, Yulan [2], Xian, Min [3]
1 University of Mississippi
2 Pacific Northwest National Laboratory
3 University of Idaho

Scientific Achievement

This study has successfully built a convolutional-RNN capable of predicting the microstructure evolution of Fe-C under any given cooling temperature, initial concentration, and initial microstructure. The model has been improved in many aspects, including the model architecture, activation functions, and loss functions, to make the model predictions more accurate. Additional physics energetic components have also been introduced to the loss function to improve the model performance. For a small dataset, this additional physics information has significantly improved the model performance. Many Python scripts were run on INL HPC to confirm these findings.

Significance

These findings will provide another tool in materials scientists' toolbox when applying ML to materials science problems. While it is typically very costly to get more experimental data, one can implement the physics components of the data in question to further improve the model performance, saving time and money. This work is in the finishing stages, and a paper will be written this summer, 2023.

Key Publications

Paper on these findings will be written this summer (2023).

Sponsor/Program

NEAMS

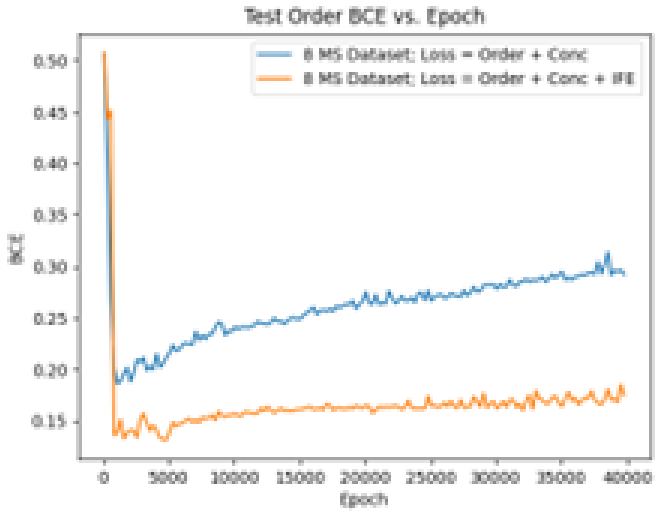


Figure 1: Error in model performance (binary cross entropy) with (orange) and without (blue) interfacial energy component in loss functions as a function of Epoch.

Figure 2: Predicted dendrite of Fe-C at the first timestep in microstructure evolution by a model trained on a large dataset.

Figure 3: The true Fe-C dendrite for a given cooling temperature and initial carbon concentration at a given timestep.

B.113 Cardinal: Accelerating Discovery in Fusion and Fission Energy

Report Participants

Novak, April [1], Gaston, Derek R[2], Merzari, E [3], Shriwise, Patrick C[1], Shaver, Dillon R[1], Fischer, P [4], Min, M [1], Martineau, R [1]
1 Argonne National Laboratory
2 Idaho National Laboratory
3 Pennsylvania State University
4 University of Illinois, Urbana-Champaign

Scientific Achievement

Cardinal is a multiphysics solver that leverages MOOSE for multiscale and multiphysics simulations of nuclear energy systems. Cardinal is intended to provide lower-length-scale simulations to benchmark coarse mesh tools, gain fundamental insights into underexplored physics, and complement experimental campaigns.

Significance

Cardinal provides detailed modeling of nuclear energy systems with explicit representation of fine-scale details in both the neutronics and thermal hydraulics domains. Cardinal leverages mixed central processing unit and GPU resources using in-memory data transfers, which enables large-scale multiscale and multiphysics simulations. Furthermore, Cardinal is intended for practical engineering due to its incorporation of CAD geometry for Monte Carlo transport and unstructured meshes for all physics domains. A flexible interface to MOOSE allows seamless plug-and-play simulations with the entire MOOSE ecosystem. Cardinal is a winner of the 2023 R&D 100 Award.

Key Publications

Sponsor/Program

NEAMS,Gateway for Accelerated Innovation in Nuclear, INL LDRD, ANL LDRD

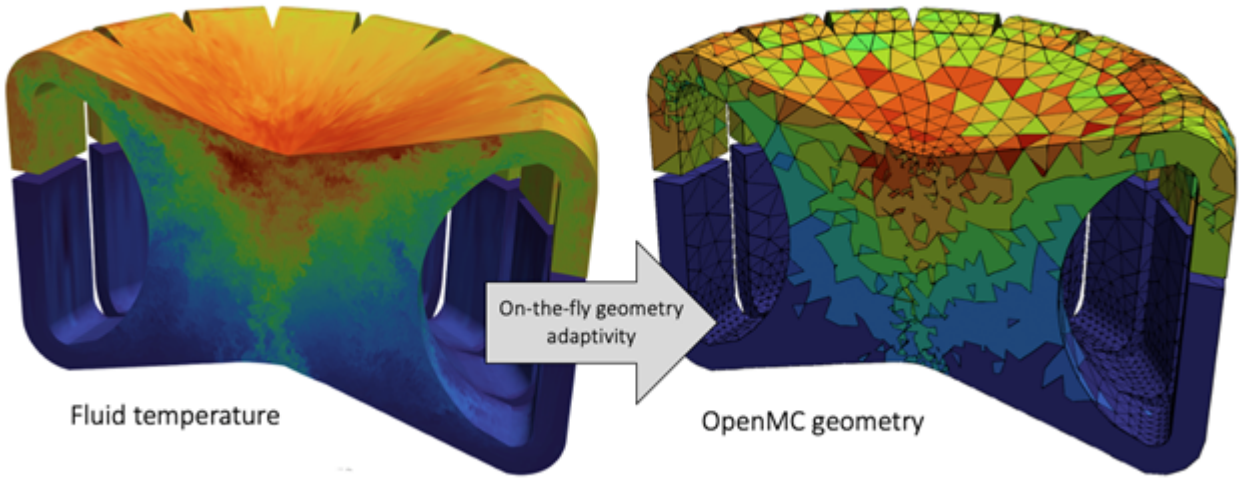


Figure 1: Multiphysics simulation of an MSR, which couples NekRS and OpenMC. Left: NekRS fluid temperature. Right: OpenMC on-the-fly regenerated cell boundaries.

B.114 AI/ML-Enhanced Neutron Source ID and Spectroscopy with RDT's NRID

Report Participants

Ochs, Taylor R[1], Bellinger, Steven [1], Anderson, Matthew W[2], Fronk, Ryan G[2]
1 Radiation Detection Technologies, Inc.
2 Idaho National Laboratory

Scientific Achievement

This project, and future work, entails utilizing INL-developed artificial intelligence (AI) and ML algorithms to enhance the neutron source localization and identification, neutron energy spectrum unfolding, and neutron dose rate calculations, capabilities of RDT's Neutron Radioisotope Identifier and Dosimeter (NRID). INL's HPC resources were used to perform MCNP simulations of the NRID for a small subset of neutron-emitting radioactive sources in various source-detector configurations. The simulation results were then used to generate over 78 million detector response spectra to train and evaluate the AI/ML algorithms. The AI/ML algorithms showed very high accuracy for source localization and the highest-to-date accuracy for source identification. Software/Algorithms " MCNP " Uhura - Application No. 17/649,031, Increasing Energy Resolution, and Related Methods, Systems, and Devices, " Spock - Application No. 63/063,183, Machine-Learned Spectrum Analysis,

Significance

A need persists for an accurate neutron spectrometer for source identification, neutron energy spectrum measurement, and high-accuracy area neutron dose monitoring. Such an instrument is useful to nuclear nonproliferation, radiation area monitoring, and neutron-related science applications. Legacy systems, like Bonner spheres, require multiple measurements with different moderator spheres and external calculations for neutron energy spectrum determinations. REM balls provide dose rate information but are inaccurate for epithermal and fast (5–10+ MeV) neutrons. To meet this need, RDT has built an advanced neutron spectrometer populated with more than 100 microstructured semiconductor neutron detectors strategically impregnated throughout a neutron moderator cylinder. RDT is seeking to utilize advanced AI/ML technologies developed at INL to perform neutron source ID and neutron energy spectrum unfolding calculations onboard the NRID system.

So far the team has probed the feasibility of using Spock and Uhura to improve NRID's source identification accuracy. Initial results on simulated data suggest that the AI/ML algorithms are more than 80% accurate when more than 25,000 counts are measured, which improves source ID accuracy by 10%–20% over the previously used template matching techniques. Work is ongoing to match the NRID's lab-measured responses to the MCNP simulations (on which the algorithms were trained), so that these improvements can be verified in the field. RDT is also continuing to pursue additional funding avenues that will allow the team to dive deeply into neutron spectrum unfolding. If successful, NRID, using INL's advanced algorithms, would be the highest performing neutron spectrometer available, thereby providing a new tool to assist the advancement of neutron science.

Key Publications

None

Sponsor/Program

Industry/Other.

Figure 1: RDT's NRID.

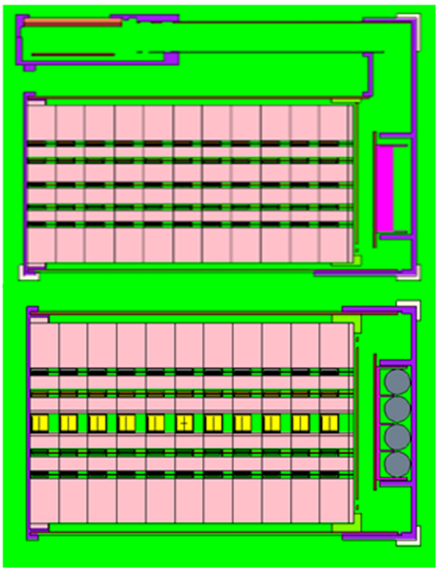


Figure 2: NRID MCNP model.

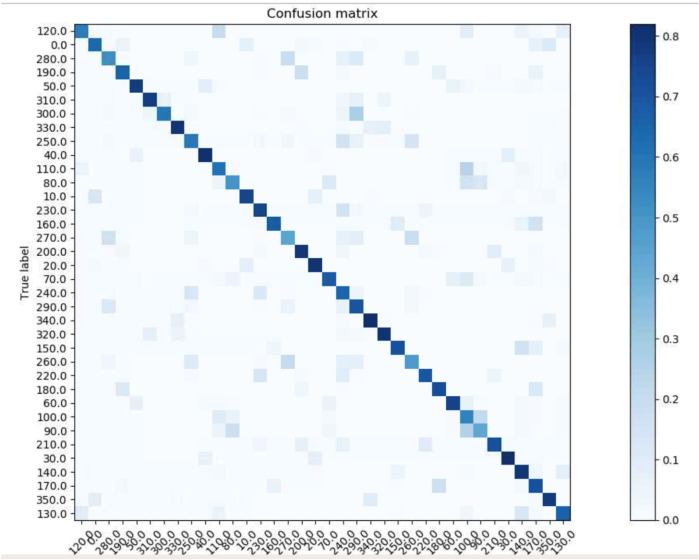


Figure 3: Confusion plot for AI/ML enhanced source localization.

B.115 Development of a MOOSE thermal-hydraulic model of the MPC-32 Canister and HI-STORM Overpack

Report Participants

Okyay, Sinan [1], Kong, Fande [1], Merzari, Elia [2], Gaston, Derek R[1], Permann, Cody J[1]
1 Idaho National Laboratory
2 The Pennsylvania State University

Scientific Achievement

This project aims to develop a thermal model of the MPC-32 canister and HI-STORM overpack using MOOSE. The HI-STORM SNF storage system is designed for high-burnup spent fuel storage, which is essential in developing advanced nuclear technologies. Thermal-hydraulic safety demonstrations of the SNF will increase the public acceptance of next-generation nuclear technologies. This study demonstrates the thermal-hydraulic capabilities of the MOOSE framework, including the modeling of natural circulation, heat transfer, porous flows, etc. The ultimate goal of the project is to verify whether MOOSE tools (including Pronghorn) are suitable for studying the thermal-hydraulic performance of the SNF dry cask storage system.

Significance

This study demonstrates the thermal-hydraulic capabilities of the MOOSE framework when applied to dry cask problems. Such problems often include natural circulation, heat transfer, and porous flows. The following accomplishments were achieved in this study: " An inclusive and reliable solution strategy was built to combat issues relating to the dry cask system. This solution method encompasses the complexity of the problem in a step-by-step fashion; therefore, potential problems can be identified and resolved in a straightforward manner. " As is often the case with such solvers, the finite volume N-S solver of the MOOSE framework was validated and compared by using the cavity case. The vast amount of experimental data available make the cavity case a unique candidate for performing validation and comparison activities on CFD software in natural circulation problems. " The capabilities of the MOOSE solver under different meshing strategies were demonstrated. This capability provides users with the flexibility to decide which meshing strategy is best suited for their studies. " A reliable thermal-hydraulic model for the MPC-32 and HI-STORM overpack was provided. The results were produced using a uniform and realistic cosine-shaped heat source for the given geometry. For validation, the output of the work was compared with the results from available literature. The results were achieved with under 10% margin of error compared to the reference study.

Key Publications

" Okyay, S., Merzari, E., Reger, D. A., Giudicelli, G., Leite, V. C., Lindsay, A., German, P., Development of HI-STORM Overpack and MPC-32 Thermal-Hydraulic Model with MOOSE Framework , International Topical Meeting on Nuclear Reactor Thermal Hydraulics - NURETH 20, Washington, US, August 20 - 25, 2023.

" Okyay, S., Merzari, E., Reger, D. A., Giudicelli, G., Leite, V. C., Lindsay, A., German, P., Development of HI-STORM Overpack and MPC-32 Thermal-Hydraulic Model with MOOSE Framework , International Topical Meeting on Nuclear Reactor Thermal Hydraulics - ICONE 30,

Kyoto, JP, May 21 - 26, 2023. " Okyay, S., Kong, F., Merzari, E., Reger, D. A., Giudicelli, G., Leite, V. C., Lindsay, A., German, P., Woods, N., Jarrel J. J., Gaston D., Permann C., Joseph R. A. "Development of a MOOSE thermal model of the MPC-32 canister and HI-STORM overpack", INL/RPT-22-68259, July 2022.

Sponsor/Program

UNF-STANDARDS

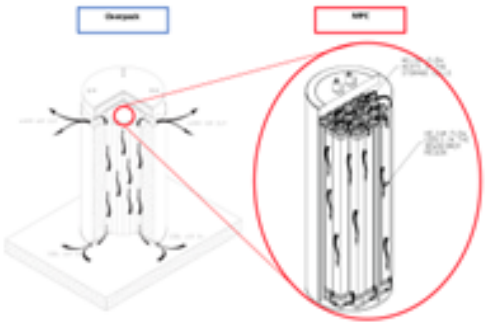


Figure 1: Flow patterns in HI-STORM SNF system.

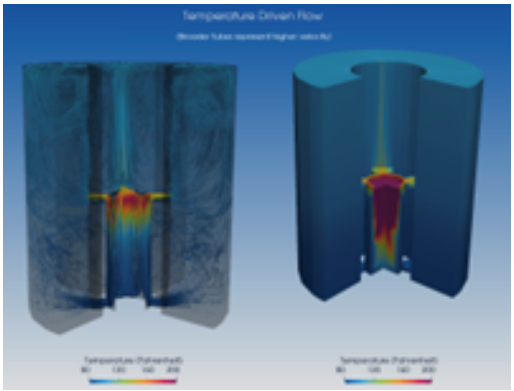


Figure 2: Velocity streamlines (left) and temperature contour (right) of the HI-STORM SNF storage system.

B.116 Modeling of a Generic Pebble-Bed High-Temperature Gas-Cooled Reactor with a Coupled SAM-Griffin Code

Report Participants

Ooi, Zhiee J[1], Zou, Ling [1], Hua, Thanh [1], Fang, Jun [1], Hu, Rui [1]
1 Argonne National Laboratory

Scientific Achievement

This project aims to couple the SAM thermal hydraulic code with the Griffin neutronics code for the modeling of a generic pebble-bed high-temperature gas-cooled reactor (PB-HTGR). The neutronics calculations are performed with Griffin, which transfers the distribution of power density to SAM, which then uses the information for thermal hydraulics calculations. The temperature distribution is then transferred back to Griffin for reactivity feedback calculations. The coupling of the codes is performed using MOOSE's MultiApp system. This project provides a better understanding on the thermal hydraulics and neutronics behavior of the PB-HTGR, which is crucial for the safety analysis of the new generation of advanced reactors. This project is still in progress.

Significance

This in an ongoing project. Preliminary results are promising where the temperature and power density distributions match the results from other models relatively well. In addition to a steady-state simulation, a load-following transient is simulated. The load-following transient is chosen to demonstrate the role of reactivity feedback in maintaining the safety of HTGRs. Additionally, the work demonstrates the capabilities of NEAMS codes and the ease of coupling different MOOSE-based codes, which is essential for multiphysics and multiscale simulations.

Key Publications

" Z.J. Ooi, L. Zou, T. Hua, J. Fang, R. Hu. 2023. System Level Modeling of a Generic Pebble Bed High-temperature Gas-cooled Reactor (PB-HTGR) with SAM and Griffin. NURETH-20. (Submitted for review)

Sponsor/Program

NEAMS

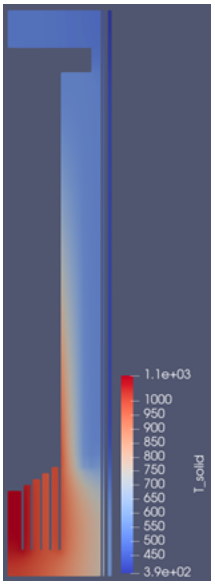


Figure 1: Steady-state solid temperature distribution of reflectors predicted by SAM.

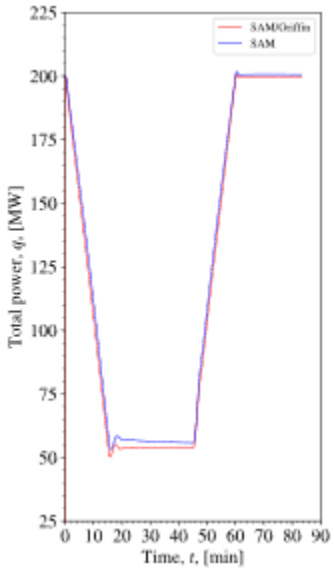


Figure 2: Comparison of the power levels during the load-following transient predicted by the SAM-Griffin and SAM-standalone models.

B.117 VERA BWR Project

Report Participants

Palmtag, Scott P[1], Lawing, Chase D[1], Al-Dawood, Khaldoon A[1]
1 North Carolina State University

Scientific Achievement

The VERA computing suite was developed under the CASL program to advance the state-of-the-art modeling and simulating of LWRs. The ability to model PWRs using advanced coupled multiphysics computational tools was developed and results were validated for over 100 cycles of PWRs. This current project is to develop and extend the VERA tools to BWRs and apply the tools to analyze the BWR fleet of reactors operated by Exelon Nuclear Generation. The results will be used to improve the eigenvalue and thermal limit predictability in BWR reactors to improve the cycle length and economic output of BWRs.

Significance

The VERA suite offers a significantly advanced modeling and simulation capability over existing industry simulation tools. The advanced capability includes detailed multigroup neutron transport for the entire core, detailed subchannel thermal-hydraulic solution over every fuel rod, and detailed pin-by-pin fuel temperature and depletion solutions.

These features of VERA should yield substantial improvement over existing industry predictions of modeling void and depletion parameters on a rod-by-rod basis instead of a bundle-average basis, and detailed modeling of different bypass flow regions. This enables a more rigorous calculation of within the bundle power distribution. This is especially important in the presence of large power gradients, such as what occurs with the insertion of control blades. The feedback of the radial void distribution, particularly at high void, is expected to have a significant impact on calculated results. In addition, it is expected that the elimination of history models in the cross-section generation and the inclusion of radial void distribution within bundles will improve eigenvalue and detector predictions.

Key Publications

" Chase Lawing, Scott Palmtag, Mehdi Asgari, VERA BWR Progression Problems, International Conference on Physics of Reactors 2022 (PHYSOR 2022), Pittsburgh, May 15-20, 2022. " Chase Lawing, Scott Palmtag, Investigation of Approximations in Modeling BWR Void Distributions, International Conference on Physics of Reactors 2022 (PHYSOR 2022), Pittsburgh, May 15-20, 2022. " Chase Lawing, Scott Palmtag, Mehdi Asgari, BWR Progression Problems , ORNL/TM-2020/1792, Oak Ridge National Laboratory, September 2021. doi.org/10.2172/1838995 " Chase Lawing, Scott Palmtag, David Kropaczek, Analysis of Approximations in Modeling of BWR Bundle Void Distributions, ORNL/SPR-2021/2241, Oak Ridge National Laboratory, August 2021. " Chase Lawing, PhD Thesis, North Carolina State University (In Progress)

Sponsor/Program

DOE FOA Modeling and Analysis of Exelon BWRs for Eigenvalue & Thermal Limits Predictability

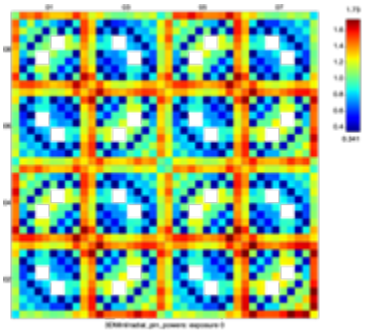


Figure 1: Radial 2D pin powers BWR 4 × 4 minicore.

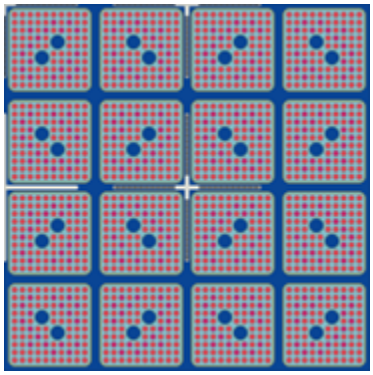


Figure 2: Radial slice of BWR 4 × 4 minicore.

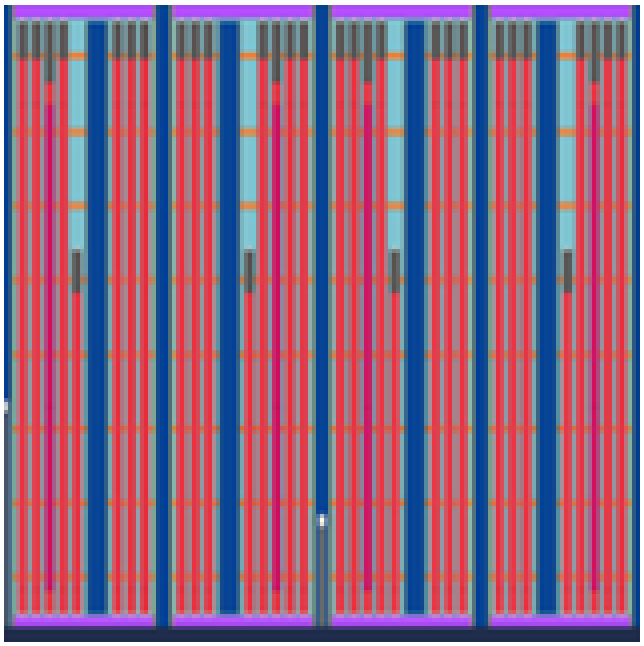


Figure 3: Axial slice from BWR minicore.

B.118 Flow Boiling and Condensation in Microgravity

Report Participants

Plawsky, Joel L[1], Woodcock, Corey [1], Khusid, Boris [2], Conboy, Thomas [3]
1 Rensselaer Polytechnic Institute
2 New Jersey Institute of Technology
3 CREARE, Inc.

Scientific Achievement

The project is designed to provide experimental data and predictive models for thermal and hydrodynamic transients and instabilities in flow boiling under microgravity by carrying out experiments on the 3M Fluorinert electronic liquid FC-72 in the International Space Station (ISS) liquid nitrogen (LN2) in parabolic flights in the Zero-Gravity aircraft. We are going to use RELAP5 to simulate the experimental results we see in microgravity and then propose changes to RELAP5 correlations (if needed) to adequately reproduce the experimental data.

Significance

We are just now running the experiment on the ISS and are collecting and storing the data for processing. Several ground-based experiments were run in preparation for the microgravity flight. At very high mass flow rates, we see little difference between the microgravity and ground-based runs. LN2 experiments are to be run at some point over the summer, but several ground-based experiments were run. There are some interesting results surrounding the behavior of the fluids near the wall, but it is unclear whether RELAP will be able to reproduce that behavior. We still need to see how the near wall behavior affects the bulk of the flow.

Key Publications

So far, we have presented at two conferences, The ASME Summer Heat Transfer Conference in Philadelphia and the ASGSR Annual Meeting in Baltimore.

Q. Lei et al. Thermal Stability of Cryogenic Fluid Flow in Microgravity SHTC2022-97391 ASME 2022 SHTC, Philadelphia, PA. July 11-13, 2022 Q. Lei et al. Transients and Instabilities in Cryogenic Fluid Flow in Microgravity (ASGSR:18) ASGSR Annual Meeting, Houston, TX, November 9-12, 2022

Sponsor/Program

NSF/CASIS

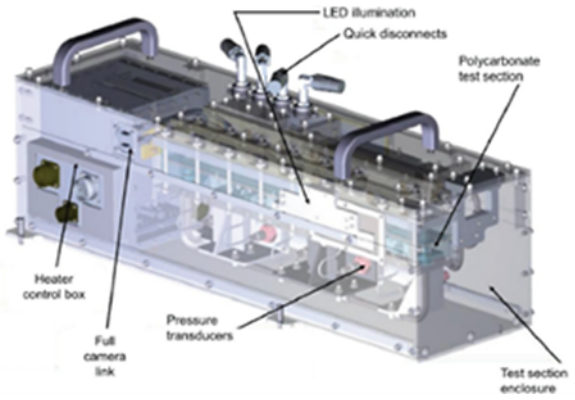


Figure 1: ISS flow boiling module.

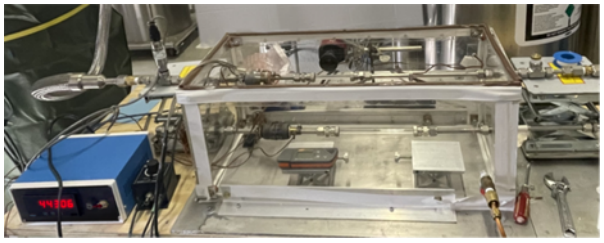


Figure 2: LN2 flow channel configuration.

B.119 eVinci Microreactor

Report Participants

Plivelich, Austin W[1]
1 Westinghouse Electric Company

Scientific Achievement

The MOOSE toolset (BISON, Sockeye, and Griffin) is used for the code-coupled modeling and analysis of the Westinghouse eVinci heat-pipe reactor. Based on the code performance in the Meitner project, it may be decided to use these codes to perform modeling and simulation activities supporting the licensing application and process for the eVinci reactor.

Significance

Performing code-coupled simulations of the eVinci heat-pipe reactor to show its perfomance in transients and inherent safety features is critical for building the first-of-its-kind reactor.

Key Publications

N/A

Sponsor/Program

Department of Energy, Los Alamos National Laboratory, Idaho National Laboratory, Argonne National Laboratory, US NRC, and any other United States or Canadian governmental agency to receive the findings as part of Westinghouse's licensing requirements.

B.120 Advanced Modeling of eVinciTM Heat-Pipe Microreactor

Report Participants

Price, Dean R[1], Roskoff, Nathan J[1], Guler, Cenk [1]
1 Westinghouse Electric Company

Scientific Achievement

A wealth of research has enabled the creation of many efficient tools for LWR analysis. As heat-pipe microreactors are a relatively new reactor design, simulation methods and tools for these reactors are not well-established. This project involves the use of high-fidelity general reactor simulation tools applied to heat-pipe microreactors. Due to the generality of these simulation tools, they require a relatively large computational burden, which leads to a requirement for HPC resources. Some specific tasks associated with these simulations are multiphysics modeling using Serpent and OpenFOAM and cross-section generation for Griffin. These tasks support the design and evaluation of the eVinci heat-pipe microreactor under development at Westinghouse Electric Company.

Significance

So far, most multiphysics simulations of heat-pipe microreactors have used homogenization techniques to perform calculations. Often, the cross sections used to homogenize the geometries were based on Monte Carlo calculations of the reactor. As homogenization techniques and cross section generation can introduce many uncertianties in a reactor analysis workflow, this work uses a Monte Carlo neutronics simulation tool to avoid the requirement for any homogenization. This technique has allowed the calculation of safety and design relevant quantities with a higher degree of accuracy than may be expected from a homogenization-based simulation tool.

Key Publications

Price, D., & Roskoff, N. (2023). Method for control drum position critical search with Monte Carlo codes. Progress in Nuclear Energy, 162, 104731.

Sponsor/Program

Westinghouse Electric Company

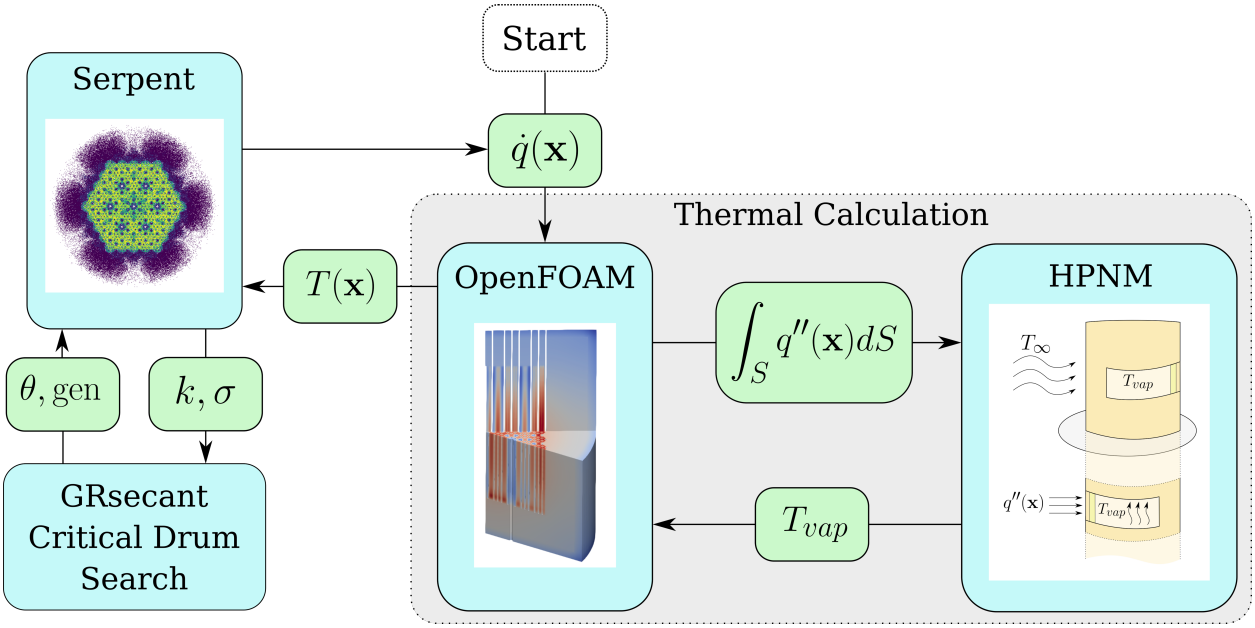
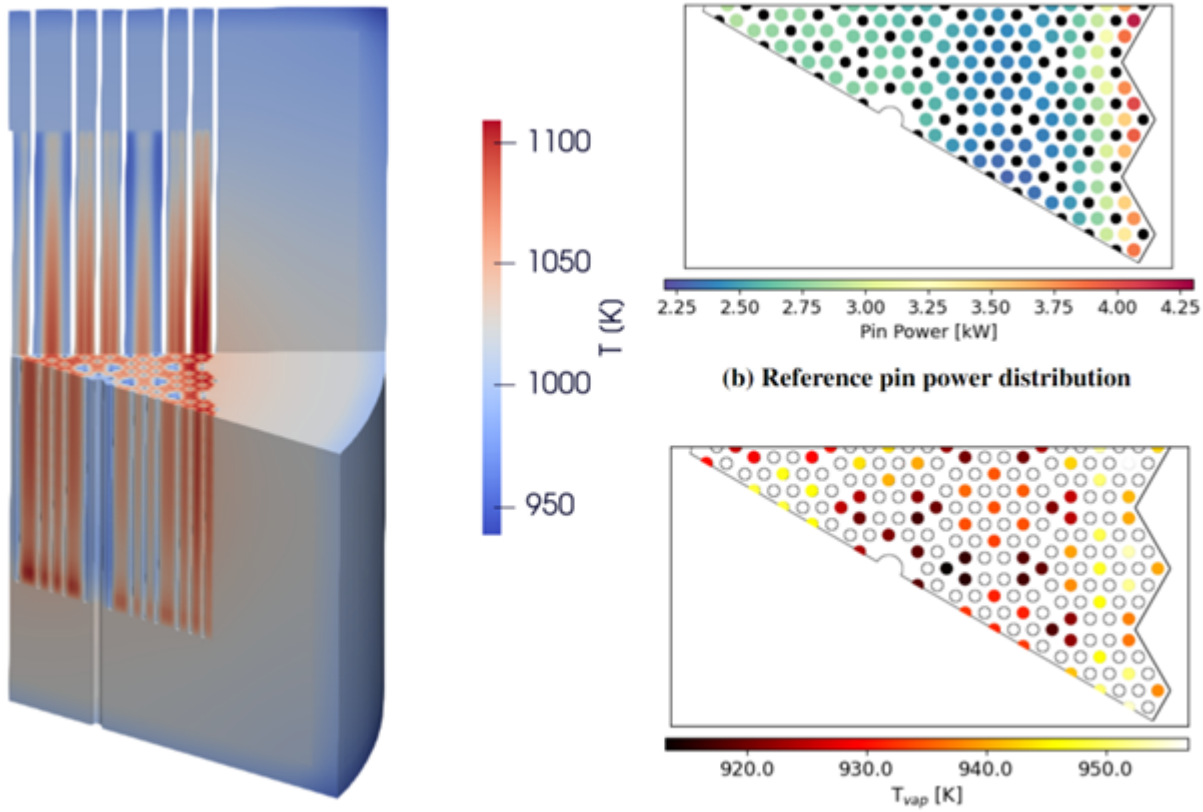


Figure 1: Coupling procedure used for simulating the heat-pipe microreactor.



(a) Reference core temperature distribution

(b) Reference pin power distribution

(c) Reference heat pipe temperature distribution

Figure 2: Reference core operating characteristics calculated with the multiphysics coupling procedure.

B.121 High-Fidelity, Data-Science-Informed Pebble-Bed Reactor Simulation

Report Participants

Ragusa, Jean C[1], Carlson, Liam N[1], Balestra, Paolo [2]
1 Texas A&M University
2 Idaho National Laboratory

Scientific Achievement

Traditional neutronics calculations of PBRs, such as those used in codes like VSOP, rely on the homogenization of macroscopic cross sections over regions called spectral zones. Since cross sections for pebbles of varying temperature and burnup are averaged over a region, there is a great deal of local information lost in a whole-core calculation. The Pebble Tracking Transport (PTT) method in Griffin allows for high-fidelity deterministic modeling of a PBR core by treating the pebble centers as nodes in an unstructured tetrahedral mesh. In PTT, macroscopic cross sections must be supplied for pebbles. These cross sections are currently being generated in Serpent using INL's HPC resources. It is very costly to generate new cross sections as pebbles change positions, burnup, and temperature during normal operation, so we are investigating implementing ML algorithms to provide approximate pebble cross sections for PTT simulations.

Significance

Several capabilities have been added to Griffin due to this research. Previously, the PTT algorithm has only been able to assign cross sections to pebbles within the same region or block. Now, cross sections may be assigned to groups of pebbles that share similar characteristics, such as burnup, temperature, and neutronic environment. Additionally, pebble-wise reaction rates may be calculated for individual pebbles in a PBR core. It was determined that the incoming particles over a pebble surface may be recorded in Serpent for a whole-core eigenvalue simulation, which can reliably reproduce the pebble-wise cross sections in a single pebble source calculation. A process for clustering pebbles into similar groups is currently being investigated.

Key Publications

N/A

Sponsor/Program

NEUP 21-24258

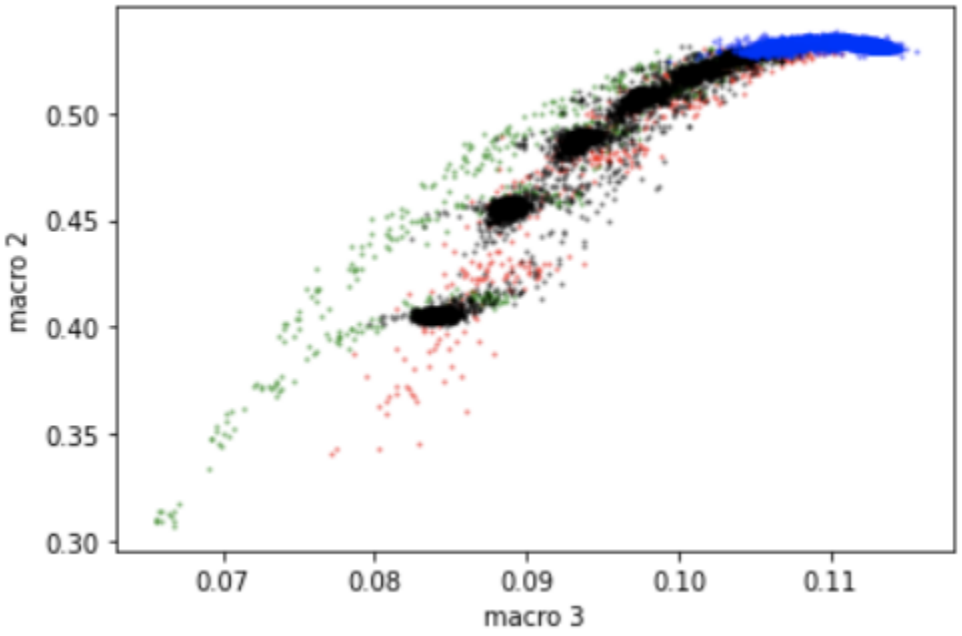


Figure 1: Clustering of neutron flux environment.

B.122 Correlation Improvement for the Near-Wall Region of Pebble-Bed Reactors

Report Participants

Reger, David A[1], Merzari, Elia [1], Balestra, Paolo [2], Schunert, Sebastian [3], Yuan, Haomin [4], Hassan, Yassin A[5]
1 Pennsylvania State University
2 Idaho National Laboratory
3 Radiant Industries Incorporated
4 Argonne National Laboratory
5 Texas A&M University

Scientific Achievement

This objective of this research is to use high-fidelity CFD simulations of PBRs to generate a dataset to improve correlations for pressure drop and heat transfer in porous media models of PBRs. Simulations of four pebble beds, ranging from 67 to 7,000 pebbles, were generated using the discrete element method with the GPU-based code Project Chrono. A novel meshing method has been developed to create all-hexahedral meshes for these cases. High-fidelity simulations have been performed using ANL's NekRS spectral-element CFD code. Time-averaged flow fields for several beds were divided into concentric subdomains to extract average flow information across multiple bed regions. This data was used to suggest improvements to the KTA drag correlation that allow for significantly improved modeling of localized features in a porous media code. This new correlation has been implemented into INL's Pronghorn thermal hydraulics code.

Significance

This project greatly improves the accuracy with which porous media models can predict velocity fields in a PBR. Through the use of a high-fidelity LES dataset, a new pressure drop correlation was developed that allows for spatial variations in bed porosity to be accurately modeled in a porous media code. This is important, as existing correlations fail to accurately predict the coolant velocity near the wall of the bed where the presence of the wall changes the pebble packing and increases the porosity. The newly developed correlation reduces errors in the prediction of the near-wall velocity from over 50% with the KTA correlation to roughly 6% or less with the new correlation, as seen in Figure 2. Future work will continue to expand the range of validity for the new correlation and will begin an investigation into heat transfer correlations for PBRs as well.

Key Publications

Reger, D., Merzari, E., Balestra, P., Schunert, S., Yuan, H., Hassan, Y., Fischer, P., & Min, M. (2022). Pressure Drop Correlation Improvement for the Near-Wall Region of Pebble-Bed Reactors. Nuclear Technology, 209. Reger, D., Merzari, E., Balestra, P., Schunert, S., & Yuan, H. (2023). A New Generalized Pressure Drop Correlation for Modeling Localized Effects in a Pebble Bed Reactor. Nuclear Engineering and Design. 403. Reger, D., Merzari, E., Balestra, P., Stewart, R. & Strydom G. (2023). Discrete Element Simulation of Pebble Bed Reactors on Graphics Processing Units. Annals of Nuclear Energy, 190. Reger, D., Merzari, E., Balestra, P., Schunert, S., King, S., Hassan, Y., Fischer, P., & Min, M. (2023). Direct Numerical Simulation and Large Eddy Simulation of a 67-Pebble Bed Experiment. Nuclear Technology.

Sponsor/Program

NEAMS Center of Excellence for Thermal-fluid Applications in Nuclear Energy DEAC02-06CH11357

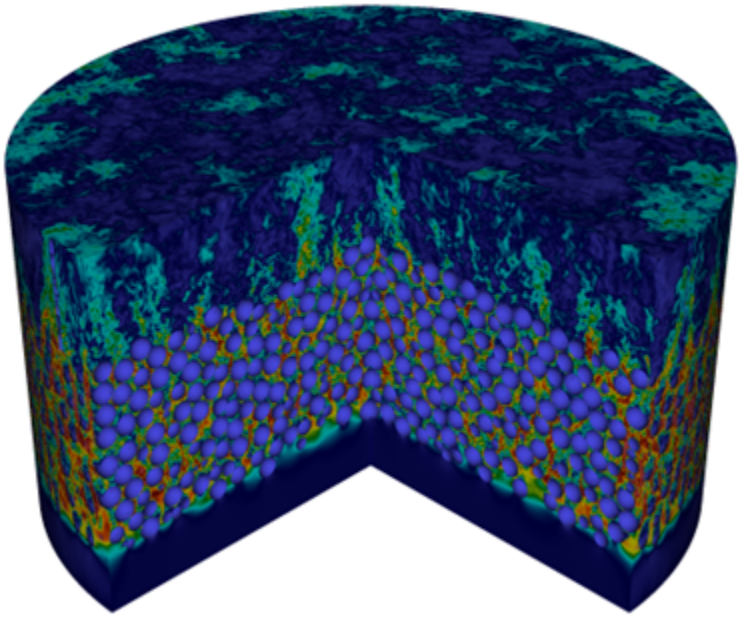


Figure 1: Instantaneous velocity field generated from LES of a bed of 7,000 pebbles.

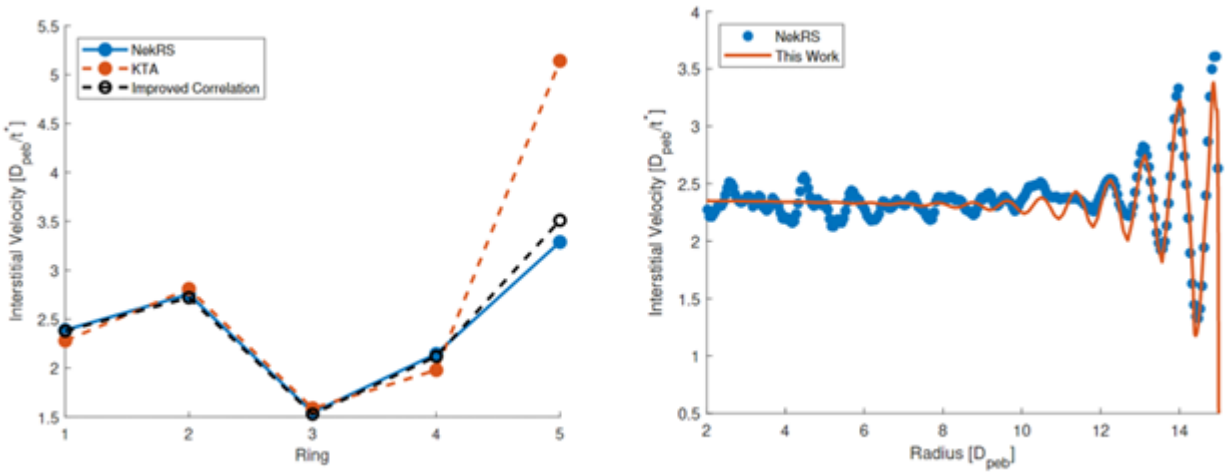


Figure 2: Radial velocity profiles from NekRS and Pronghorn with coarse (left) and fine (right) bed discretization, showing significant improvement over the KTA correlation.

B.123 Bayesian Calibration with Summary Statistics for Predicting Xenon Diffusion in Uranium Oxide Nuclear Fuel

Report Participants

Robbe, Pieterjan [1], Andersson, David [2], Bonnet, Luc [1], Casey, Tiernan [1], Cooper, Michael W[2], Matthews, Christopher [2], Sargsyan, Khachik [1], Najm, Habib [1]
1 Sandia National Laboratories
2 Los Alamos National Laboratory

Scientific Achievement

The evolution and release of fission gas impacts the performance of UO2 nuclear fuel. In this project, we have created a Bayesian framework to calibrate a novel model for fission gas transport that predicts diffusion rates of uranium and xenon in UO2 under both thermal equilibrium and irradiation conditions. Our calibration strategy uses synthetic data sets taken from historical diffusion, gas release, and thermodynamic experiments to estimate the parameters in the model, such that the resulting model predictions agree with the reported summary statistics. We demonstrate good agreement between the calibrated xenon diffusivity and the established fit from Turnbull et al. (1982), indicating that the dominant uranium vacancy diffusion mechanism in the model is able to capture trends in the data.

Significance

The fission gas diffusivity coefficient is one of the crucial parameters used in many nuclear fuel performance models. Reconciling existing models, such as the cluster dynamics simulation software Centipede, with historical gas release and thermodynamic data is crucial to predict the behavior of fission gas for both current and novel nuclear fuel types. Our results are in good agreement with the Turnbull et al. fit for the xenon diffusivity. The latter analysis has been used as a starting point for many higher-level fission gas release models, as it sets the timescale for the subsequent percolation of gas bubbles at grain boundaries. The excellent agreement between the estimated xenon diffusivity from calibration and the empirical fits based on experimental data confirms that a uranium vacancy-based mechanism can describe the xenon diffusion under irradiation conditions predicted from the experimental data.

Key Publications

P. Robbe, D. Andersson, L. Bonnet, T. Casey. M. W. D. Cooper, C. Matthews, K. Sargsyan, H. Najm. 2023. Bayesian Calibration with summary statistics for predicting xenon diffusion in uranium oxide nuclear fuel. Computational Materials Science, under review.

Sponsor/Program

This work was supported by the U.S. Department of Energy, Office of Nuclear Energy and Office of Science, Office of Advanced Scientific Computing Research through the Scientific Discovery through Advanced Computing project on Simulation of Fission Gas.

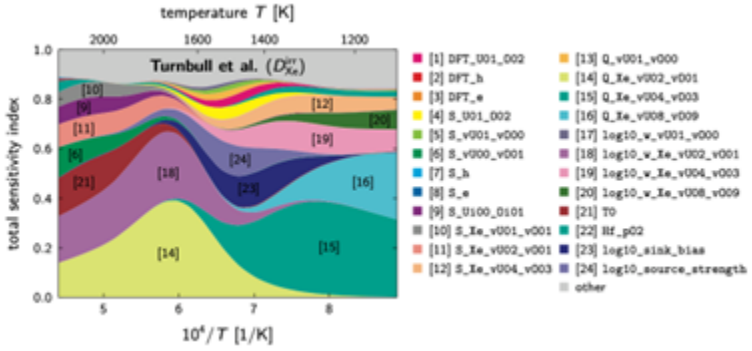


Figure 1: Parameter sensitivities as a function of temperature for xenon gas release under irradiation conditions under the conditions reported in Turnbull et al. (1982).

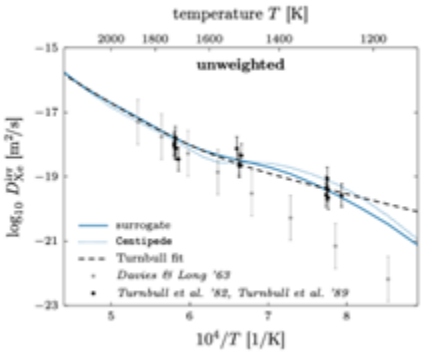


Figure 2: Estimated model predictions for the xenon diffusivity under irradiation conditions compared to the experimental data from Turnbull.

B.124 Modeling and Simulating a Heat-Pipe-Cooled Microreactor

Report Participants

Roskoff, Nathan J[1], Kucukboyaci, Vefa N[1]
1 Westinghouse Electric Company

Scientific Achievement

This work involved the continued evaluation of DireWolf's ability to model the transient behavior of a heat-pipe microreactor, the development of a homogenized reactor mesh using the NEMO tool, and the development and evaluation of the efficacy of a Serpent-generated cross-section library.

Significance

This work demonstrated DireWolf's ability to perform code-coupled simulations, used NEMO to generate a 3D assembly-homogenized mesh, and used Serpent to develop a multigroup cross-section library as input for Griffin.

Key Publications

None

Sponsor/Program

DOE (DE-FOA-0001798), LANL, INL

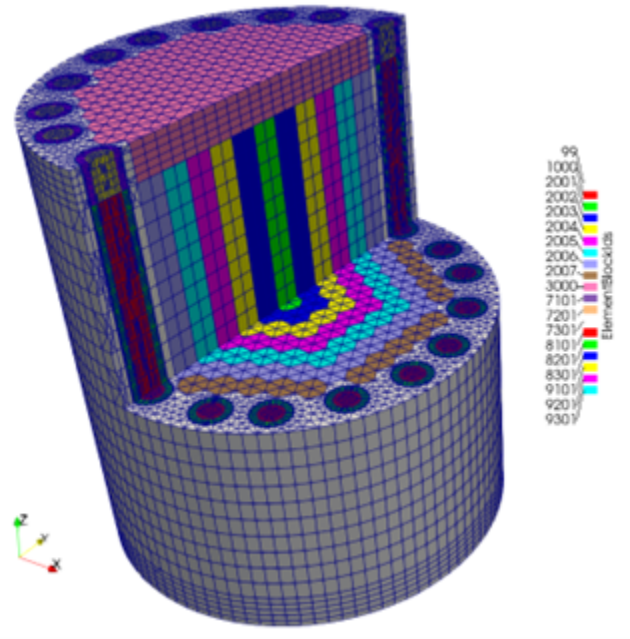


Figure 1: Griffin neutronics mesh (colors represent Block IDs).

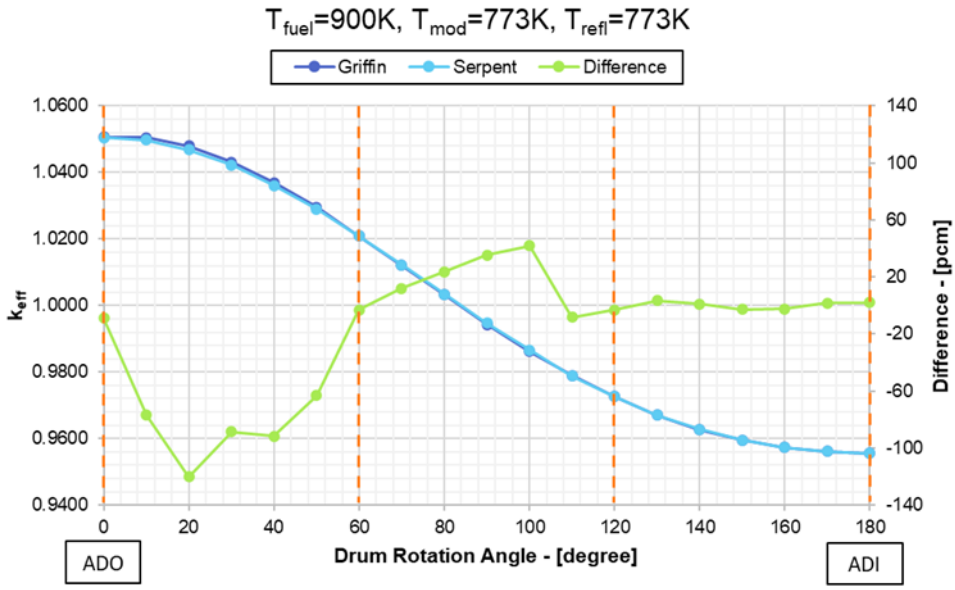


Figure 2: Example of cross-section efficacy study (dashed lines indicate cross-section evaluation point; Serpent uncertainty on keff <10 pcm).

B.125 Advanced Test Reactor Power Uprate Support

Report Participants

Ruppert, John J[1], England, Jonas [1], Bonnin, Ross B[1]
1 MPR Associates

Scientific Achievement

To increase capabilities for high-power irradiation experiments in ATR, an effort is currently in progress to increase the ATR maximum lobe operating limit from 60 to 70 MW. In support of this task, MPR is performing thermal hydraulics modeling of safety-basis transient events to support increasing the lobe power to 70 MW. This ongoing effort involves simulating reactor flow conditions using RELAP5 and performing a Monte-Carlo simulation of the limiting fuel plate hot stripe using ATR-SINDA and SINDA-SAMPLE to assess conformance to required safety criteria.

Significance

An increase to the maximum lobe operating limit will expand the ability for ATR to support irradiation experiments for key clients around the world.

Key Publications

No external publications. All documents produced are stored in the INL document management system

Sponsor/Program

ATR

B.126 Data-Driven Surrogate Model Development for MOOSE

Report Participants

Ruybalid, Andre P[1], Matthews, Christopher [1], Capolungo, Laurent [1]
1 Los Alamos National Laboratory

Scientific Achievement

Simulating the thermomechanical creep response of real-world steel alloy structures used in nuclear energy applications. Several creep surrogate models of the Los Alamos Reduced Order Models for Advanced Nonlinear Constitutive Equations family for the MOOSE framework have been developed using a data-driven approach. The surrogate models have been improved by calibrating them on the full-field crystal plasticity framework of elasto-viscoplastic fast Fourier transform models, instead of the previously used mean-field method of VPSC. To this end, approximately 50,000 physics-based elasto-viscoplastic fast Fourier transform simulations, as well as mean-field VPSC simulations, have been run on the INL HPC system Sawtooth. Various polynomial-based surrogate models have been calibrated on the resulting data, and after being implemented in the MOOSE framework, a multitude (hundreds) of finite-element simulations have been run on Sawtooth. This allows the surrogate model to simulate creep response as a function of irradiation effects and microstructure (e.g., dislocation and precipitate content) within the finite-element framework of MOOSE.

Significance

The surrogate model is capable of simulating creep experiments and allows to understand the effect of the microstructure on the mechanical creep response. The insights can be used to direct material processing and design processes and improve the accuracy of lifetime predictions of steel alloy structures used in nuclear energy applications.

Key Publications

A.P. Ruybalid, A. Tallman, M. Arul Kumar, C. Matthews, L. Capolungo. 2023. Data-driven surrogate model with microstructure internal state variables for P91 steel alloys. Status: in progress.

Sponsor/Program

NEAMS

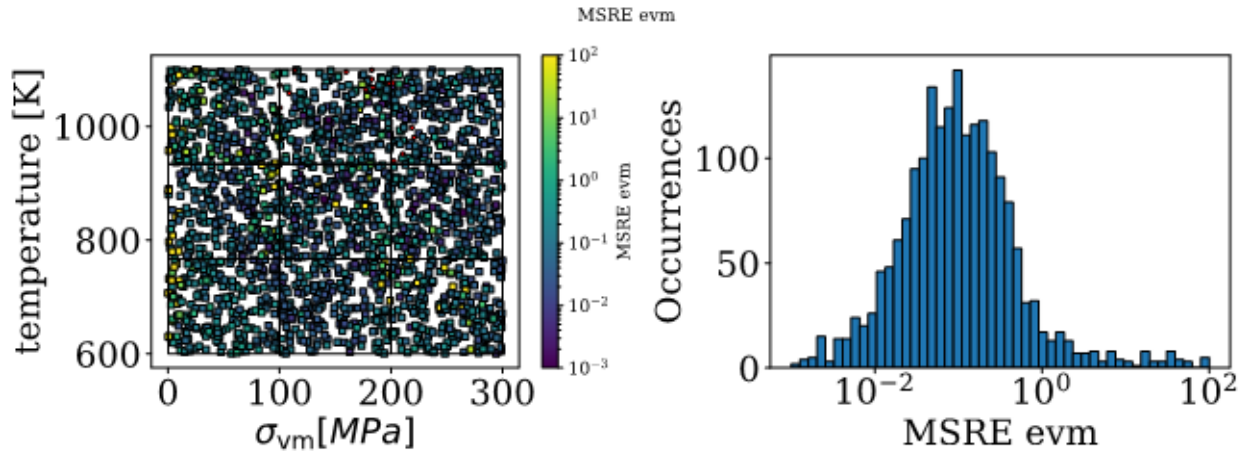


Figure 1: Validation results of 2,000 surrogate model simulations compared to physics-based simulations in terms of the mean squared relative error (MSRE) on the computed accumulated strain ("evm"). The training set, corresponding to this model, consists of 16,000 training and 2,000 testing simulations.

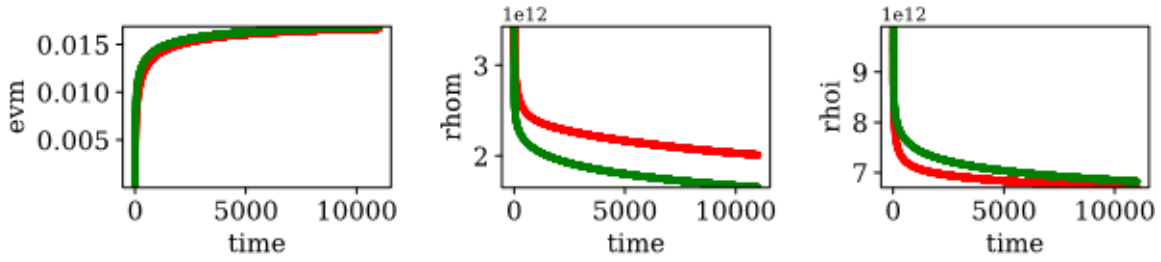


Figure 2: Example of a single output response at the same input parameter set from a physics-based simulation (red) and surrogate model (green) for the strain output (evm), the cell dislocation density (rhom), and the cell-wall dislocation density (rhoi).

B.127 Development of VERA for BWRs

Report Participants

Salko, Robert K[1], Asgari, Mehdi [1], Graham, Aaron M[1], Kropaczek, Dave [1]
1 Oak Ridge National Laboratory

Scientific Achievement

This work developed and validated a new T/H solver, Alternative Nonlinear Two-Phase Subchannel (ANTS), and incorporated it into VERA for BWR analyses and further developed VERA for modeling BWR depletion cycles.

Significance

This work has the goal of developing a core simulator with higher fidelity than current industry methods and can therefore capture operation effects not captured by current tools. This will allow for improving the core design and potentially recapturing lost margin.

Key Publications

Robert Salko, Belgacem Hizoum, David Kropaczek, Mehdi Asgari, Verification and validation of the Alternative Nonlinear Two-phase Subchannel (ANTS) code, Nuclear Engineering and Design, Volume 397, 2022, 111930, ISSN 0029-5493, https://doi.org/10.1016/j.nucengdes.2022.111930.

Robert Salko, Belgacem Hizoum, Aaron Graham, Benjamin Collins, and Mehdi Asgari, Summary of CTF Modeling and Numerical Improvements for Boiling Water Reactor Simulations,

Sponsor/Program

NEAMS

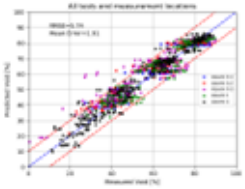


Figure 1: ANTS prediction of BFBT void.

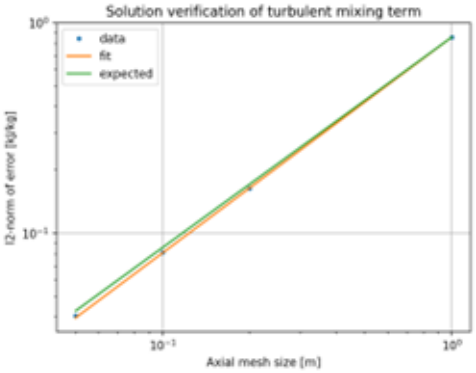


Figure 2: Solution verification of ANTS turbulent mixing term.

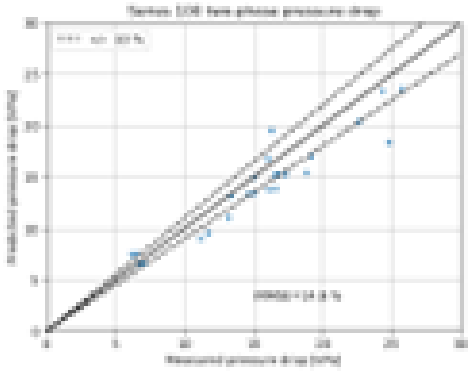


Figure 3: ANTS prediction of two-phase pressure drop in RISO tests.

B.128 Comparison of Liquid Temperature Between the 13- and 49-Level Models

Report Participants

Schappel, Daniel P[1], Linton, Kory [1], Helmreich, Grant [1], Keever, Tamara [1], Petrie, Christian [1]
1 Oak Ridge National Laboratory

Scientific Achievement

This work developed methods to estimate the stresses in the SiC matrix due to TRISO particles at high temperatures, using homogenized particles at discrete locations. Meshing techniques were developed to prevent the need for creating spherical regions for the particles, which reduced the mesh size to a large but practical level.

Significance

Previous methods used a homogenized fuel meat. This produced a tensile exterior and compressive interior. While this is close enough for low-temperature work where the particles are pulling away from the matrix, at high temperatures, the particles expand towards the matrix and create stress concentrations both in the can wall and interior matrix. This allows for estimating where the cracks are likely to initiate and the probable extent of the propagation.

Key Publications

Danny Schappel, Kory D. Linton, Grant W. Helmreich, Tamara J. Keever, Christian M. Petrie Failure Analysis of Nuclear Transient-Tested UN Tristructural Isotropic Fuel Particles in a 3D Printed SiC Matrix Journal of Nuclear Materials. 586 (2023) 154691.

Sponsor/Program

NSUF

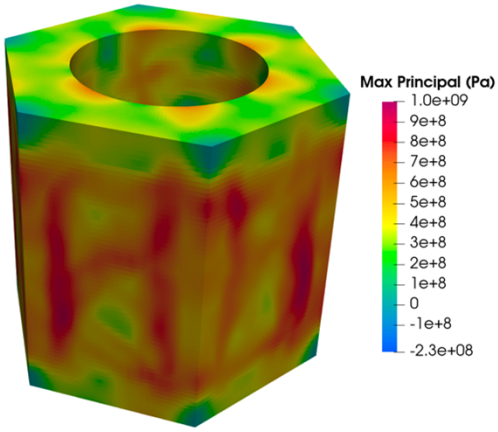
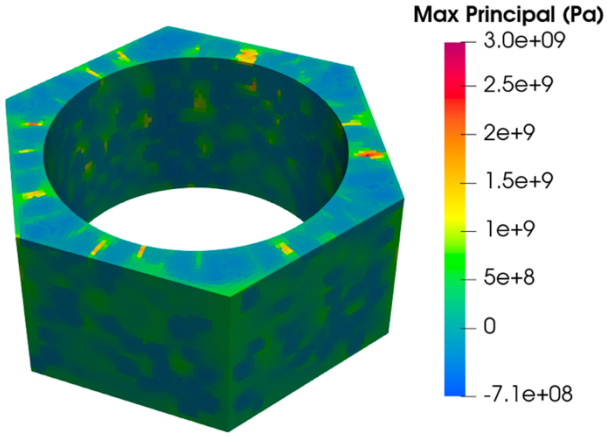


Figure 1: a) Can stress and b) matrix stress at about 7× the expected energy deposition for the maximum accident condition for HTGRs.



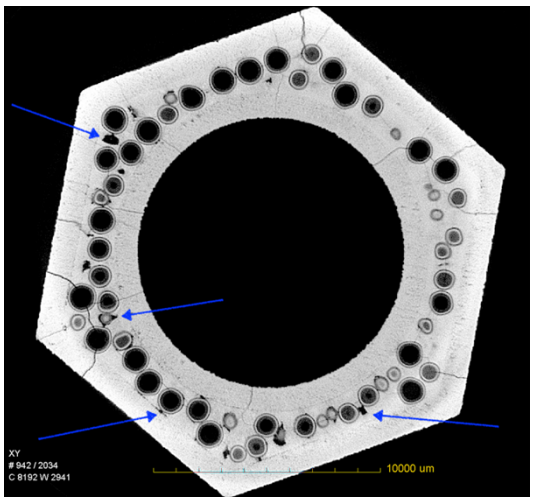


Figure 2: XCT image of a compact after 3,097 J/g-UN (99 ms FWHM) deposition, which is about 7× the maximum HTGR accident condition.

B.129 Fuel Performance Modeling of High-Burnup and Advanced Fuels

Report Participants

Shirvan, Koroush [1], Gauthier, Vincent [1], Halimi, Assil A[1], Che, Yifeng [2]
1 Massachusetts Institute of Technology
2 Idaho National Laboratory

Scientific Achievement

Realistic modeling of nuclear reactor fuel is essential in its determination of safety and economic performance. This is why modeling engineering-scale fuel responses with MOOSE and BISON that provides an effective multiphysics framework is the focus of our work. Specifically, challenges with prediction of fuel cracking and fission gas release as the fuel approaches high burnups are tackled with the multiscale modeling capability of the MOOSE-BISON tool. The next generation of nuclear fuels require the careful assessment of their structural performance for their applications. MOOSE and BISON allowed modeling ATF forms and Generation IV reactor fuels to support various DOE activities. The advent of ML allows to accelerate such modeling approaches to scale the domain of the analysis.

Significance

This work demonstrates the value of multiscale and multiphysics fuel performance simulations of existing and advanced fuels. The work is aimed to impact near-term and future trends in fuel performance research and development. Specifically, robust numerical techniques for fuel cracking simulations are being developed. ATF are being assessed for both existing and future nuclear technologies. An effective surrogate modeling strategy was demonstrated for both normal and transient fuel performance simulations.

Key Publications

Che Y., Yurko J., Seurin P., Shirvan K., Machine learning-assisted surrogate construction for full-core fuel performance analysis, Annals of Nuclear Energy, December 2021, 108905
https://doi.org/10.1016/j.anucene.2021.108905

Sponsor/Program

NEUP Projects 18-14893, 20-19912, 22-27048

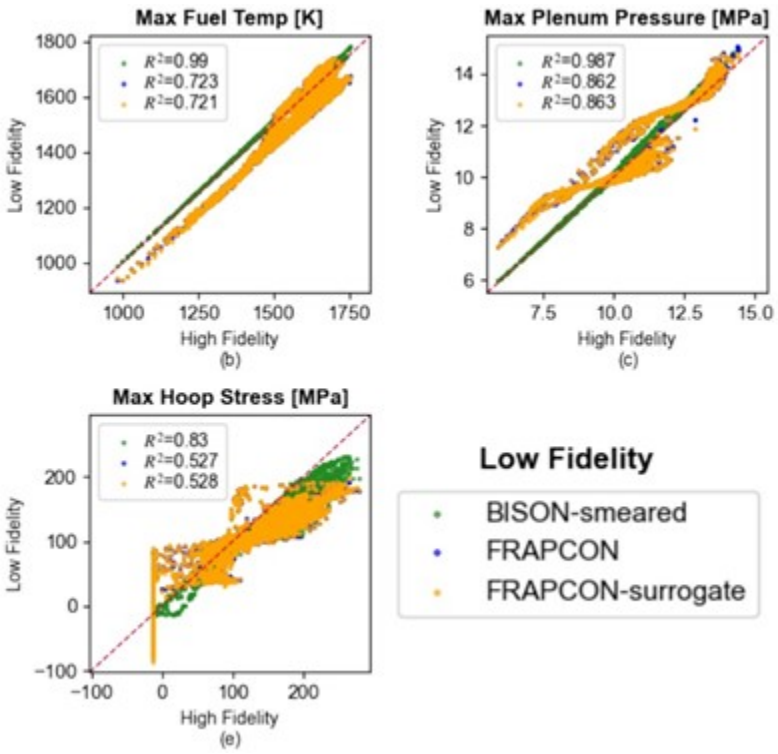


Figure 1: Comparison of BISON to FRAPCON on full-core PWR scale.

B.130 Investigation of Thermodynamic, Magnetic, and Structural Properties of -UZr2 using Density Functional Theory

Report Participants

Shousha , Shehab H[1], Beeler, Benjamin W[1]
1 North Carolina State University

Scientific Achievement

In this project, we used DFT and ab initio molecular dynamics to study the low-temperature phase of the U-Zr alloy. The initial goal of this work was to identify the optimal configuration ordering that reflects an accurate description of -UZr2. We employed different ordering of the U and Zr atoms in the hexagonal unit cell and we also utilized the special quasirandom structure (SQS) with different cell sizes. The goal was to achieve reasonable accuracy compared to experiment properties, including the volume per atom and enthalpy formation, while maintaining a magnetic state close to the true paramagnetic structure of -UZr2. Since paramagnetic structures are challenging to simulate using DFT, paramagnetic systems are often either described as nonmagnetic or antiferromagnetic. Both magnetic structures were considered at 0 K and at finite temperatures ranging from 100 to 500 K. It was observed that finite temperature calculations were required to obtain a nonmagnetic or antiferromagnetic state, the first time this has been achieved for the -UZr2 phase. The results for the volume per atom and formation enthalpy, with and without Hubbard U utilization, are shown in Figures 1, 2, 3, and 4, respectively. The SQS structure with an antiferromagnetic ordering most closely predicts the experimental volume, while adding the Hubbard U decreases the enthalpy of formation. The calculation of temperature-dependent properties, such as thermal expansion coefficients and heat capacities, are currently underway, as is an examination of the ratio of lattice constants as a function of the temperature. Subsequently, the effects of off-stoichiometry will be explored by incorporating antisite defects and the construction of novel SQS systems, examining the entire compositional regime of stability of the -UZr2 phase.

Significance

The U-Zr metallic fuels are developed for use in fast reactors for their advantages in thermal conductivity, high-fissile density, and ease of fabrication. Understanding the structure and phase stability of the Zr-rich -UZr2 is of great importance to the processing of U-Zr fuels and for assessing long-term performance in nuclear reactors.

Key Publications

S. Shousha, and B. Beeler, Magnetism and Finite Temperature Effects in -UZr2: A Density Functional Theory Analysis, 2023 (In progress)

Sponsor/Program

NEAMS, LDRD, NSUF

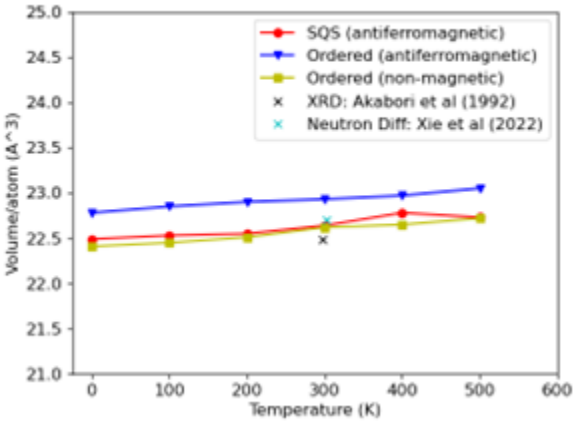


Figure 1: Volume per atom versus temperature using GGA.

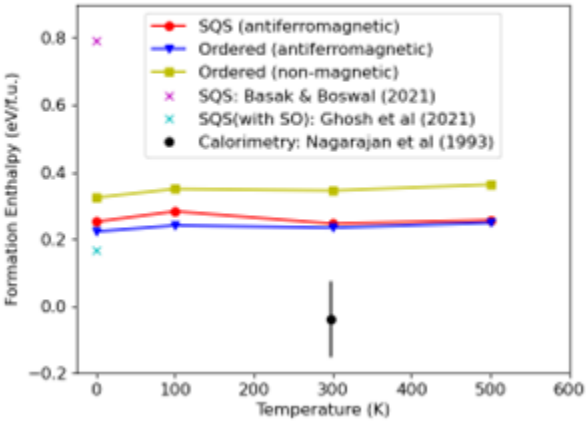


Figure 2: Formation enthalpy per unit formula of -UZr2 using GGA.

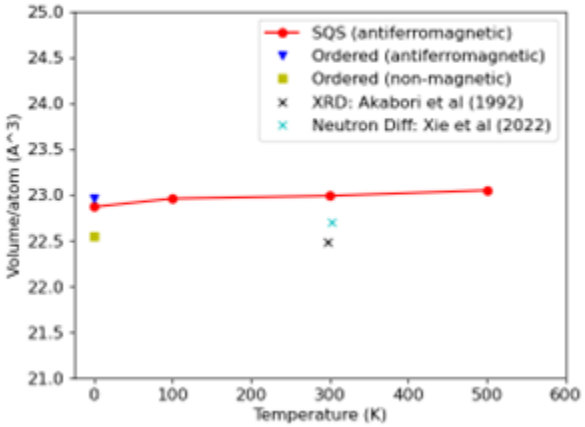


Figure 3: Volume per atom versus temperature using GGA+U with U = 1 eV.

B.131 BANR/ARDP Particle Design Optimization

Report Participants

Shrier, Alex [1]
1 BWX Technologies, Inc

Scientific Achievement

BWX Technologies' (BWXT's) Advanced Gas Reactor Program (ARDP) project utilizes INL's fuel performance code MOOSE and BISON in order to assess, characterize, and down select a modified TRISO particle, specifically, a UN kernel TRSIO particle with modified layer thicknesses. Computationally, the modeling methodology utilizes sampling plans for thousands of particles which incorporate thermal-physical stress analysis (Figure 1–2), failure modes (Figure 1–2), and as-fabricated distributions to assess a design space (Figure 3) and inform upon particle design down selection.

Significance

As mentioned above, the sampled particle design space is used to inform particle design down selection and will ultimately define BWXT's Advanced Nuclear Reactor (BANR) and ARDP reactor core design. The fuel design and optimization study for the particle architecture is essential in defining the core's operational envelope, providing the base case for design limits and tolerances.

Key Publications

None

Sponsor/Program

ARDP and BANR

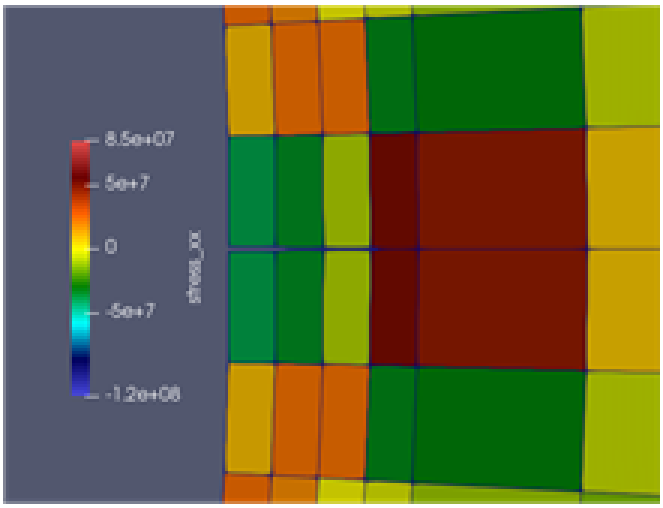


Figure 1: UN TRISO IPyC crack failure mode.

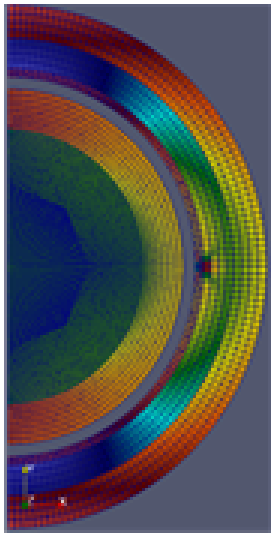


Figure 2: UN TRISO failure mode stress analysis.

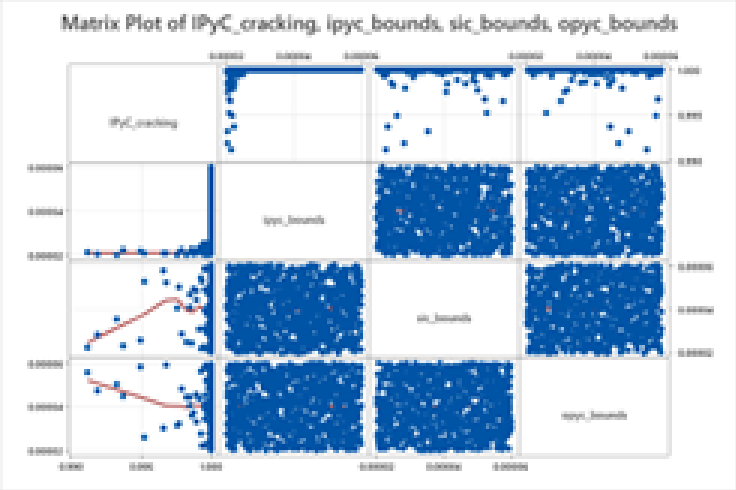


Figure 3: UN TRISO design optimization.

B.132 Nuclear Thermal Propulsion

Report Participants

Shrier, Alex [1]
1 BWX Technologies, Inc

Scientific Achievement

Using MOOSE and BISON to assess exotic and extreme environments on proposed ceramic-ceramic (Cer-Cer) and ceramic-metal (Cer-Met) fuel materials. As many materials will require testing at these exotic and extreme environments, scoping studies are required to verify and validate fuel designs. Further, the modification and adaption of the source code is critical in assessing possible phenomena and subsequently informing design-based decisions.

Significance

The generation of a base set of proposed fuel materials and their thermophysical properties will be needed during each design phase of the BWXT Nuclear Thermal Propulsion reactor engine. The generation of material data sheets with respect to material properties and phenomena observed in extreme environments is critical in the reactor engine design as well as component and component subsystem design selections. Utilizing MOOSE and BISON, sensitivity studies assess, verify, and validate proposed fuel materials, designs, and possible thermal-physical phenomena.

Key Publications

None

Sponsor/Program

NASA-NTP

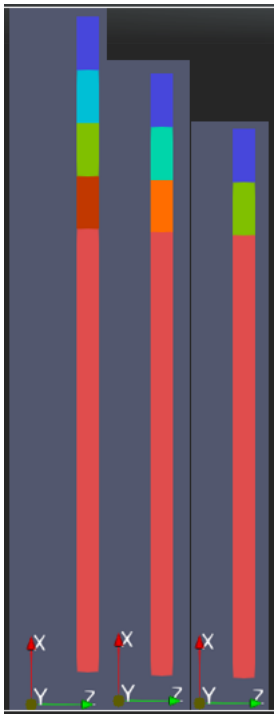


Figure 1: 1D Cer-Cer particle design comparison.

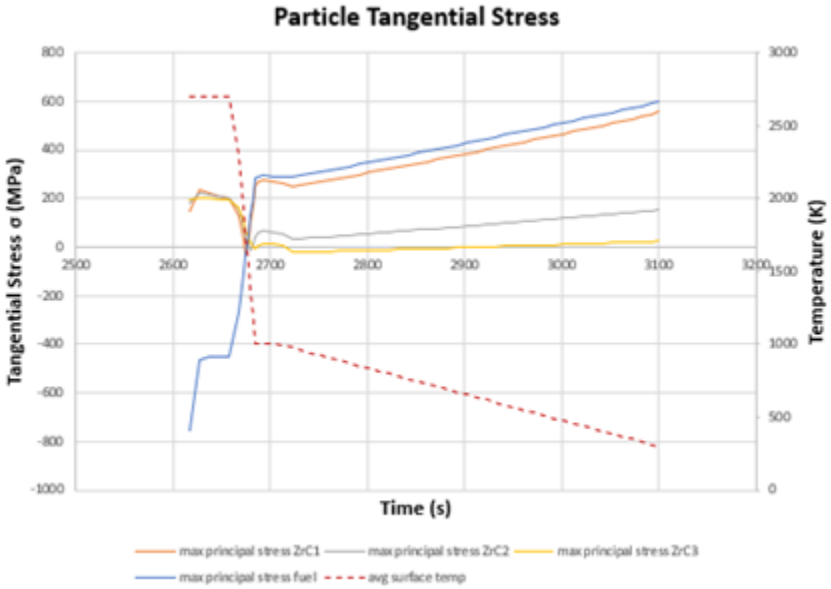


Figure 2: Operation thermal stress assessment on a multilayer Cer-Cer particle design.

B.133 Multiphysics Fuel Performance Modeling of TRISO Fuel in Advanced Reactor Environments

Report Participants

Siaraferas, Tatiana [1], Robert, Yves [1], Fratoni, Massimiliano [1]
1 University of California Berkeley

Scientific Achievement

This project aims to develop and validate precise and computationally efficient multiphysics TRISO particle fuel performance models for advanced pebble-bed fluoride- and gas-cooled high-temperature reactor concepts. Specifically, the aim is to assess the thermal-mechanical response of TRISO particles during normal operation, develop multiphysics neutronics and thermohydraulics models to predict the fuel's operational conditions in normal operation, AOOs, and DBA conditions, and use this information as input for fuel performance models. INL's HPC resources will be leveraged to use NEAMS tools such as Griffin and Pronghorn. Specifically, the goal is to develop models that couple the Monte Carlo code Serpent and Griffin with Pronghorn and, based on the power distribution from the neutronics analysis, to derive the temperature of the pebbles and TRISO particles during normal and off-normal operating conditions. The results of the developed models will be used to determine the fuel behavior and radionuclide release during normal operation, AOOs, and DBA conditions of a reactor design. Lastly, through this project, the goal is to quantify the acceptable limits during transient conditions using information about the fuel failure fraction and radionuclide release inventory.

Significance

This project is a crucial stepping stone in deploying and licensing advanced nuclear reactors that use TRISO fuel particles. TRISO-coated particle fuel has been found to be a desirable fuel choice for FHRs, HTGRs, and microreactors. These types of reactors have gained interest and are currently being developed in the United States and worldwide to cover rising energy demands and reach decarbonization goals. Though these types of reactor technology and fuel have been developed and researched in the past; currently, there is no validated capability for predicting TRISO fuel behavior for advanced reactors during normal operation, AOOs, and DBAs. The results of this project will provide critical data to support the designing, licensing, and deploying of advanced nuclear reactors.

Key Publications

Robert, Y., Fratoni, M., & Siaraferas, T. 2022. Proof of concept for hyper-fidelity depletion of full-scale pebble bed reactors. Retrieved from https://ssrn.com/abstract=4194599 " Wirth, B. 2020. Multi-physics fuel performance modeling of TRISO-bearing fuel in advanced reactor environments.

Sponsor/Program

NEUP IRP Project 20-22094

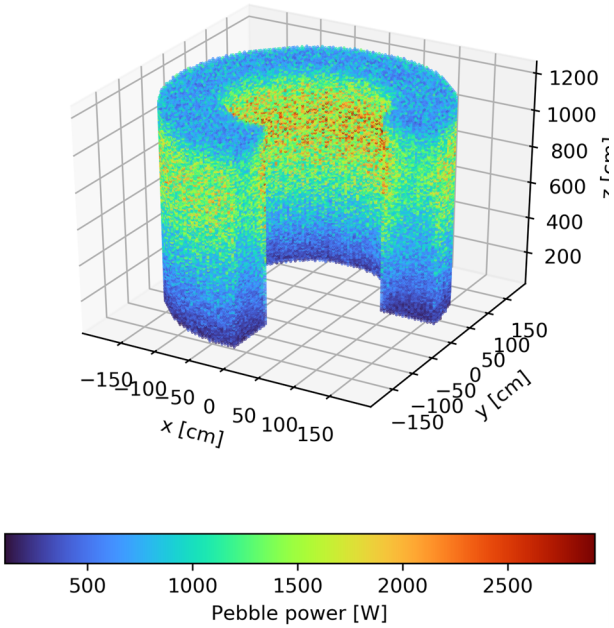


Figure 1: 3D representation of pebbles in an HTGR core showing pebble power distributions at equilibrium.

B.134 Modeling of Liquid-Metal-Bonded ADOPT Fuel with SiC-SiC Cladding

Report Participants

Yingling, J [1], Stephan, Adam D[1]
1 University of South Carolina

Scientific Achievement

Several simulations have been run, and the results are promising. At this point in time, I don't think I'm able to publicly share much of the testing results. The results will be published soon, but the work is still in progress. I can share that, after the initial rise to power, the liquid-metal-bonded Advanced Doped Pellet Technology (ADOPT) SiC has the lowest centerline temperature with a 210 K temperature advantage relative to He-bonded ADOPT-SiC. This result is comparable to the results of Wongsawaeng [4] but somewhat lower than the results of Sweet et al., which include the effect of thermal shunting [2].

Significance

This study aims to fully model the potential of using ADOPT fuel with SiC/SiC cladding with a liquid metal bonding. The primary goal is to analyze this particular setup as it applies to accident tolerance and consider its viability under normal operation. From this point, I intend to utilize the code to model SiC cracking if and when the ADOPT pellet contacts the inner cladding wall as well as to add some simulations for using a coated cladding and other material alterations.

Key Publications

1. L. H. Jr. Hallman, Westinghouse Advanced Doped Pellet Technology (ADOPT) Fuel, WCAP-18482-NP Rev. 0, May 2020. 2. R. T. Sweet, K. A. Terrani, and B. D. Wirth, EFFECT OF HELIUM OR LEAD-BISMUTH FILLED CRACKS ON TEMPERATURE PROFILE OF LWR FUEL PELLETS, p. 22. 3. D. Wongsawaeng and D. R. Olander, Effect of Replacing Helium with a Liquid Metal in the Fuel-Cladding Gap on Fission Gas Release, Nucl. Technol., vol. 146, no. 3, pp. 211–220, Jun. 2004, doi: 10.13182/NT04-A3500. 4. D. Wongsawaeng and D. Olander, Liquid-Metal Bond for LWR Fuel Rods, Nucl. Technol., vol. 159, no. 3, pp. 279–291, Sep. 2007, doi: 10.13182/NT07-A3876. 5. Still in progress

Sponsor/Program

University of South Carolina

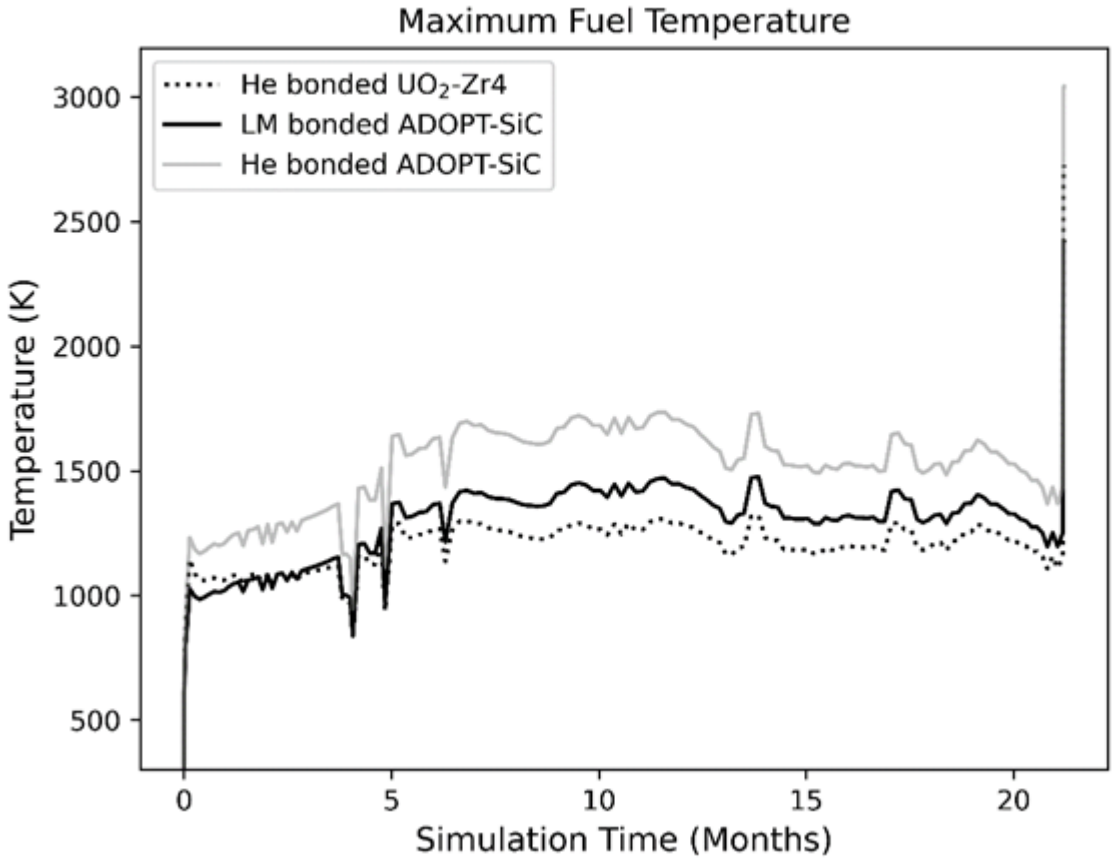


Figure 1: Calculated maximum fuel temperature comparison.

B.135 NRC Non-LWR Advanced Reactors and HTTR LOFC Projects in the Office of Research (RES)

Report Participants

Tehrani, Nazila H[1]
1 Nuclear Regulatory Commission

Scientific Achievement

As a member of the NRC non-LWR team in the Office of Research, I am responsible for developing and modifying plant models to perform independent confirmatory analyses and evaluations related to applicant submittals. I will use the BlueCRAB suite (SAM, BISON, Griffin, Pronghorn, and Sockeye) to accommodate the development and modification needs for those advanced reactor plant models under development. I used Griffin to run the molten-salt-cooled pebble-bed reactor model for transient analysis and gas-cooled pebble-bed reactor model DLOFC and PLOFC transient analysis. I used Griffin and SAM codes to run MHTGR models on VTB.

Significance

The NRC is responsible for performing independent analyses and evaluations of applicant submittals to ensure the safe and reliable operations of nuclear reactors in the United States.

Key Publications

None

Sponsor/Program

NRC

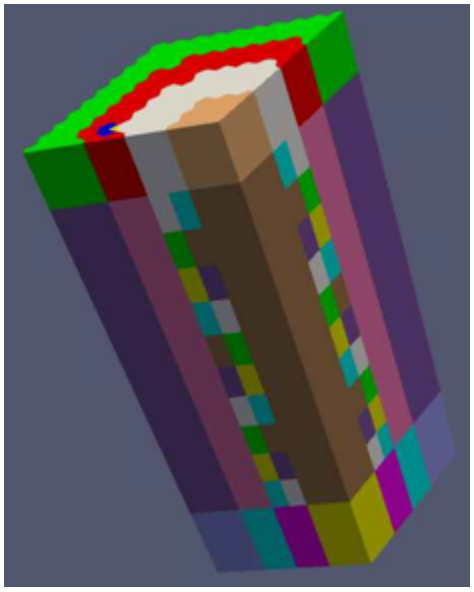


Figure 1: MHTGR Griffin model (prismatic).

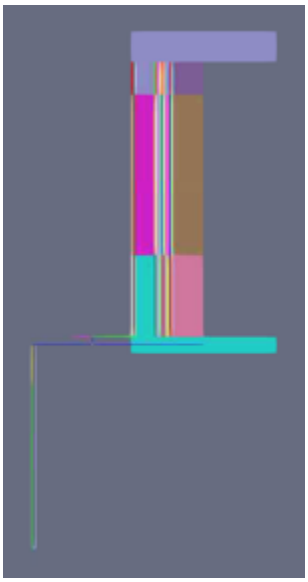


Figure 2: MHTGR primary loop SAM model.

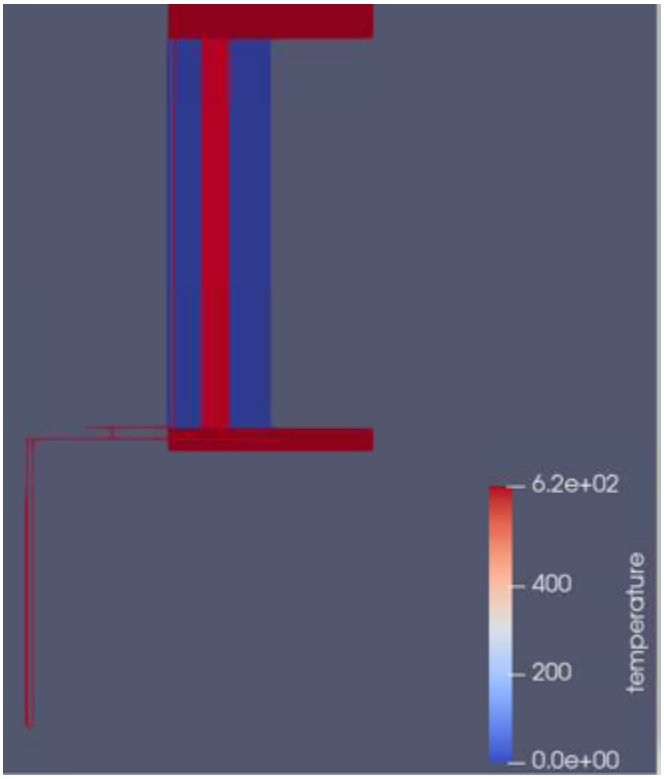


Figure 3: MHTGR SAM model.

B.136 LOWE Fuel Element Heating for Transport

Report Participants

Temme, Tyler N[1], Harroff, Brandon H[1], Brown, Curtis A[1], Hardtmayer, Douglas E[1]
1 MPR Associates

Scientific Achievement

To support the development of the U-10Mo monolithic fuel concept and the design of the ATR's LEU fuel element, LOWE, irradiation tests are planned with full-size LOWE elements in ATR core driver positions. These tests are referred to as an ET. Following the ETs, ATR will be qualified for unrestricted use of LOWE in ATR, allowing LOWE fuel elements to be used in any ATR position and in any quantity. Addendums to the ATR SAR are being prepared to allow the insertion of LOWE for ET-3 and unrestricted LOWE operation. At present, spent fuel storage and shipping containers are being evaluated for future LOWE fuel. These evaluations require the heat generation of the LOWE fuel elements as a function of time.

Significance

The expected heat generation curves of a heavily depleted LOWE fuel element is still being analyzed.

Key Publications

MPR Associates. 2023. MPR Calculation 1129-0280-CALC-003, Rev. 0 (in progress)

Sponsor/Program

ATR
USHPRR Program

B.137 BISON-Informed Whole-Core TRISO Fuel Performance Modeling

Report Participants

Tompkins, James B[1], Schunert, Sebastian [1], Chin, Roger [1], Jiang, Wen [2]
1 Radiant Industries Incorporated
2 Idaho National Laboratory

Scientific Achievement

In recent years, NEAMS' BISON code has seen significant development efforts devoted to TRISO fuel performance modeling with a particular emphasis on particle failure and fission product release. While BISON validation efforts have been undertaken utilizing AGR program experiment data, BISON simulations are typically performed at fuel scale. Gas-cooled reactor designs monitor the bulk primary loop coolant for radionuclides, and thus fuel performance in operating reactors is monitored at the system scale. To bridge this gap between fuel and system scales to integrate BISON simulation results into whole-core models, this work presents a methodology in which TRISO particle failure fractions are predicted over a performance envelope in BISON, calculated particle failures are classified to identify impacted layers, the fission product diffusion from TRISO layers is quantified, and bulk release is determined for homogenized spatial regions.

Significance

With this methodology, the BISON fuel performance code may be utilized to quantify a conservative estimate of fission product release within a reactor design. These assessments can be used as a source term for mechanistic modeling under various reactor operational conditions to inform the specified acceptable core radionuclide release design limits and ensure even under accident conditions that regulatory site boundary dose limits are not exceeded and establishing a regulatory case for functional containment. Development for these capabilities is under way, with expected completion in April 2023. TRISO failure calculations have been run using HPC resources, and we will next work to develop correlation functions for several conditions in the particles known to contribute towards failure. This would conclude the failure model development and then we would work to implement this in conjunction with the diffusion model into a digital twin developed using the Radiant SimEngine software package.

Key Publications

(In-progress) Tompkins, J. B., Schunert, S., Chin, R., Jiang, W. (2023, June 11-14). BISON-informed Whole Core TRISO Fuel Performonce Modeling [Conference presentation]. 2023 American Nuclear Society Annual Meeting, Indianapolis, IN, United States.

Sponsor/Program

This work is primarily sponsored by a DOE SBIR with joint award for Radiant and INL.

Figure 1: Diagram of the singular particle per element methodology.

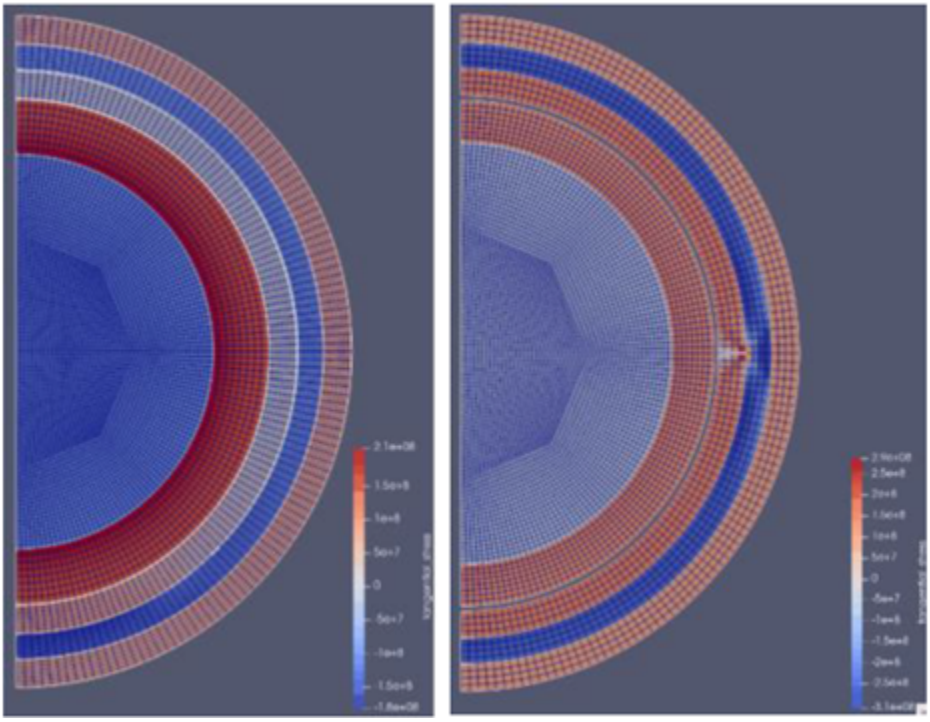


Figure 2: (left) 2D TRISO particle with IPyC layer debonding from SiC and (right) 2D TRISO particle model with crack in IPyC layer subjecting SiC to tensile stresses.

B.138 Nanoindentation Modeling for Investigating Alpha Uranium Grain Size Response & Aluminum Stress Relaxation

Report Participants

VandenBroeder, Gavin T[1], Chen, Tianyi [1], Yushu, Dewen [2], Pitts, Stephanie A[2], Frazer, David [2]
1 Oregon State University
2 Idaho National Laboratory

Scientific Achievement

This work aims to employ a model of nanoindentation using the current crystal plasticity capabilities of INL's MARMOT. The base hardening model is applied to two different scenarios: the relaxation of stress in pure aluminum and grain-size-dependent parameterization of wrought alpha uranium for comparing hardness. The basis for each of these simulations is a newly developed model for nanoindentation. Berkovich and spherical indentation tips were developed within CUBIT on the HPC resources. The first set of computations was used to tune the model's contact, time stepping, and stability. It was then split into two versions, one using Kalidindi crystal plasticity parameterized after aluminum and the other using alpha uranium crystal plasticity parameterized after coarse- and fine-grain alpha uranium. In both cases, Paraview is used on the HPC recources for data visualization and output.

Significance

Nanoindentation is a widely used submesoscale mechanical testing method for determining fundamental material properties. A model of this method will allow for a better understanding of experiments and visualizations of acting phenomena. The aluminum model is being used to gather data on stress relaxation during the indentation-holding phase with varied stress exponent values. This work has been coupled with experimentation to provide insights into understanding the dislocation behavior during nanoindentation stress relaxation. A manuscript is being prepared for journal publication. On the other hand, recent nanoindentation experiments have prompted the opportunity for rapid model validation. As an example, an existing alpha-uranium crystal-plasticity model is being compared with the experimentally measured hardness of wrought alpha uranium. Simulations are being performed under both Berkovich and Spherical tip indentations. This work is not yet completed and would require extended access to HPC and MARMOT to finish.

Key Publications

Gavin VandenBroeder, David Frazer, Dewen Yushu, Stephani Pitts and Tianyi Chen. 2023. Crystal Plasticity Nanoindentation Modeling of Depleted -Uranium using Marmot. Submitted to the 2023 ANS Annual Meeting, Indianapolis, IN, June 11-14.

Sponsor/Program

Work supported through the Idaho National Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517

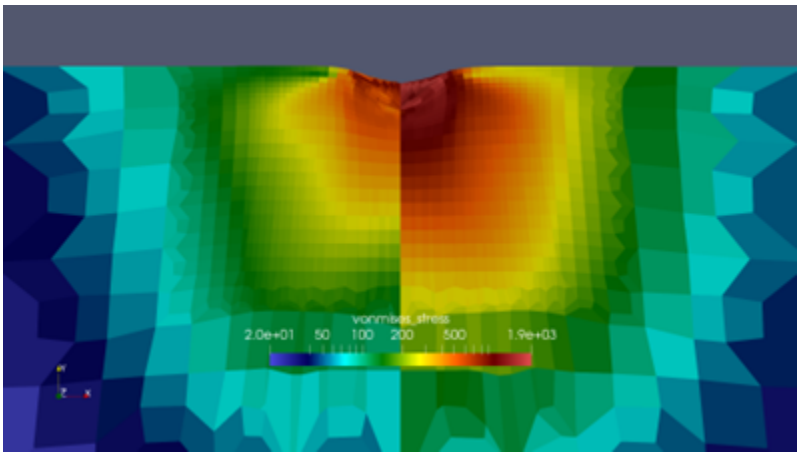


Figure 1: Von Mises stress 0.0 seconds into the holding phase comparing loading rates of 100 and 800 nm/s with a stress exponent of 10. The stress in 800 nm/s is much higher.

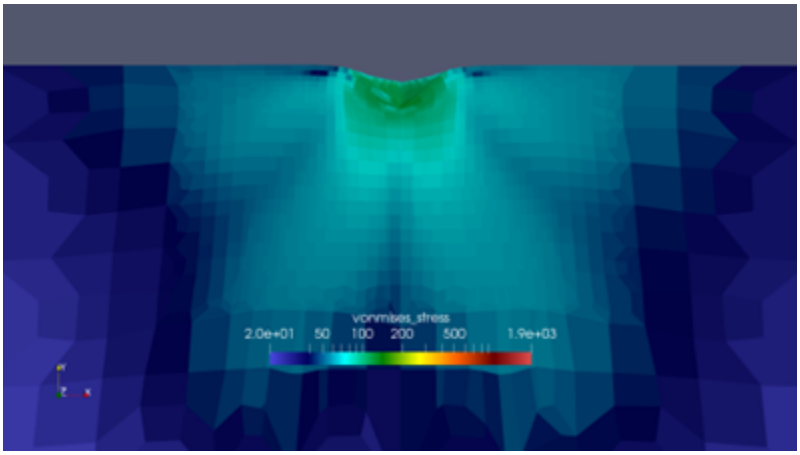


Figure 2: Von Mises stress 2.0 seconds into the holding phase comparing loading rates of 100 and 800 nm/s with a stress exponent of 10. Both loading rates relax to nearly the same stress distribution.

B.139 Atomistic study of fundamental bulk and defect properties in -uranium

Report Participants

Wang, Yuhao [1], Beeler, Benjamin W[2], Jokisaari, Andrea M[3]
1 University of Michigan
2 North Carolina State University
3 Idaho National Laboratory

Scientific Achievement

Alpha-uranium plays an important role in the performance and structure evolution of metallic fuels under irradiation. It is a highly anisotropic material that demonstrates a complex microstructural response to irradiation dependent on the irradiation temperature, and the mechanisms that control this behavior are not well understood. In this work, fundamental bulk properties and energetic and thermodynamic properties of single point defects and di-defects in -uranium are determined using molecular dynamics over the range of 400–750 K. The constant pressure heat capacity, total volumetric thermal expansion, anisotropy of the thermal expansion, and single vacancy and single interstitial formation energies all agree well with previous experimental and ab initio results, lending support to the di-defect formation and binding energies and the diffusivity results. We find that the diffusion of vacancies and di-vacancies is strongly anisotropic, while interstitial and di-interstitial diffusion is slightly anisotropic, and the most rapidly migrating species changes depending on the temperature. The formation energy of vacancies and di-vacancies increases slightly with temperature, while the formation energy of interstitials and di-interstitials increases strongly with temperature. In addition, di-vacancies are very loosely bound over the entire temperature range, with an average binding energy of 0.017 eV. Conversely, di-interstitials are strongly bound (0.64 eV) until approximately 600 K, above which the binding energy decreases significantly, with an average binding energy of 0.31 eV. These results provide valuable new insights into the possible mechanisms of the complex irradiation damage behavior of -uranium.

Significance

In this work, we investigated several fundamental bulk and defect properties of -uranium via classical molecular dynamics and compared the results, when possible, with experimental results, density functional theory calculations, and ab initio molecular dynamics. We have shown good agreement of the specific heat capacity, volumetric thermal expansion, anisotropy of the thermal expansion in the a, b, and c directions, and vacancy and self-interstitial formation energies, lending confidence that our results of defect diffusivity and di-defect binding energies are physically significant. We find that the vacancy and di-vacancy diffusivity is strongly anisotropic, with slow diffusion in the b, or [010], direction. We also find that the total diffusivity and diffusivity in each of the a, b, and c directions are very similar for vacancies and di-vacancies. Conversely, self-interstitial diffusivity is less anisotropic, with slow diffusion in the a direction, and while self-interstitials generally transport faster than vacancies and di-vacancies, di-interstitials move much more slowly at low temperatures. Furthermore, the vacancy and interstitial formation energies increase with temperature, though the interstitial formation energy increases much more than the vacancy formation energy. The binding energy of di-vacancies is near zero over the entire temperature range, while it is strongly positive at temperatures below 600 K and much weaker above 600 K for di-interstitials.

The complex behavior of the defect energetics and transport could explain the complex behavior of -uranium under irradiation as a function of temperature, as the exact degree of vacancy and interstitial clustering, recombination, loss to sinks, and anisotropic transport through the crystal is altered. Further investigation is required to test the interplay of these behaviors and understand their effect on microstructure evolution under irradiation. With further research, these results will improve the fundamental understanding of the effect of temperature on radiation damage and support the development of physics-based models of metallic fuel behavior in reactors.

Key Publications

" (Under review) Wang, Y., Beeler, B., Jokisaari, A. An atomistic study of fundamental bulk and defect properties in -uranium. (Journal of Nuclear Materials)

" (In Progress) Wang, Y., Beeler, B., Jokisaari, A. Atomic assessment of anisotropic elastic response for defects in -uranium. (Targeted Journal: Journal of Nuclear Materials)

" Beeler, B., Mahbuba, K., Wang, Y., Jokisaari, A. (2021). Determination of thermal expansion, defect formation energy, and defect-induced strain of -U via ab initio molecular dynamics. Frontiers in Materials, 8, 188.

Sponsor/Program

This work is supported through the INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office Contract DE-AC07-05ID14517 under the LDRD 20A44-121, Modeling and characterization of alpha-U to accelerate metallic fuel development.

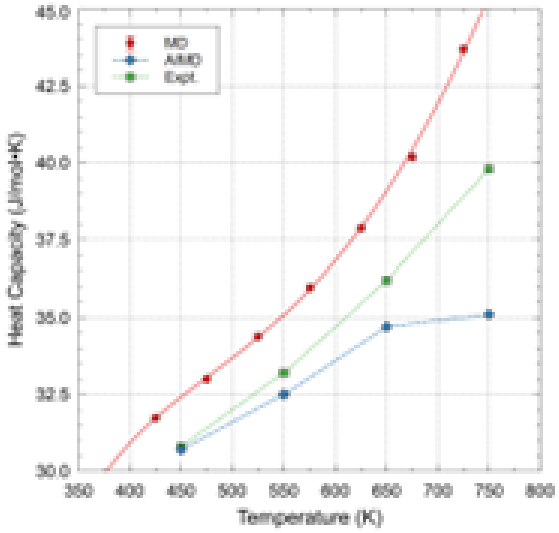


Figure 1: The constant pressure heat capacity of -uranium versus temperature.

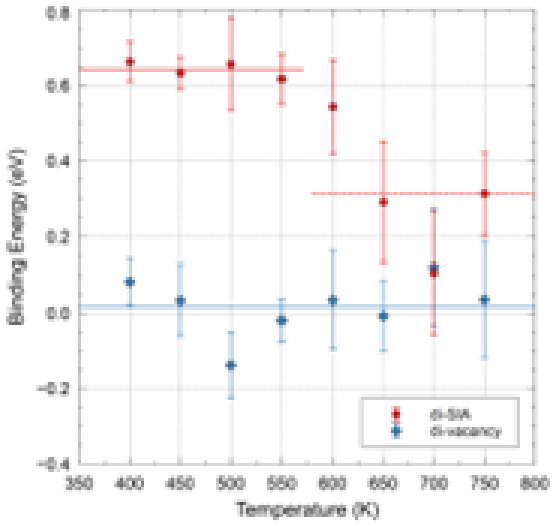


Figure 2: Binding energies for a di-SIA and a di-vacancy in -uranium.

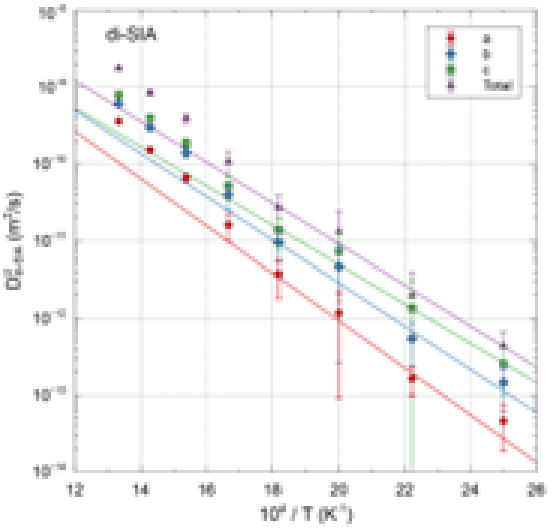


Figure 3: Atomic diffusivity of di-SIA as a function of temperature.

B.140 SpaceX Falcon Heavy Mass Constraints as Design Driver for Practical Heat Pipe Stirling Microreactors

Report Participants

Watson, Daniel L[1], Gatchalian, Ronald Daryll E[1], Hsieh, Hui-Yu [1], Bhat, Pramatha [1], Tsvetkov, Pavel [1]
1 Texas A&M University

Scientific Achievement

A nuclear reactor system was designed with a SpaceX Falcon Heavy as the design driver (mass and size constraints). Neutronics, depletion, shielding, and criticality safety analyses were performed with MCNP6.2 on the INL Sawtooth cluster. Ansys was performed on local Texas A&M resources to assess heat-pipe performance.

Significance

The project outcomes delineated the maximum power yields achievable with the current commercial heavy-lift rocketry utilizing a nuclear power system. Acceptable neutron radiation doses were observed at the 300 kWt power range with LiH shielding, however, photon doses surpassed NASA FSP SoW DR-3's threshold (combined 5 Rem/yr). The reactor, modeled on INL's "Special Purpose Heat Pipe Microreactor Design A," exhibited safe shutdown margins during oceanic submersion incidents and control drum malfunctions.

Key Publications

Watson, D. L. P., Gatchalian R. D. E., Hsieh H., Bhat P., & Tsvetkov P. V (2023). SpaceX Falcon Heavy Mass Constraints as Design Driver for Practical Heat Pipe Stirling Micro Reactors. Proceedings of Nuclear and Emerging Technologies for Space (NETS 2023), Idaho Falls, 305-311. doi.org/10.13182/NETS23-41911

Sponsor/Program

This project was completed as an assignment within a course at Texas A&M University (NUEN610 - Reactor Design). Maturation of the evaluations yielded a conference paper that was accepted to NETS 2023, and ultimately invited to a special (upcoming) publication of Nuclear Technology .

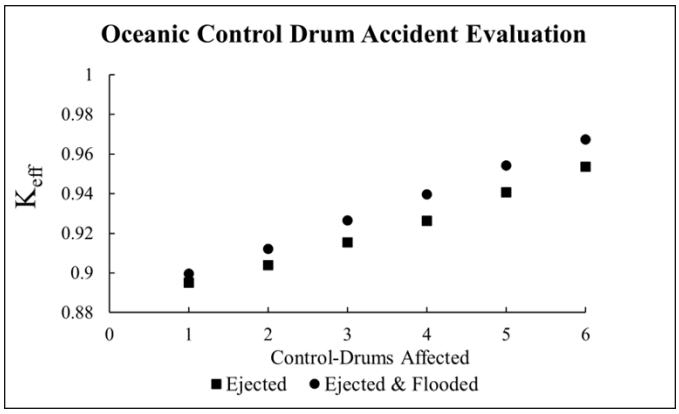


Figure 1: Criticality safety evaluation for a launch failure and subsequent oceanic submersion with affected control drums.

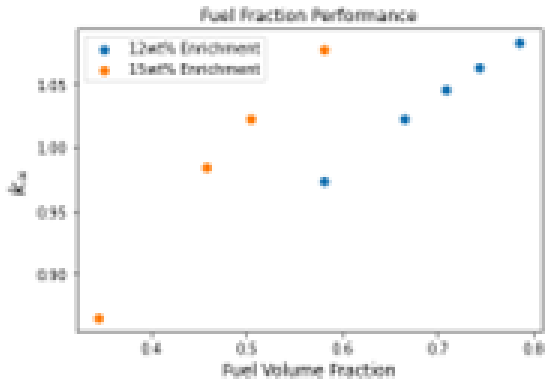


Figure 2: K-eigenvalues for differing enrichments and fuel volume fractions.

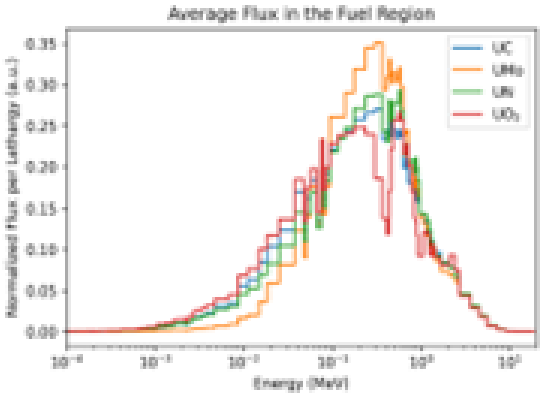


Figure 3: Flux energy spectrum in fuel for differing fuel materials.

B.141 Modeling of NBSR and NNS Multiphysics Behavior

Report Participants

Weiss, Abdullah G[1], Celikten, Osman S[1], Gurgen, Anil [1], Sahin, Dagistan [1]
1 National Institute of Standards and Technology

Scientific Achievement

This work involved modeling the behavior of an NBSR fuel element in MOOSE. Ongoing work will attempt to further improve the model and validate it with available operations data. Upon validating the NBSR model, a twin model will be developed for the NNS to help the design efforts.

Significance

The work is still in-progress. The word performed to-date yielded two benefits: familiarizing the NIST Center for Neutron Research staff with MOOSE and MOOSE tools (yielding new users for INL-developed software) and finishing the first step of building a one-of-a-kind multiphysics model for the NBSR.

Key Publications

None

Sponsor/Program

NIST

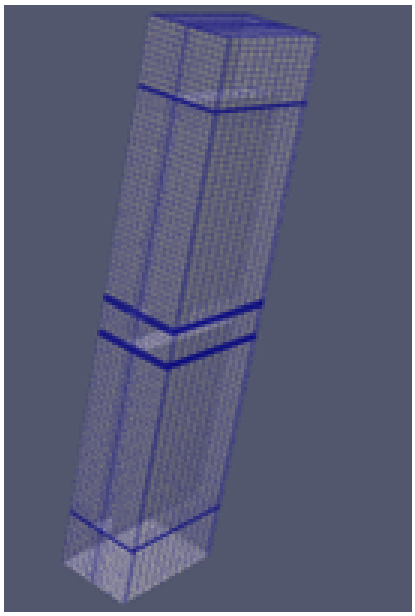


Figure 1: Mesh for NBSR fuel element.

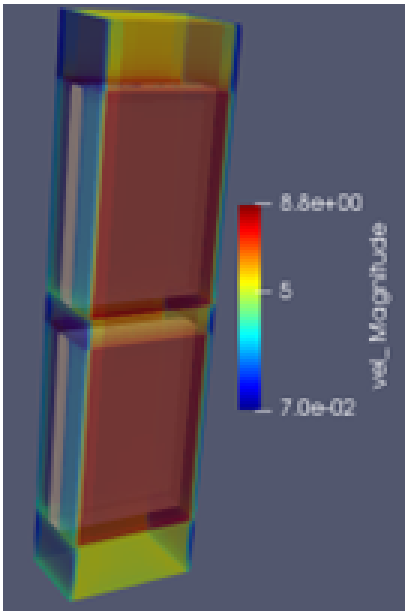


Figure 2: Velocity distribution in fuel element.

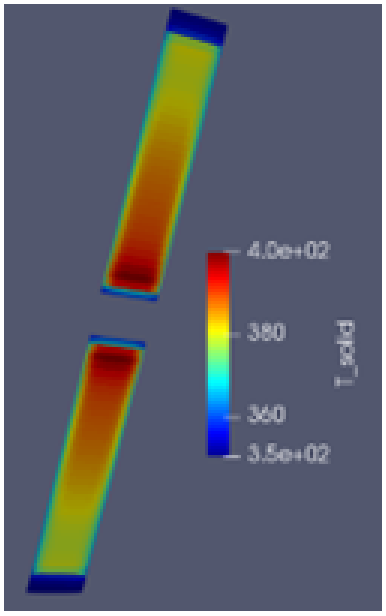


Figure 3: The fuel and cladding temperature distribution.

B.142 Artificial-Intelligence-Based Process Control and Optimization for Advanced Manufacturing

Report Participants

Yaseen , Mahmoud T[1], Wu, Xu [1], Yushu, Dewen [2], German, Peter [2]
1 North Carolina State University
2 Idaho National Laboratory

Scientific Achievement

For this LDRD project, North Carolina State University's goal is to develop physics-informed ROMs by enforcing physical laws in the data-driven ROMs to provide predictive capabilities with physical meaning, thus improving the interpretability of the data-driven ROMs. Our original plan was to build physics-informed ROMs by including physical knowledge during the training phase of the ROMs. We first explored physics-informed neural networks (PINNs) to build DNN-based ROMs. However, after careful investigation, we concluded that directly solving the governing equations for INL's MOOSE-based AM model with PINNs is infeasible due to the following difficulties: a changing geometry due to melting and a moving laser power source cannot be modeled by PINNs; PINN cannot track the moving melt pool surface, thus the convective boundary condition cannot be implemented in the loss function (physical consistency term); cannot couple the thermal model with the mechanical model, especially for complicated geometries. For complicated engineering-scale multiphysics problems, such as AM, we plan to still make use of the training data generated by the MOOSE-based AM model developed and validated in other tasks. To demonstrate the improvement of the physics-informed data-driven ROMs, we will quantify the advantages (if any) over purely data-driven ROMs. We also plan to leverage Fourier Neural Operator and deep operator networks (DeepONets) to build the ROMs, given the parametric nature of the governing equations (changing process parameters including the power, scanning speed, etc.).

Significance

The AI-based process control and optimization (PC&O) method will leverage existing INL investments in multiscale, multiphysics M&S for AM. Compared to commercial software (e.g., STAR-CCM+), MOOSE provides the unique control capability to adjust AM simulation models during the runtime, which is fundamental for enabling online PC&O. A significant challenge is that the existing AM models are usually computationally prohibitive, making them unable to provide timely predictions that can be employed by deep reinforcement learning to make decisions. To reduce the computational cost, we will develop physics-informed ROMs using deep learning algorithms that can accurately predict physical phenomenon ranging from the microstructural level to engineering scale. When training the ROMs, in addition to the accuracy and simplicity terms in the loss function, we will add a third term for physical consistency. In this way, the ROMs can be trained with physical knowledge embedded, instead of being purely data driven. Our developed ROM will significantly reduce the time for deep-reinforcement-learning-based PC&O methodology.

Key Publications

Yaseen, M., Yushu, D., German, P., and Wu, X. (2023). Reduced Order Modeling of a Moose-based Advanced Manufacturing Model with Operator Learning. In Proceedings of the 2023 In-

ternational Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2023). Niagara Falls, Ontario, Canada, August 13-17, 2023 (in preparation)

Sponsor/Program

INL Laboratory Directed Research & Development (LDRD) Program under DOE Idaho Operations Office contract no. DE-AC07-05ID14517

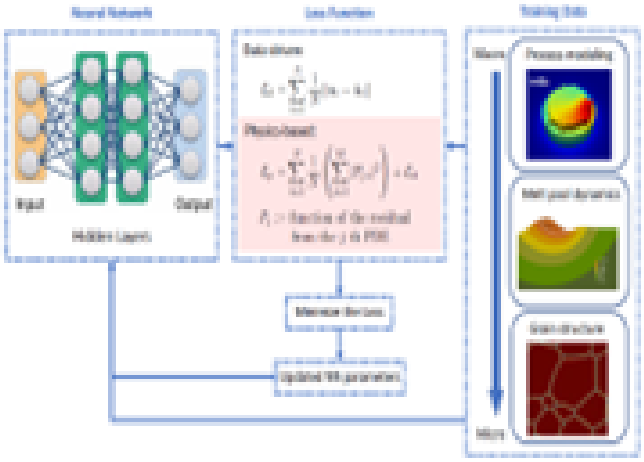


Figure 1: Comparison of MOOSE-based AM simulation for max bead temperature with deep-neural-network-based ROM predictions.

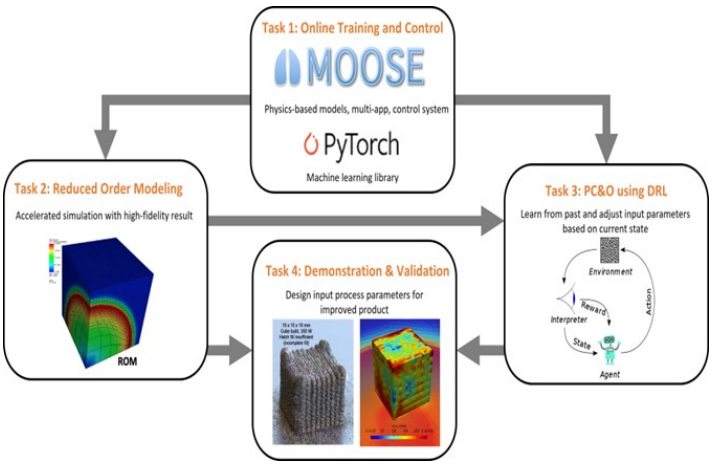


Figure 2: Bead temperature of the melt pool along the scanning path.

B.143 Thermal Hydraulic Evaluation of Large Break LOCA Under High-Burnup Conditions

Report Participants

Wysocki, Aaron J[1], Hirschhorn, Jake [2], Capps, Nathan A[1], Greenquist, Ian T[1]
1 Oak Ridge National Laboratory
2 Idaho National Laboratory

Scientific Achievement

TRACE thermal hydraulic (TH) LBLOCA analyses were performed for a realistic 24 month high-burnup PWR equilibrium cycle to inform subsequent transient BISON high-burnup FFRD susceptibility evaluations. Realistic LBLOCA system behavior was first established by configuring to and comparing with the BEMUSE OECD LBLOCA benchmark. Fuel and operating conditions were then applied from high-burnup VERA depletion calculations. LBLOCA simulations were performed for 281 selected high-burnup rods, for which transient TH boundary conditions were collected for later use in BISON.

Significance

Increasing the peak rod average burnup of PWR fuel beyond 62 GWd/tU may increase FFRD susceptibility during a LBLOCA. The calculations performed in this project provide needed insight into the TH and fuel conditions of PWR fuel during LBLOCAs, allowing an estimation of FFRD susceptibility and informing future LOCA experiments to support LWR high-burnup operation. The TRACE results indicated that rod linear heat rate (rather than burnup) is the main predictor of PCT during the event. PCT typically occurred at a local burnup lower than the rod-average burnup, especially for twice-burned fuel.

Key Publications

A. Wysocki, J. Hirshhorn, N. Capps, I. Greenquist, Multiphysics Analysis of Fuel Fragmentation, Relocation, and Dispersal Susceptibility Part 3: Thermal Hydraulic Evaluation of Large Break LOCA Under High-Burnup Conditions, Annals of Nuclear Energy, 2023 (In Review).

N. Capps, I. Greenquist, A. Wysocki, J. Hirshhorn, Multiphysics Analysis of Fuel Fragmentation, Relocation, and Dispersal Susceptibility Part 2: High Burnup Steady State Operating and Fuel Performance Conditions, Annals of Nuclear Energy, 2023 (In Review).

I. Greenquist, A. Wysocki, J. Hirshhorn, N. Capps, Multiphysics Analysis of Fuel Fragmentation, Relocation, and Dispersal Susceptibility Part 1: Overview and Code Coupling Strategies, Annals of Nuclear Energy, 2023 (In Review).

Sponsor/Program

NEAMS

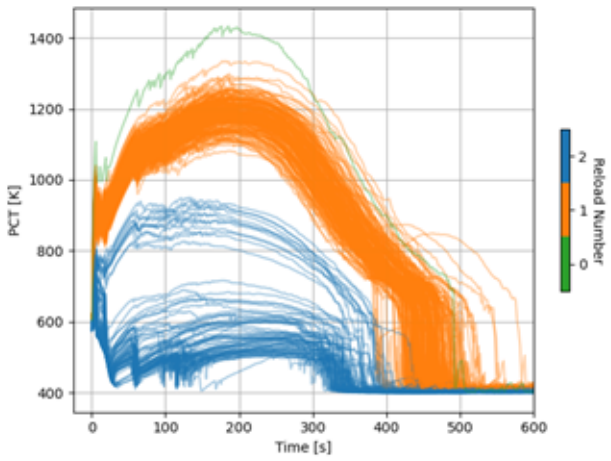


Figure 1: LBLOCA PCT versus time for 281 high-burnup rods (blue and orange lines) and the highest power rod in the core (green line).

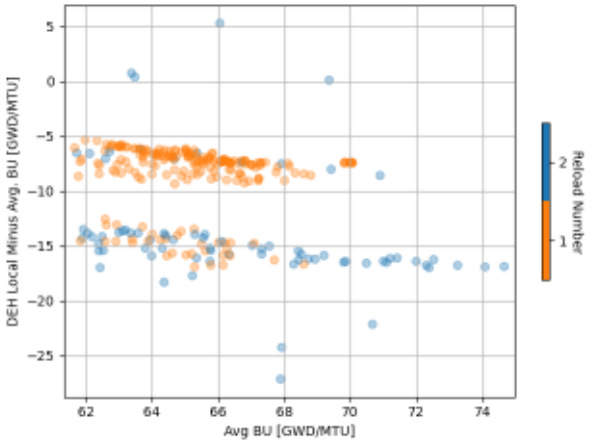


Figure 2: Difference between the local burnup at the PCT location and rod average burnup.

B.144 Post CASL VERA Applications to Departure from Nucleate Boiling Challenge Problem and ATF Development

Report Participants

Xu, Yiban [1], Sung, Yixing [1], Boychenko, Mykola [1]
1 Westinghouse Electric Company

Scientific Achievement

In support of industry's initiatives for safer and more efficient reactor operation and power generation, VUG has continually developed the multiphysics code system VERA that couples the neutron code MPACT with the thermal-hydraulic code CTF for addressing the DNB (departure from nucleate boiling) 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 RIA or other flow reduction events. In 2022, CTF was used for evaluating RIA test result from TREAT as part of the high-burnup (HB) ATF development program.

Significance

As it is subject to continuous improvements and regulatory licensing, the VERA code system is being evaluated and applied to the HB ATF development and provides an advanced tool to the industry for PWR safety analysis and operational support. Based on the study results, a potential application of the VERA code system is to evaluate margin improvement from ATF features without DNB-induced fuel failure under non-LOCA conditions, such as a locked rotor event. In addition, CTF is being applied to RIA test data analyses for establishing HB fuel acceptance criteria in collaboration with INL under the High-Burnup Experiments for Reactivity initiated Accident Program.

The advanced fuel rod models in the newly released CTF versions can help to determine cladding burst criteria under various operation conditions for different fuel designs, such as dupped pellets and high burnups. CTF parallelzation provides opportunities for coupling with statistical codes, such as Dakota for applications of uncertainty quantification and parameter sensitivity analyses, which are important areas for improving operational safety and regulatory confidence.

Key Publications

1. C. S. Brown, et al., Best Estimate Plus Uncertainty Analysis of Departure from Nucleate Boiling Limiting Case with CASL Core Simulator VERA in Response to PWR Main Steam Line Break Event, Nuclear Engineering and Design, Vol. 309, pp.8-22 (2016). 2. Y. Xu and Y. Sung, Validation of Improved CTF Transient Fuel Rod Model, L3:AMA.CP.P18.07, CASL-U-2019-2865, 2019. 3. Y. Sung, et al, CASL VERA Applications to Departure from Nucleate Boiling Challenge Problem, 2020 ANS Winter Conference, CASL Symposium, .November 16-19, 2020 4. R. K. Salko, et al., CTF: A modernized, production-level, thermal hydraulic solver for the solution of industry-relevant challenge problems in pressurized water reactors, Nuclear Engineering & Design, NED-22-00254, 2022.

Sponsor/Program

The current VERA/CTF development work at Westinghouse is supported by DOE through the HB ATF program.

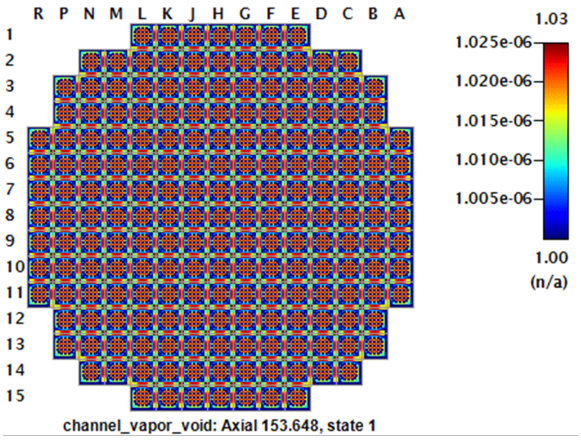


Figure 1: VERA simulation of reactor core void fraction distribution.

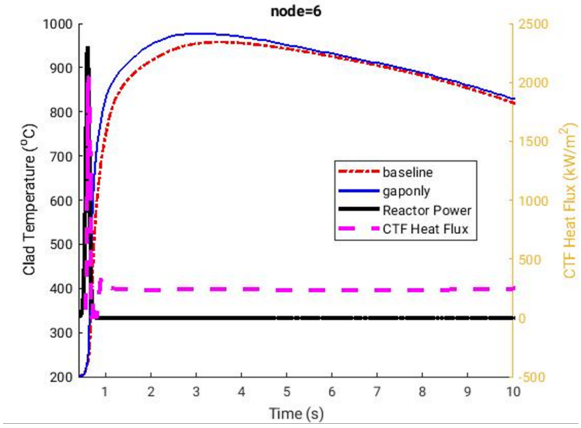


Figure 2: VERA simulation of fuel rod responses in a RIA scenario.

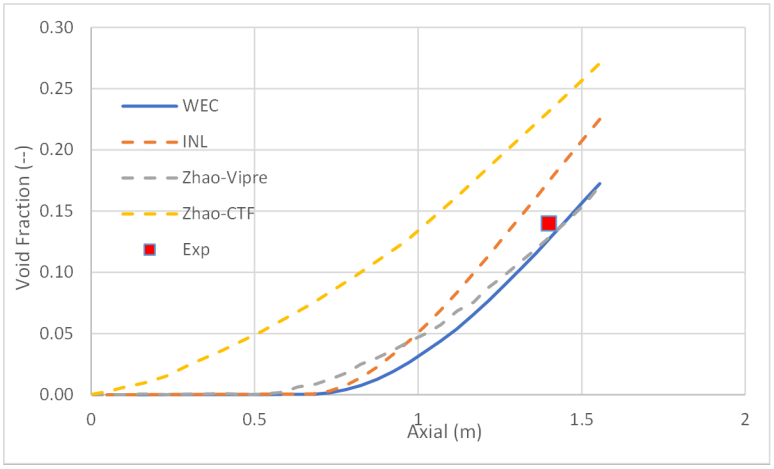


Figure 3: VERA simulation benchmark with PSBT test data.

B.145 Multiscale Multiphysics Modeling and Simulations of Advanced Nuclear Reactors

Report Participants

Hu, Rui [1], Zou, Ling [1], Yang, Gang [1], Ooi, Zhiee J[1], Mui, Travis [1], O'Grady, Daniel J[1]
1 Argonne National Laboratory

Scientific Achievement

The primary goal of this work was to develop a multiscale multiphysics modeling capability for analyzing advanced nuclear reactors. Simulating advanced nuclear reactors requires capturing the phenomena of several fields of physics, including reactor kinetics, thermal hydraulics, thermomechanics, fuel performance, etc. The models are simulated in BlueCRAB and its submodules, such as GRIFFIN, SAM, Pronghorn, and BISON. The GRIFFIN module is used to simulate the reactor kinetics behavior of the reactor; the SAM and Pronghorn modules are used to simulate the heat transport in the reactor core and heat removal through the primary loop and decay heat removal systems; and the BISON module is used to simulate the fuel performance and thermal mechanics of the reactor cores. The different submodels are coupled together using the MultiApp system in MOOSE. The BlueCRAB multiphysics modeling was demonstrated by performing a steady-state analysis and transient simulations of typical reactor design basis events.

Significance

For plant systems analyses and assessing the adequacy of the emergency core cooling features of a design, the NRC is developing a suite of codes called BlueCRAB. BlueCRAB is the coupled combination of NRC codes and codes developed by DOE under the NEAMS Program and is capable of simulating a broad range of conventional and advanced reactor designs. To prepare for independent analysis as part of the review and to demonstrate the capabilities of BlueCRAB, this work supported the NRC in developing reference plant models for various advanced reactor types. The purpose of a reference plant is to provide both a test bench for the BlueCRAB system and a means to identify potential modeling and simulation challenges before a design review is underway.

Key Publications

Gang Yang, Ling Zou, Joseph Kelly, and Rui Hu, Updated SAM Model of a Reference Fluoride-Salt-Cooled High-Temperature Reactor for Multi-Physics Simulations, ANL-NSE-23/17, March 2023. Gang Yang, Ling Zou, and Rui Hu, Updated SAM Model for the Molten Salt Reactor Experiment (MSRE), ANL-NSE-23/8, Feburary 2023 Hu, R; J. Fang, D. Nunez, M. Tano, G. Giudicelli, R. Salko, Development of Integrated Thermal Fluids Modeling Capability for MSRs, ANL/NSE-22/56, August 2022.

Sponsor/Program

DOE-NEAMS, NRC

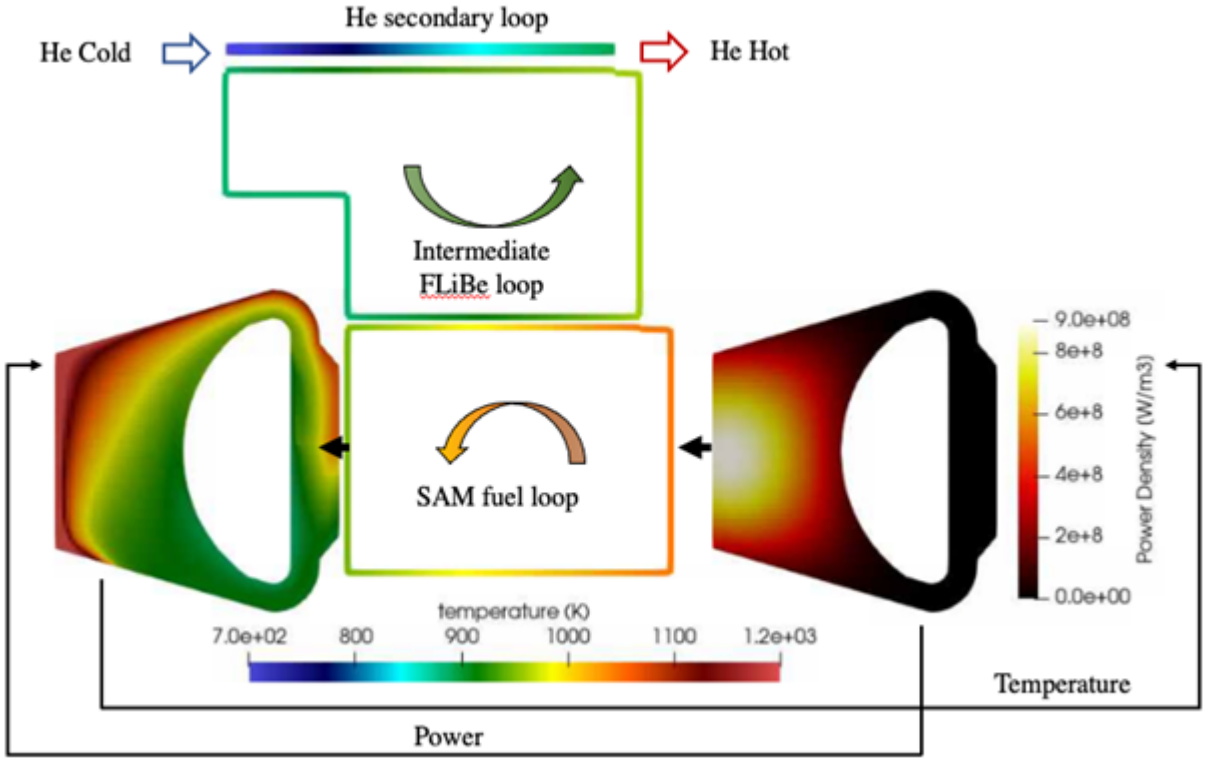


Figure 1: Steady-state results of coupled SAM-Pronghorn-Griffin of an MSR.

B.146 Molecular Dynamics Studies of the Effect of Chemical Ordering on Defect Formation Energies

Report Participants

Zhang, Yongfeng [1], Manzoor, Anus [2], Beeler, Benjamin W[3]
1 University of Wisconsin Madison
2 Idaho National Laboratory
3 North Carolina State University

Scientific Achievement

Using molecular dynamics simulations adopting the LAMMPS simulation package, the point defect formation energies in U-10Mo are computed with and without equilibrating the chemical ordering of Mo. The results from hybrid molecular dynamics and Monte Carlo simulations indicate that Mo atoms repel each other, exhibiting substantial short-range order (SRO). Such SRO improves the stability of the body-centered-cubic solid solution phase and increases the formation energies of vacancy, interstitial dumbbells, and Xe substitutionals. A large amount of data has been obtained to establish the probability distributions of the formation energies and to elucidate the dependence of the formation energies on local atomic environments.

Significance

The fundamental properties of point defects (i.e., vacancies and interstitials) govern the irradiation damage evolution and consequent property degradation in materials. The results here not only provide more accurate atomistic data for basic defect parameters to upper scale modeling but also indicate the critical importance of accounting for the impact of chemical ordering. The results and findings will be wrapped up for a journal publication in the short future. Following the current and previous work, we will revisit the diffusion properties of point defects and how they affect the elastic properties of U-10Mo.

Key Publications

1. Benjamin Beeler, James Cole, Gerald Hofman, ATM Jahid Hasan, Shenyang Hu, Curt Lavendar, Anus Manzoor, Zhi-Gang Mei, Aaron Oaks, Maria Okuniewski, Gyuchul Park, Aashique Rezwan, Kelley Verner, Abdellatif Yacout, Bei Ye, Yongfeng Zhang, Microstructural-Level Fuel Performance Modeling of U Mo Monolithic Fuel. September 2023, Idaho National Laboratory. 2. B. Beeler, Y. Zhang, The reconciliation and validation of a combined interatomic potential for the description of Xe in U-Mo, Front. Nucl. Eng. 2 (2023) 1185448.

Sponsor/Program

USHPRR.

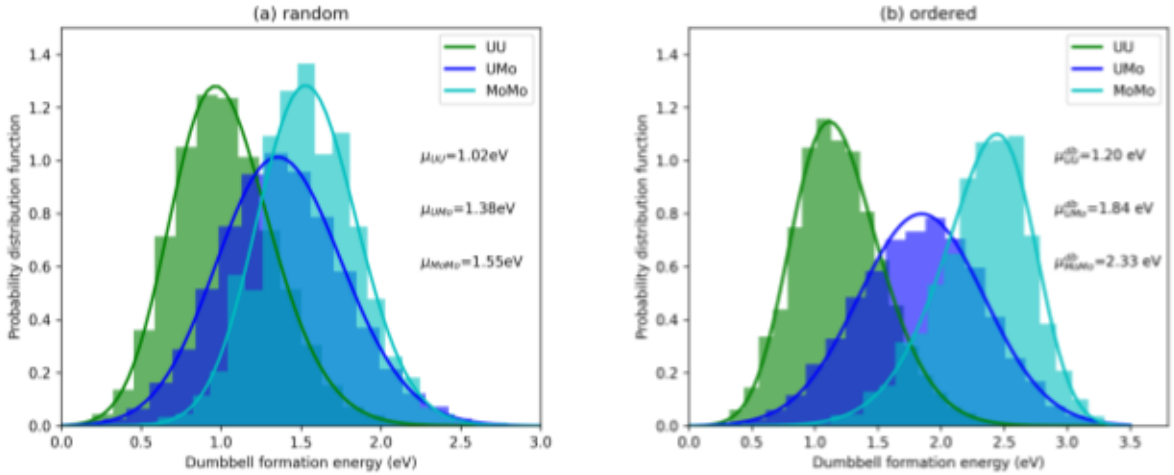


Figure 1: Distributions of interstitial dumbbell formation energies in the (a) random solid solution and (b) the SRO state at 300 K. Substantial increases can be seen in the formation energies of different dumbbells because of SRO.

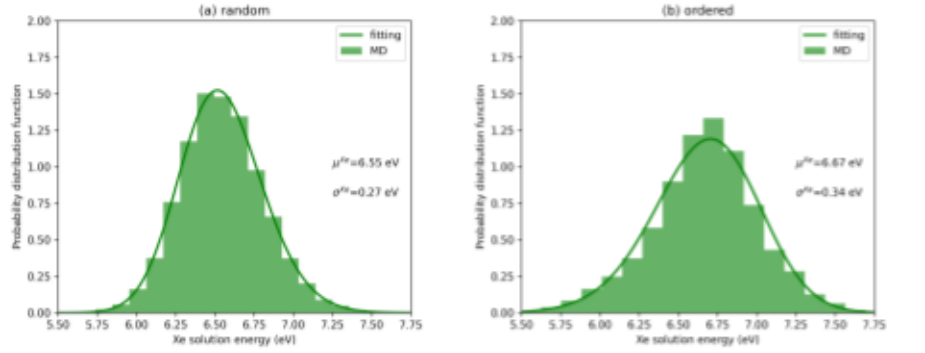


Figure 2: Distributions of Xe solution energies in the (a) random solid solution and (b) the SRO state at 300 K. There is a slight increase in the mean solution energy and a noticeable broadening of the distribution.

B.147 Computational Modeling of Damage and Plasticity in Multifractured Fault Zones with Fluid Injection

Report Participants

Zhao, Chunhui [1], Elbanna, Ahmed [1]
1 University of Illinois Urbana-Champaign

Scientific Achievement

This work examined understanding how ruptures propagate and interact within a multifractured fault zone. In this project, our focus is to mimic the process of fluid injection and characterize the spatial and temporal distribution of the resulting seismicity in the presence of obscene of pre-existing natural fractures. We will also incorporate models to quantify damage and plasticity within the fault zone. This serves as a continuation of our current exploration on simulating dynamic ruptures using cohesive zone models provided in the MOOSE framework within our newly developed MOOSE app: MOOSE FARMS.

Significance

This project serves to provide guidance from a theoretical and numerical perspective on injection-induced seismicity, which is commonly encountered in oil and gas operations, geothermal energy applications, and CO2 sequestration activities. We would like to systematically characterize how the pressure change due to the fluid injection affects the pre-existing faults or fault zones in the subsurface, how damage and plasticity evolve during the process, and how new fractures may nucleate, propagate, or get activated, to guide safe operations under realistic circumstances. We have been working on developing the code structure in the MOOSE framework and have achieved several milestones so far: 1. Verification of code implementation on a planar fault using the Southern California Earthquake Center Benchmark Problem TPV205, in both 2D and 3D versions, and we have presented the results during the meetings with Utah-Forge Project and FORGE Group. 2. Verification of code implementation to simulate a dynamic rupture on a fault with branch problems using Southern California Earthquake Center Benchmark Problem TPV14 (left-lateral sense of motion) and TPV15 (right-lateral sense of motion). Testing both cases was necessary to ensure the code's ability to simulate potential reversal in slip. 3. Implement a code framework to automatically generate a complex fault network. 4. Utilize the code capability to model and understand the 2023 Turkey-Syria earthquake, as an example of a destructive dynamic fracture on a geometrically complex fault network, focusing on identifying super-shear and sub-Rayleigh ruptures and comparing with the station records, characterizing the conditions that govern the rupture jumps between the fault segments and the relation between liquefaction and ground velocity profile.

Key Publications

Abdelmegrid, M., Zhao, C., AJ Rosakis & Elbanna, A. E. (n.d.). The Supershear Rupture that Triggered the Feb 6th 2023 Mw 7.8 Kahramanmara Turkey Earthquake: Evidence from Near-Field Records. (In Progress)

Sponsor/Program

Utah Forge Project

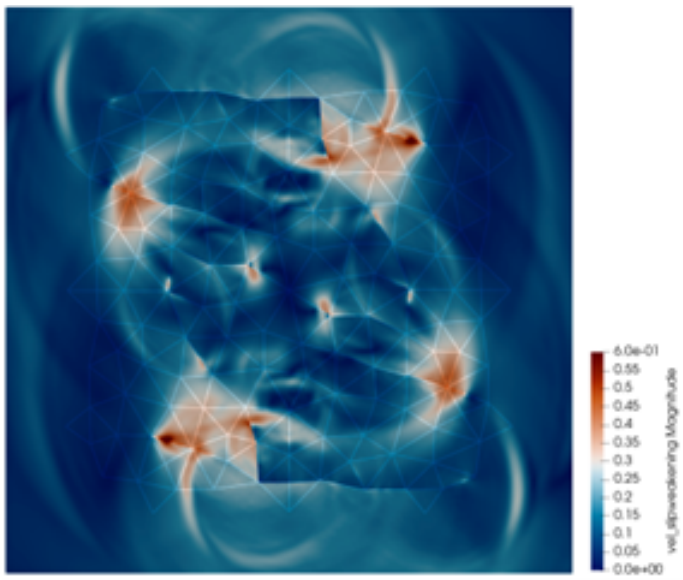


Figure 1: Velocity magnitude of overstressing multifault zones.

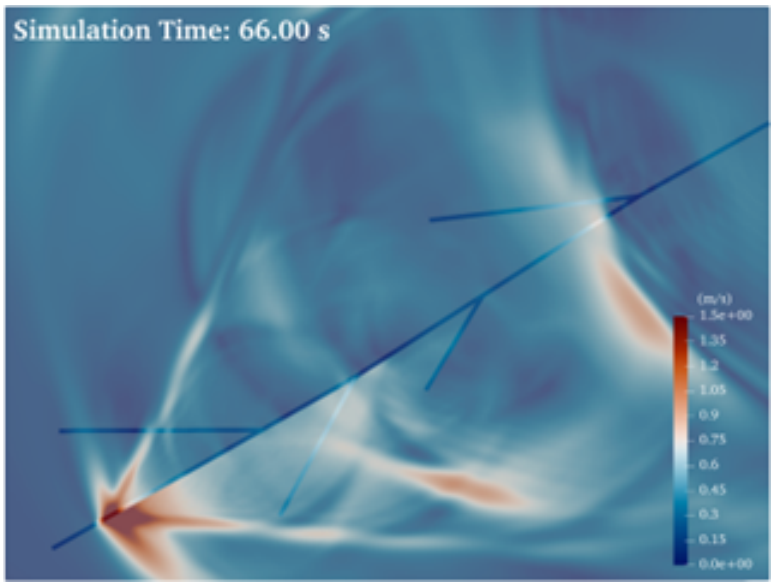


Figure 2: Velocity magnitude of supershear rupture on the south end of the 2023 Turkey-Syria Earthquake.

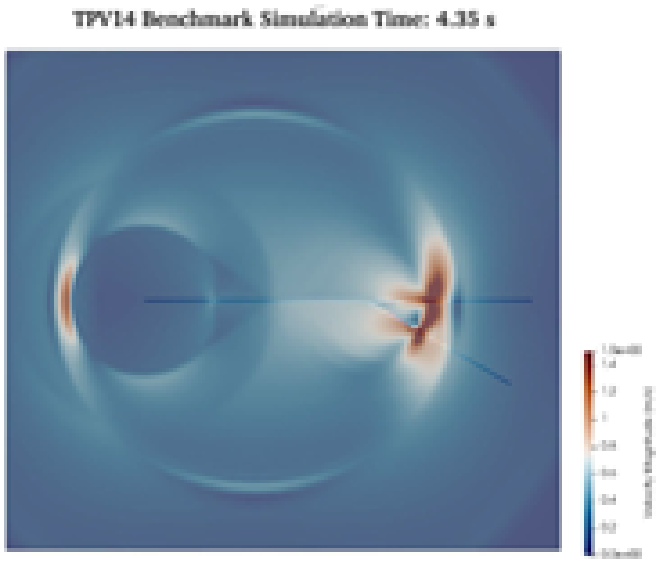


Figure 3: Velocity magnitude of Benchmark TPV 14

B.148 Effect of Heterogeneous Diffusivity on Gas Bubble Evolution in UO2: A Coupled 3D Xolotl-MARMOT Study

Report Participants

S. Chatterjee[1], S.Blondel[2], M. Muntaha [1], S. Biswas[3], L. Aagesen [3], M.Tonks [1]
1 Department of Materials Engineering, University of Florida
2 University of Tennessee
3 Idaho National Laboratory

Scientific Achievement

The gas bubble evolution in UO2 fuel rods at the mesoscale is important because it causes a swelling and degradation of fuel rods due to fission gas release. In this project, we investigated the behavior of intergranular and intragranular gas bubbles in 3D polycrystalline UO2 microstructures during in-reactor operations using a multiscale coupled Xolotl-MARMOT code, assuming heterogeneous chemical diffusivities. It should be noted that previous works have considered simple bi-crystal or hexagonal UO2 grain configurations to reduce computational costs. Specifically, we performed 10-grain and 100-grain simulations using the coupled code. The 10-grain simulation with 1.2 billion DOF required 578 cores on the Sawtooth cluster at INL. While the 100-grain simulation with 10 billion DOF required 9,600 cores. Further, these simulations were run for a simulation time of 12 and 3 days, respectively. In the future, we plan to execute similar runs for longer simulation times to capture the fission gas release during reactor operations realistically.

Significance

Based on the 10-grain simulations, we find that the assumption regarding the chemical diffusivities along the grain boundaries and bubble surface plays a significant role in intergranular bubble evolution. More specifically, for the case with heterogeneous gas diffusivity, we observe bubble coalescence in 12 days simulation time (Fig 1b) compared to the homogeneous diffusivity case (Fig 1c). Nevertheless, the computation time for the heterogeneous case was almost 12× that of the homogeneous case (Fig 1d). Despite the higher computational cost, it is only in the heterogeneous case that we find an intergranular bubble network through which fission gases vent out to the environment (Fig 2), as presumed in experiments.

Key Publications

Blondel et.al, 2022. "Coupled, 3-dimensional Xolotl – MARMOT simulations of fission gas evolution in UO2", Milestone report, MS-22CH0101092

Sponsor/Program

DOE-NE SciDAC

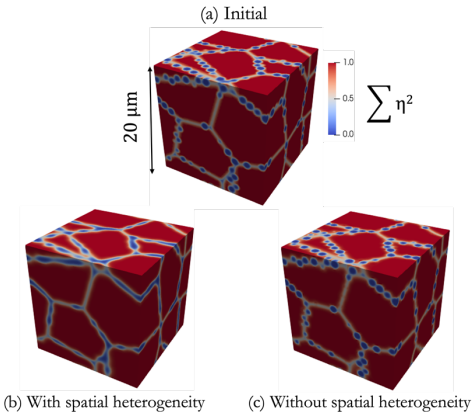
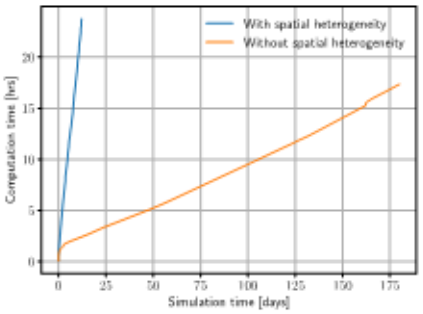


Figure 1: Bubble evolution in a 203 μm3 UO2 polycrystal with 10 grains and 600 initial intergranular bubbles. The initial microstructure is shown in (a), the simulation after 12 days with spatial heterogeneity in the Xe diffusivity is shown in (b), and the simulation after 180 days without spatial heterogeneity is shown in (c). (d) Computation time as a function of simulation time.



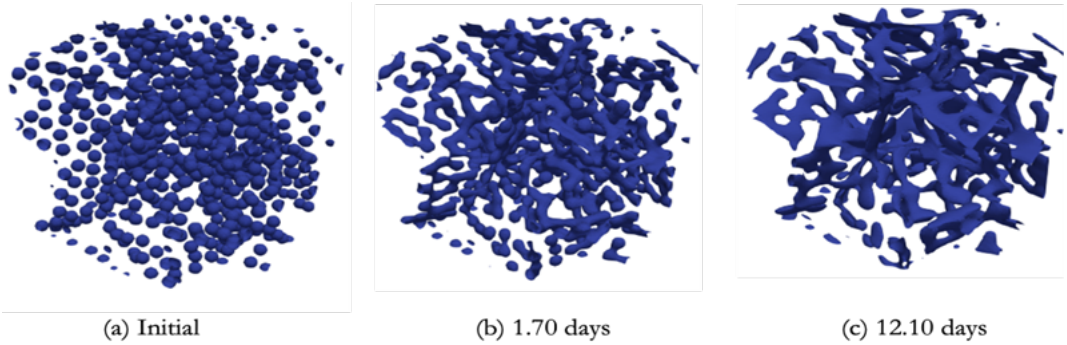


Figure 2: Intergranular gas bubble evolution for the 203 μm3 10-grain polycrystal with spatially heterogeneous diffusivities at the initial condition, t = 1.7 days, and 12.1 days in (a)–(c), respectively. However, the very short time reached in this coupled simulation precludes any meaningful analysis of the intragranular xenon clustering and bubble evolution.

B.149 Use of Nanocalorimetry to Measure Radiation Damage Annealing in Metals

Report Participants

Hirst, Charles A.[1]
1 Massachusetts Institute of Technology

Scientific Achievement

MD simulations have been used to anneal radiation damage in metals to investigate the energy release and power output from irradiated materials. The Creation-Relaxation Algorithm was used to create a defected supercell containing isolated Frenkel pairs, as an analogue to electron irradiation. These cells were annealed from 0.001 Tm to the melting point (Tm) over different durations, from 0.2 ns to 2 µs. The energy release as a function of time was differentiated to determine the power output associated with this microstructural evolution, as a function of heating rate.

Significance

The simulated power output was fit to a power law and extrapolated across 10 orders of magnitude in time to compare to prior literature. Remarkably, the results match within a factor of 2. This match between our atomistic simulations and historical calorimetry experiments demonstrates the ability to connect the modeling and characterisation of radiation damage through energy space. This has the potential to validate decades of damage cascade simulations and, inversely, to yield mechanistic insight into the evolution of defects at the nm-scale and below.

Key Publications

Hirst C. A., Connick, R. C., Cao P., Kemp R. S. & Short M. P. On the use of nanocalorimetry to measure radiation damage annealing in metals. (In progress)

The Minerals, Metals & Materials Society (TMS) – Talk, March 2023 Hirst C. A., Connick, R. C., Cao P., Kemp R. S. & Short M. P. Energy: a path forward to connect radiation damage simulations and experiments.

Sponsor/Program

LDRD “Moving beyond DPA: A new approach for rapidly quantifying radiation damage”

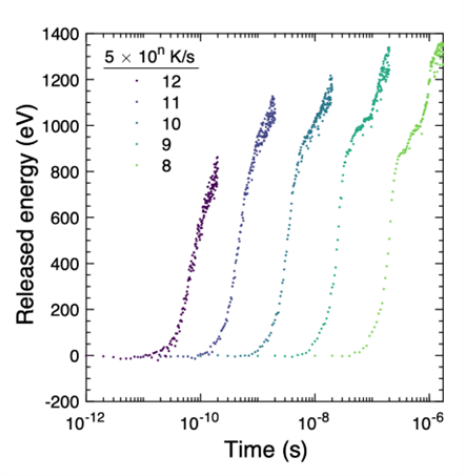


Figure 1: MD simulations determine the energy release associated with radiation damage annealing at different heating rates (K/s).

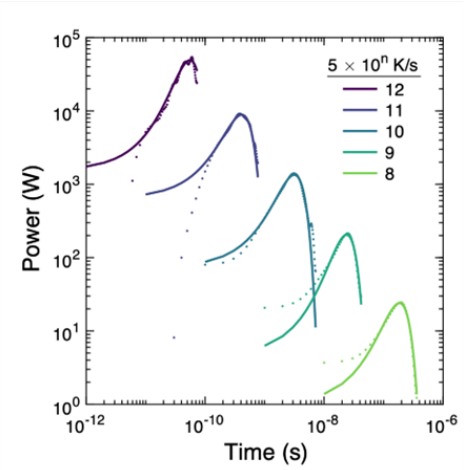


Figure 2: The energy release is differentiated to determine the power output associated with defect recovery.

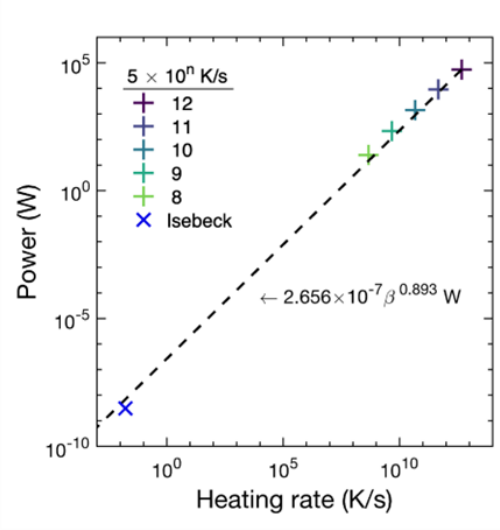


Figure 3: Simulated results are extrapolated to experimental heating rates, demonstrating an excellent match with prior experiments.

B.150 Heat-Pipe Reactor Code-Coupled Simulations

Report Participants

Durse, Megan E[1]
1 Westinghouse Electric Company

Scientific Achievement

The MOOSE toolset (BISON, Sockeye, and Griffin) is used for the code-coupled modeling and analysis of the Westinghouse eVinci heat-pipe reactor. Based on the code performance in the Meitner project, it may be decided to use these codes to perform modeling and simulation activities supporting the licensing application and process for the eVinci reactor.

Significance

An ability to perform code-coupled simulations of the eVinci heat-pipe reactor to show its performance in transients and inherent safety features is critical for building the first-of-its-kind reactor.

Key Publications

N/A

Sponsor/Program

Department of Energy, Los Alamos National Laboratory, Idaho National Laboratory, Argonne National Laboratory, US NRC, and any other United States or Canadian governmental agency to receive the findings as part of Westinghouse's licensing requirements.

B.151 Scalable Framework of Hybrid Modeling with Anticipatory Control Strategy for Autonomous Operation of Modular and Microreactors

Report Participants

Lin, Linyu [1], Oncken, Joseph E[1], Poudel, Bikash [1], Agarwal, Vivek [1], Gribok, Andrei [1], Boring, Ronald L[1], Permann, Cody J[1], McJunkin, Timothy R[1], Eggers, Shannon [1]
1 Idaho National Laboratory

Scientific Achievement

The purpose of this research is to develop and validate a scalable autonomous control system for microreactors that uses hybrid modeling (physics-based and artificial intelligence techniques) and anticipatory control techniques. Such capabilities will enable emerging microreactors to safely regulate their operations, take optimized control actions in a (semi-)autonomous manner, aid operators, and proactively protect against potential anomalies. Figure 1 shows the configurations of the anticipatory control system, which is connected with a 37 heat pipe (HP) system simulated by MOOSE-based tools. Through numerical study, this work validates the controller's performance in achieving target transients for temperatures and heat fluxes. Figure 2 shows the performance of an MPC with different data-driven approaches in achieving the target reference trajectory. Overall, though a sparse identification of nonlinear dynamics with control (SINDYc) based MPC produces stabler and more accurate validation results, the inherent variance of NN models produces higher change speeds in their control actions, and the MPCs based on feedforward and recurrent neural networks are better able to track any drastic setpoint changes. Figure 3 compares the performance of the SINDYc- and LSTM-based MPCs in tracking power reference trajectories with different final setpoints and ramping speeds. LSTM is one class of recurrent neural network, which deals with the vanishing gradient problem better than other types of recurrent networks. Overall, the LSTM-based MPC is more fluctuated than the SINDYc-based MPC, especially when the ramping speeds are high. However, such fluctuations better adapt the system to fast transients. This is consistent with the observations made in the temperature control scenario. This work also investigates the event of a system anomaly, such as an HP failure. The control system needs to be capable of controlling the reactor in the degraded state. A detection module was built into the MPC to detect HP failure and, should a failure be detected, to adapt the predictor model within the controller accordingly. The dual HP failure phase begins at t = 500 with the failure of HP C. Two primary benefits of the adaptive MPC (A-MPC) control are observed during this phase. The first benefit once again involves accurate reference tracking. When the reference power output level drops at t = 600, the non-adaptive MPC controller is incapable of following the reference power output trajectory despite that trajectory being within the performance envelope of the system even in the failed HP state. However, as was the case with a single HP failure, the A-MPC controller accurately tracks the reference trajectory from t = 600:900. This behavior can be seen in Figure 6. The second benefit is constraint adherence. At t = 1,060, the non-adaptive MPC controller allows the evaporator temperature of HP B to significantly overshoot, 1330 K, above the upper constraint value of 1200 K, as shown in Figure 4. In contrast, the A-MPC controller does not produce this overshoot behavior and maintains an HP B evaporator temperature within the higher limits.

Significance

This research develops and assesses an MPC system to enable the anticipatory control strategy for an HP microreactor simulated by MOOSE-based tools. Such capabilities will enable emerging microreactors to safely regulate their operations, take optimized control actions in a (semi-)autonomous manner, aid operators, and proactively protect against potential anomalies. These capabilities will enable emerging reactors to safely regulate their operations, take optimized control actions in a semiautonomous manner (or autonomous, in the case of microreactors), aid operators, and proactively protect against potential disturbances. The overall outcomes of this research will provide an enhanced understanding (not readily achievable otherwise) of how the plant or system of interest must be able to respond to fluctuating loads and adapt to various operating conditions with minimal (or no) human intervention, aid in our understanding of the role of plant operators engaging in semiautonomous or remote operations, and offer a solid argument for reducing the conservatism associated with building and operating reactors.

Key Publications

" L. Lin, J. Oncken, and V. Agarwal, 2023, Anticipatory control strategy for autonomous operation of heat-pipe microreactor , in preparation, Annals of Nuclear Energy " J. Oncken, L. Lin, V. Agarwal, 2023, Adaptive model predictive control for heat-pipe cooled microreactors under normal and heat pipe failure conditions , in preparation, Nuclear Technology. " L. Lin, J. Oncken, V. Agarwal, 2023, Data-Driven Model Predictive Control for Temperature Management of Heat Pipe Microreactor , NPIC/HMIT, Knoxville, TN. " L. Lin, Benjamin Zastrow, J. Oncken, V. Agarwal, 2023, Adaptive Data-Driven Model Predictive Control for Heat Pipe Microreactors , NPIC/HMIT, Knoxville, TN. " J. Oncken, L. Lin, V. Agarwal, 2023, Adaptive Model Predictive Control for Heat-Pipe cooled Microreactors under Normal and Heat Pipe Failure Conditions , NPIC/HMIT, Knoxville, TN. " B. Poudel, L. Lin, T. Phillips, S. Eggers, V. Agarwal, T. McJunkin, 2022, Operational Resilience of Nuclear-Renewable Integrated-Energy Microgrids , Energies, 15(3), pp.789. " L. Lin, J. Oncken, V. Agarwal, C. Permann, A. Gribok, T. McJunkin, S. Eggers, and R. Boring, 2022, Development and assessment of a model predictive controller enabling anticipatory control strategies for a heat-pipe system (under review) , Progress in Nuclear Energy. " L. Lin, J. Lee, B. Poudel, T. McJunkin, N. Dinh, V. Agarwal, 2021, Enhancing the Operational Resilience of Advanced Reactors with Digital Twins by Recurrent Neural Networks , ResilienceWeek2021, Virtual

Sponsor/Program

INL LDRD Program

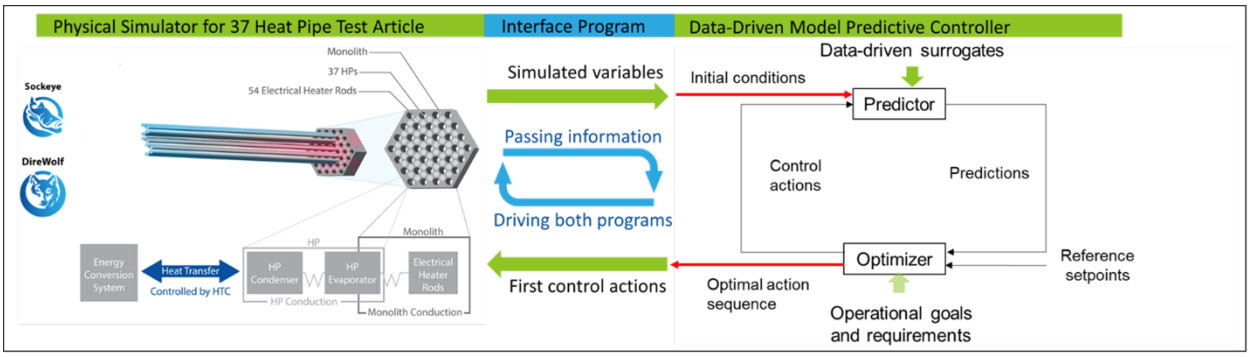


Figure 1: Schematic configurations for the anticipatory control system coupled with a 37 HP system with monolith block.

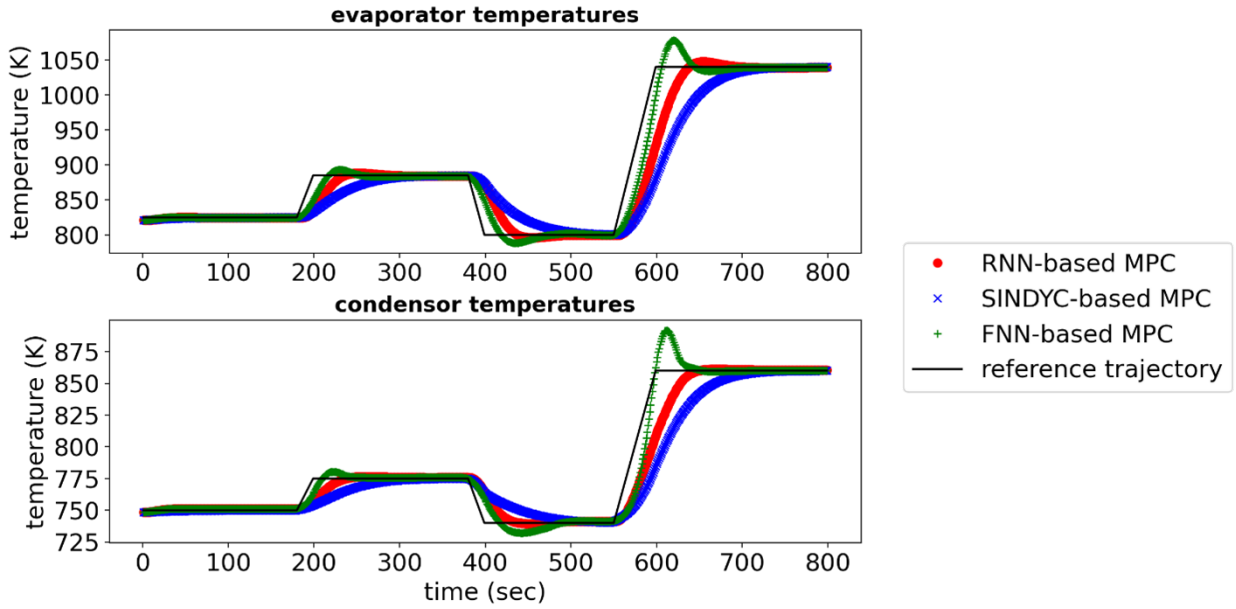


Figure 2: Performance of the FNN-, LSTM-, and SINDYc-based MPCs in tracking the reference temperature setpoints of the central HP evaporator and condenser.

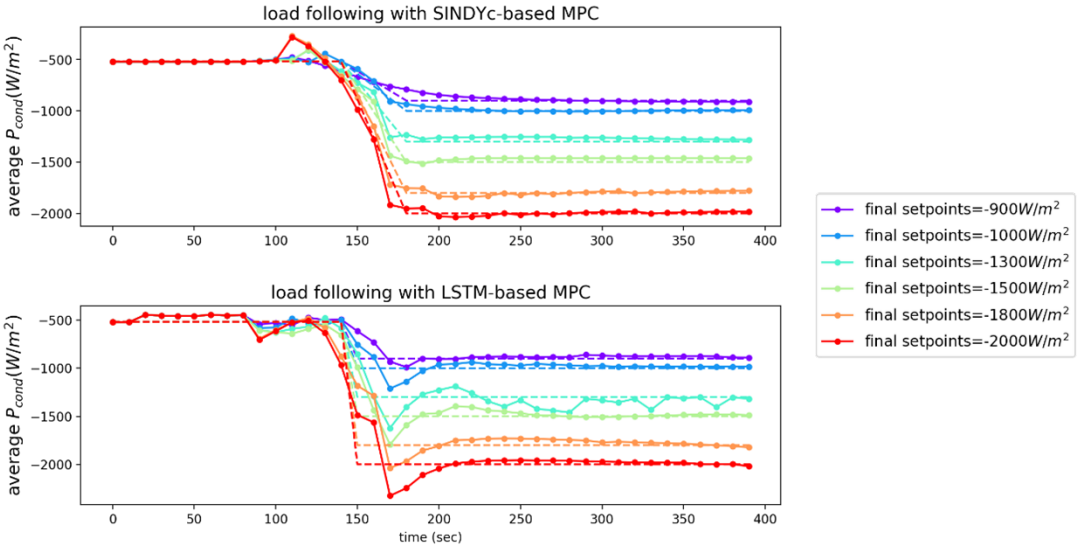


Figure 3: Comparison between the SINDYc- and LSTM-based MPCs in regard to tracking reference trajectories with different final setpoints and ramping speeds. Load following with SINDYc- and LSTM-based MPCs, with different magnitudes of final setpoints.

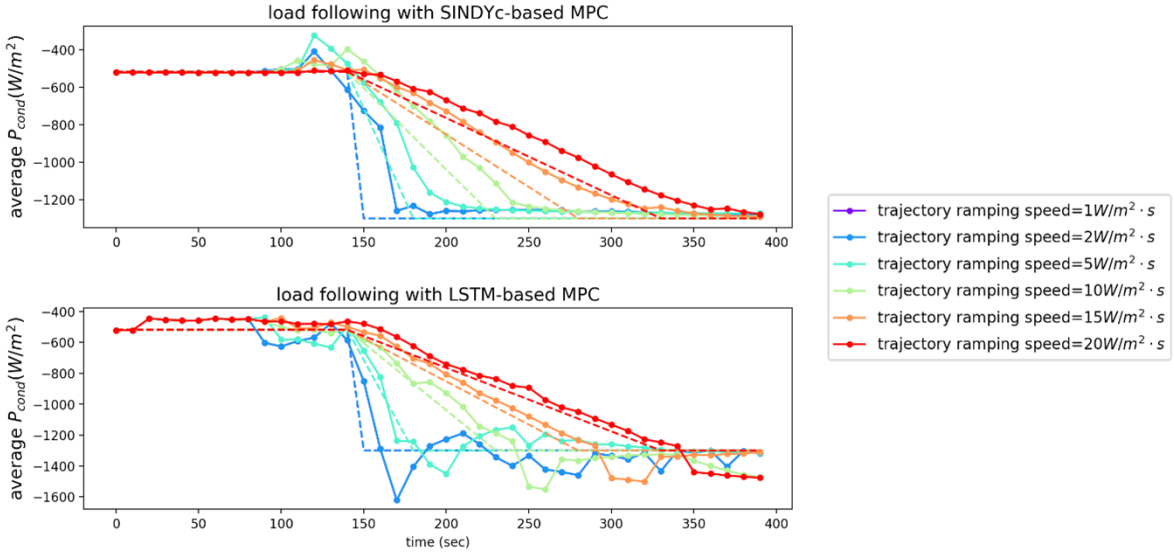


Figure 4: Load following with SINDYc- and LSTM-based MPCs, with different magnitudes of final setpoints.

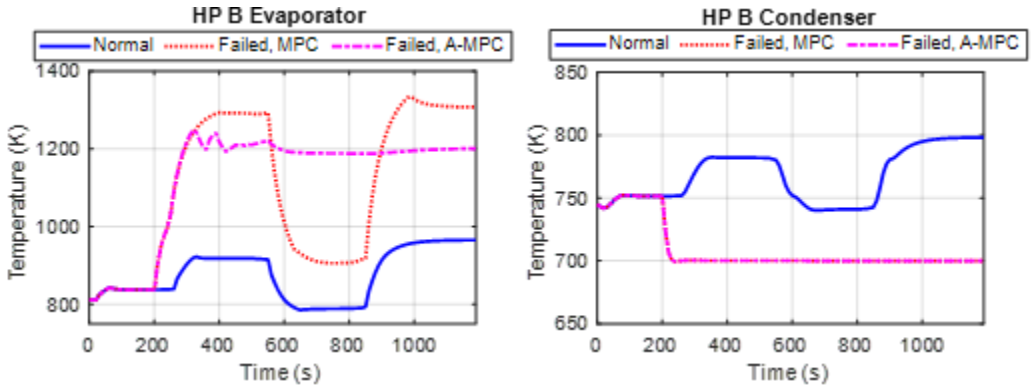


Figure 5: HP B temperature under HP B and C failure conditions.

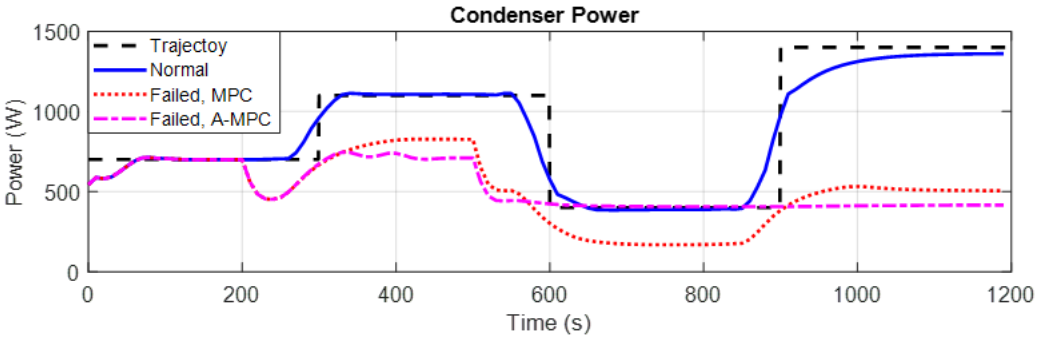


Figure 6: Average HP condenser power output under HP B and C failure conditions.

B.152 Kairos Power—INL BISON Usage and Collaboration

Report Participants

Hackelton, Jonathan [1], Novascone, Stephen [2], Permann, Cody [2]
1 Kairos Power
2 Idaho National Laboratory

Scientific Achievement

Kairos Power (KP) is an industry user, collaborator, and developer of BISON, Grizzly, and SAM MOOSE-based codes. That being said, access to the INL HPC is required to update and contribute to the codes through GitLab. INL resources may be used for collaborative research and publications.

Significance

KP is the first industry user to use MOOSE-based tools in a regulatory manner, meaning results from the simulations using these tools will be sent to the NRC for safety and building approval.

Key Publications

None

Sponsor/Program

KP – INL work is funded by multiple mechanisms including: NEAMS, KP FOA, IRP

B.153 Development and Integration of a Stochastic Clad Damage Propagation Model into Pronghorn-SC Subchannel Analysis Code

Report Participants

Karahan, Aydin [1], Tano, Mauricio [2], Kyriakopoulos, Vasileios [2], Yang, Gang [1]
1 Argonne National Laboratory
1 Idaho National Laboratory

Scientific Achievement

The project aims at implementing a stochastic clad damage propagation model into Pronghorn-SC, which is a MOOSE-based subchannel analysis program. The resulting implementation will allow users to model fuel failures due to creep rupture in a probabilistic manner, accounting for operational, manufacturing, and modeling uncertainties. Furthermore, the model will simulate the possible propagation of the stochastic failures in various design basis and beyond design basis scenarios.

Significance

Modeling fuel failures is a key concept that advanced reactor designs have to demonstrate to license their reactor design. Fuel failures lead to radioactivity release. Quantifying the fuel failures and tracking post-failure and its effects could be very attractive for vendors to optimize their design and demonstrate the safety of advanced reactor designs.

Key Publications

None

Sponsor/Program

NEAMS

Appendix C Security

Table of Contents

C.1 Use of HPC for Classifying Radio Frequency Signals

Report Participants

Reese, Randall D[1], Quach, Anna T[1]
1 Idaho National Laboratory

Scientific Achievement

We built a collection of machine learning models for classifying radio frequency (RF) signals related to the locomotive industry. These models were based on the You Only Look Once (YOLO) object detection framework. Implementation was in Python. Model training took place on the HPC using Hoodoo.

Significance

Benefit to sponsor was a collection of machine learning models they can use to secure their signal environment and detect unwanted RF traffic in bands of need.

Key Publications

None

Sponsor/Program

Department of Homeland Security, WhiteFox Corporation

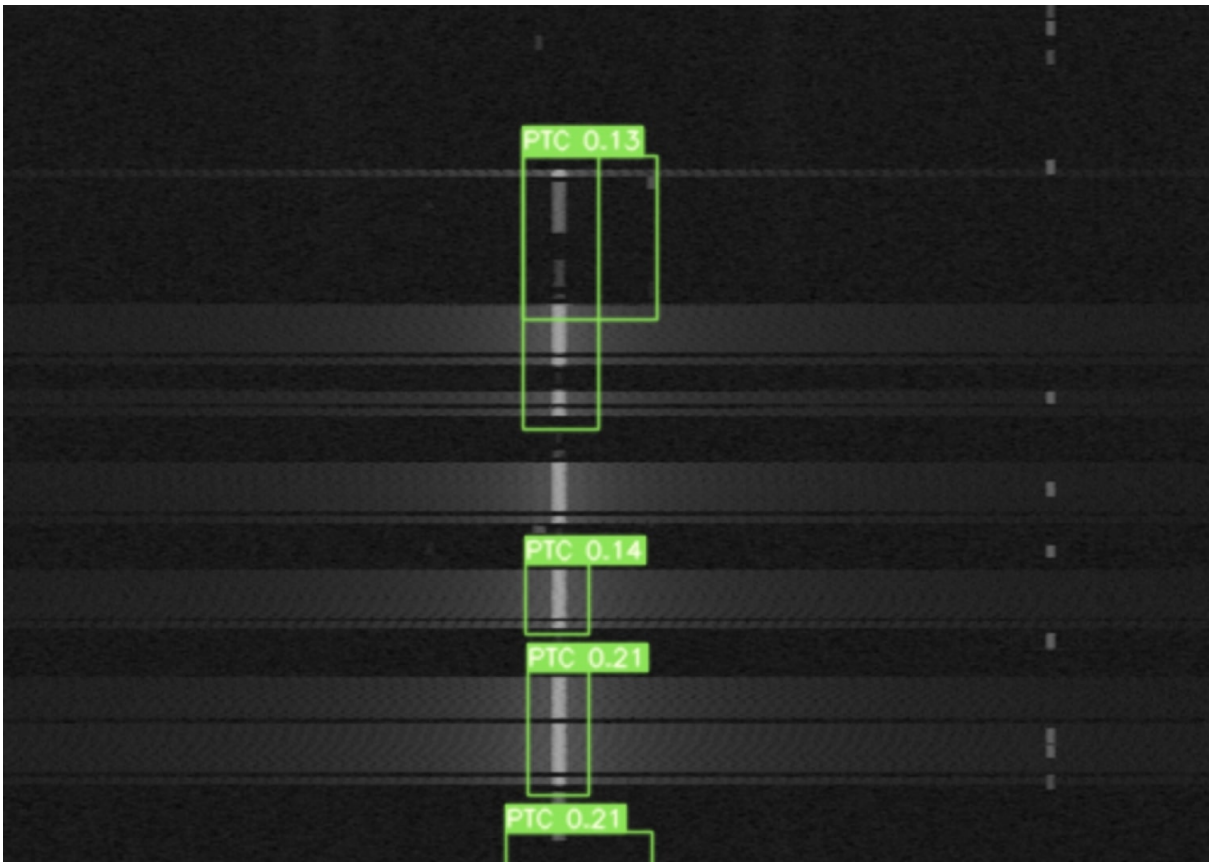


Figure 1: Identification of positive train control and narrow band FM RF signals.

C.2 Summer Project Summary

Report Participants

Martin, Candan [1]
1 Idaho National Laboratory

Scientific Achievement

The primary objective of this adapted project is to employ data labeling, log file merging, and data visualization techniques to extract meaningful insights. These insights are intended to facilitate the development of an advanced machine learning model utilizing supervised learning. The model's overarching goal remains unchanged: to enhance network visibility, streamline system identification, and strengthen cybersecurity measures, all within the context of identifying IT and OT systems in a network environment. This work used Python.

Significance

This adaptation remains impactful, addressing the intricate challenges posed by the coexistence of IT and OT systems. The importance of precise system identification and categorization remains paramount. Neglecting this challenge could result in suboptimal network operations, compromised security strategies, and an insufficient ability to effectively protect critical assets. By embracing supervised learning and data-driven insights, the project aims to enhance network dynamics and fortify security measures.

Key Publications

None

Sponsor/Program

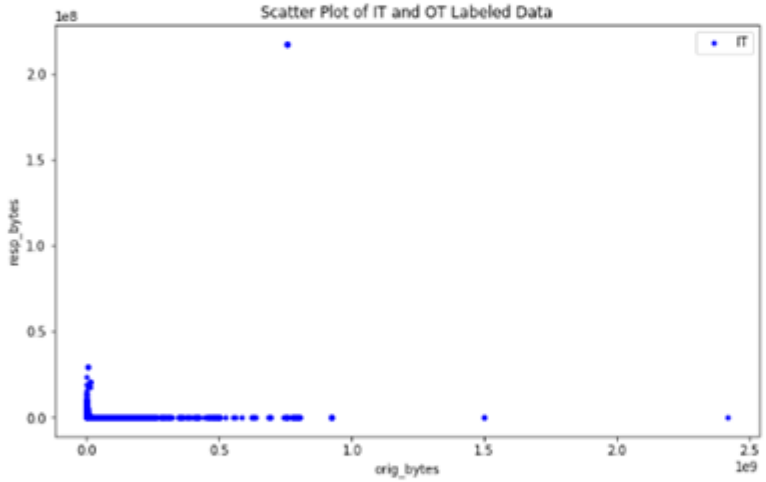
Cyber Sentry

```
16]: # Step 1: Plotting IT and OT labeled data with different colors
plt.figure(figsize=(10, 6))
plt.scatter(df[df['IT_Label_Origin'] == 1]['orig_bytes'], df[df['IT_Label_Origin'] == 1]['resp_bytes'], c='blue', label='IT', s=10)
plt.xlabel('orig_bytes')
plt.ylabel('resp_bytes')
plt.legend()
plt.title('Scatter Plot of IT and OT Labeled Data')

# Set the x and y-axis limits to zoom into the data
xmin, xmax = 0, 1e9   # Adjust the range according to your data
ymin, ymax = 0, 1e9   # Adjust the range according to your data

# Plot the data using DataFrame.plot() with specified x and y limits
df.plot(x='orig_bytes', y='resp_bytes', xlim=[xmin, xmax], ylim=[ymin, ymax])

plt.show()
plt.show()
```



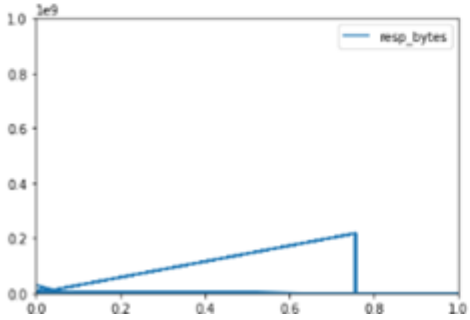


Figure 1: 2D plot visualizing distribution of resp and orig bytes.

C.3 Target-Aware Fuzzing

Report Participants

Ivans, Robert C[1], Koffi, Koffi A[2], McCarty, Michael V[1], Kolias, Constantinos [2]
1 Idaho National Laboratory
2 University of Idaho

Scientific Achievement

The goal of this project is to introduce novel fuzzing techniques that lead to the discovery of more bugs in less time, particularly for software supporting industrial control systems. Angr was used to perform symbolic execution on a user-provided binary program and automated the process of reconstructing the control flow graph (CFG) of the program as well as the extraction of path constraints. To minimize the path explosion problem, paths were prioritized that targeted basic blocks of interest, based on the user-provided target functions. In other words, unlike de facto fuzzing tools like AFL, this work provides a mechanism to govern the fuzzing process and force it to converge to specific paths according to human experience and intuition. The main issue with this approach is that Angr cannot interpret some instructions for certain platforms. This generates the issue of a partial reconstruction of the CFG for a given number of programs. Without a complete CFG, the exploration strategy will fail to converge to some solutions. Regardless, for basic CFGs like those expected to be found in industrial control system applications (e.g., ones with a shallow branch depth), an increase in speed of several orders of magnitude over AFL was observed. Figure 1 depicts a log plot of the speedup of the proposed technique over AFL. Moreover, the speedup was consistent across several programs with different characteristics, including a variety of branch depth, branch width, branch condition complexity, and the number of vulnerable functions considered. Figure 2 depicts a log box plot demonstrating the massive consistent speedup across several programs with different characteristics.

Significance

Finding bugs in software in an automated fashion is key to shining light on zero-day vulnerabilities and writing patches for them. Fuzzing is the best method available for finding bugs and vulnerabilities. The ultimate goal is to find bugs and vulnerabilities before bad actors do, so they can be patched before they get exploited.

Key Publications

Koffi Anderson Koffi Efficient Seed Generation for Expert-based Directed Fuzzing , April 2023

Koffi Anderson Koffi, Constantinos Kolias, Jia Song, Robert C. Ivans, Michael Cutshaw Terror from the Deep: A Guided Depth-First Software Fuzzing Approach. (Under Submission, MDPI Future Internet)

Koffi Anderson Koffi, Constantinos Kolias, Rajiv, Robert C. Ivans, Michael Cutshaw Fuzzing Visualizing and Interaction based on Workload Flows (Under Submission, MDPI Sensors)

Sponsor/Program

Idaho National Laboratory

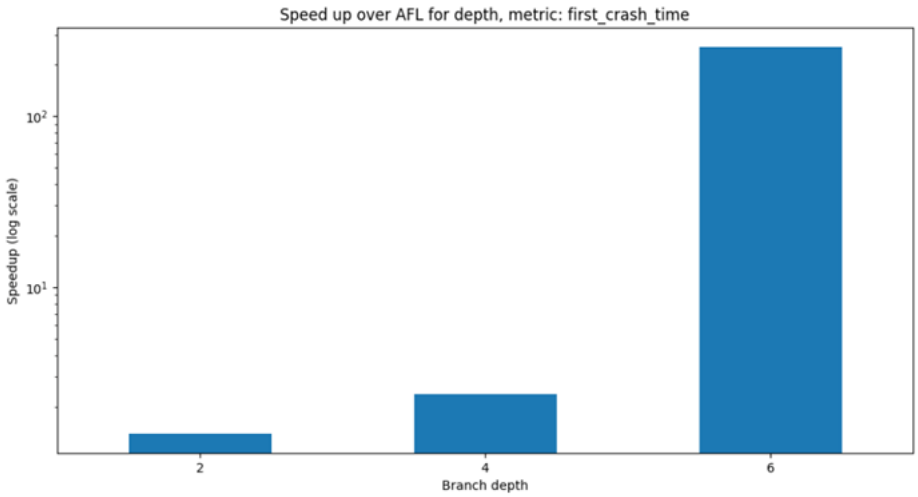


Figure 1: Speedup of our approach over AFL versus nested branch depth.

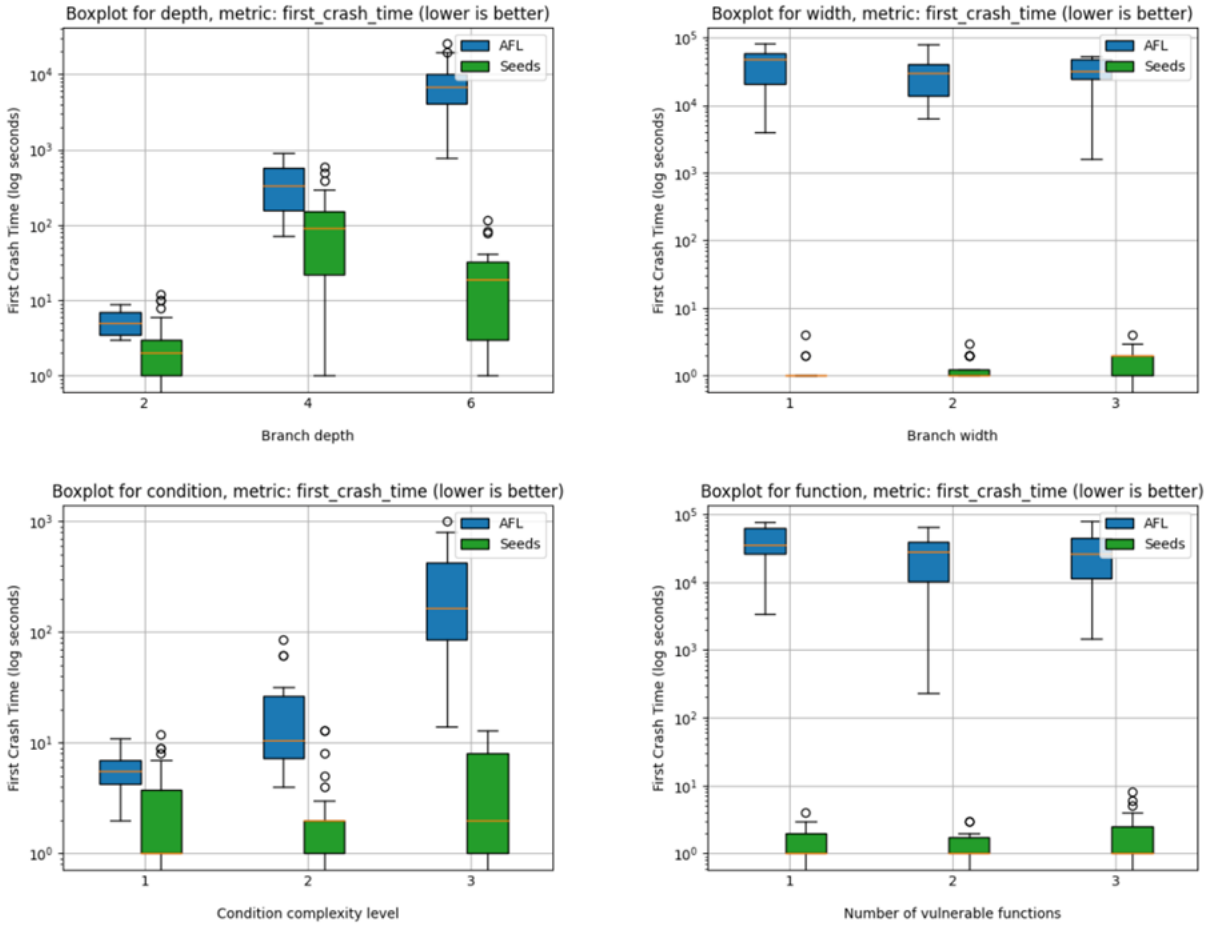


Figure 2: Log box plots of our preliminary experimental results.

C.4 Thermal Safety and Programmatic Analyses of the MP-2 and MURR-DDE Experiments in the Advanced Test Reactor

Report Participants

Hawkes, Grant L[1], Fishler, Joshua D[1]
1 Idaho National Laboratory

Scientific Achievement

Thermal safety and thermal programmatic analyses have been performed for the United States High Performance Research Reactor experiments known as Miniplate 2 (MP-2) and Missouri University Research Reactor Design and Demonstration Element (MURR-DDE) irradiated in the Advanced Test Reactor (ATR). Six irradiation positions are used for the MP-2 experiment, while a flux trap is used for the MURR-DDE experiment. The tests are fueled experiments designed for irradiation in multiple test locations in ATR and are considered noninstrumented drop-in tests where aluminum-clad fuel plates are cooled directly by the ATR primary coolant system water. These fueled experiments contain aluminum-clad fuel miniplates consisting of monolithic U-10Mo. A thermal safety evaluation was performed to demonstrate that the experiments comply with the thermal-hydraulic safety requirements of the ATR safety analysis report. Calculations showing safety margins to critical heat flux and flow instability are met considering a reactivity insertion accident, loss-of-coolant accident, and free convection cooling in the reactor and natural convection horizontal in water and air. Calculations were also performed for cladding oxide growth and its effect on peak fuel temperature. The ABAQUS finite-element structural analysis and heat transfer code from Dassault Systemes was used. The RELAP5 code was used for the flow calculations.

Significance

All thermal safety and thermal programmatic requirements for these experiments to be irradiated in ATR have been met. Departure from nucleate boiling ratio (DNBR) and flow instability ratio are required to be above 2.0 for all transient and steady-state events analyzed. The limiting scenario was found to be the reactivity insertion accident condition 2 (RIA2) for the minimum DNBR and flow instability ratio. The oxide growth was predicted with the ATR-modified Griess correlation and conservatively predicts the oxide growth during irradiation as a function of time and cladding surface temperature. The amount of oxide grown during simulations does not cause the fuel plate to be insulated to the point that the inner fuel temperatures exceed the blister threshold temperature.

Key Publications

G. L. Hawkes, D. Choe, M. Marshall, Thermal Safety/Programmatic Results for the MP-2 B 11 EXPERIMENT IN ATR, paper # 42204, INL/CON-23-72962, 2023 ANS Annual Meeting, Indianapolis, IN, Jun 11-14, 2023.

G. L. Hawkes, D. O. Choe, Thermal Model for Horizontal in-water and in-air Mini-pate Experiments in the Advanced Test Reactor, paper # 37019, INL/CON-21-63340-Rev000, 2021 ANS Winter Meeting and Technology Expo, Washington DC, Nov 30, Dec 3, 2021.

G. L. Hawkes, Thermal Safety margin Calculation of the MP-2 Experiment in the Advanced Test

Reactor, paper # ICONE28-POWER2020-16592, INL/CON-20-57467, ASME ICONE28-POWER2020 Conference, Anaheim, CA, Aug 3-6, 2020.

G. L. Hawkes, D. O. Choe, Thermal Model of Oxide Growth in Mini Plate Experiments in the Advanced Test Reactor, paper # 29034, INL/CON-19-52463, ANS Annual Meeting, Minneapolis, MN, Jun 9-13, 2019.

Sponsor/Program

United States High Performance Research Reactor

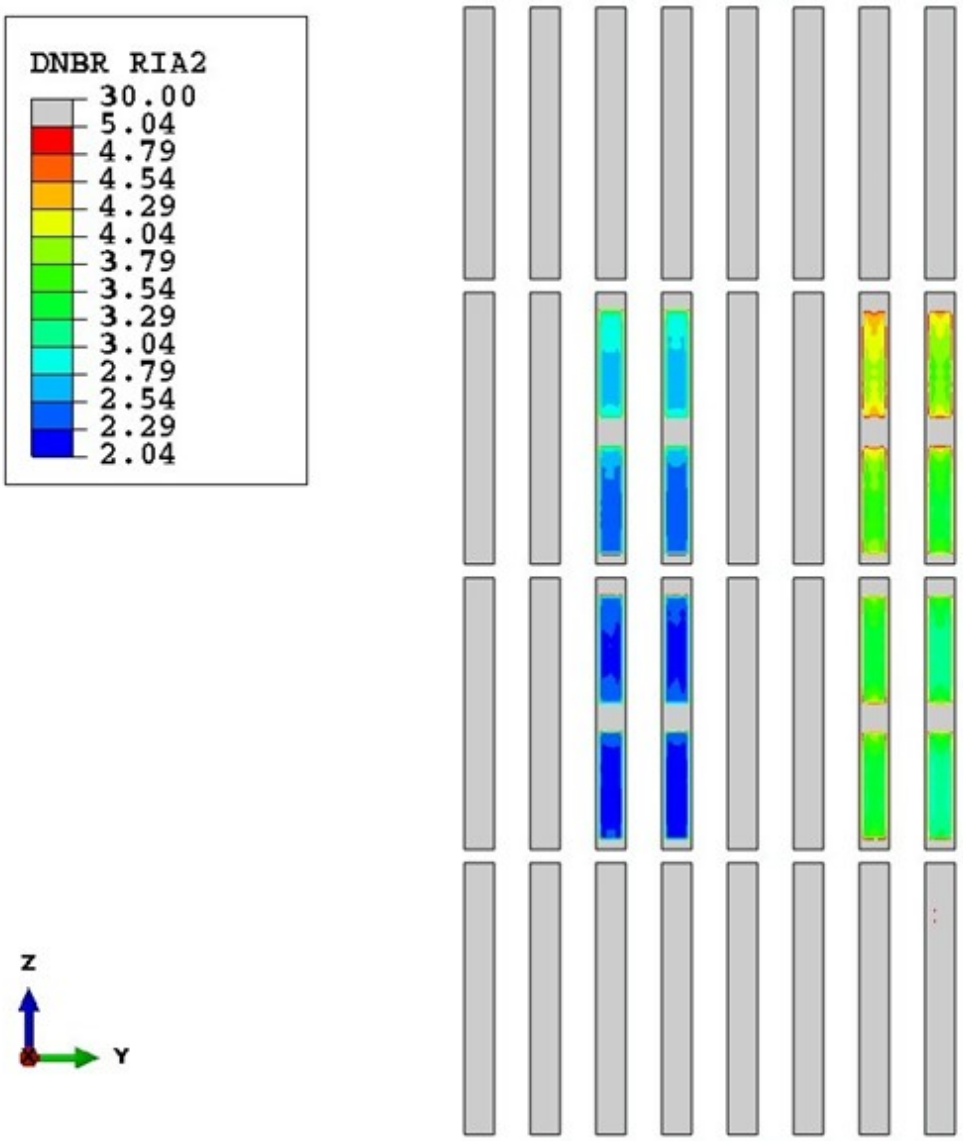


Figure 1: MP-2 minimum DNBR on plate surfaces during RIA2 transient.

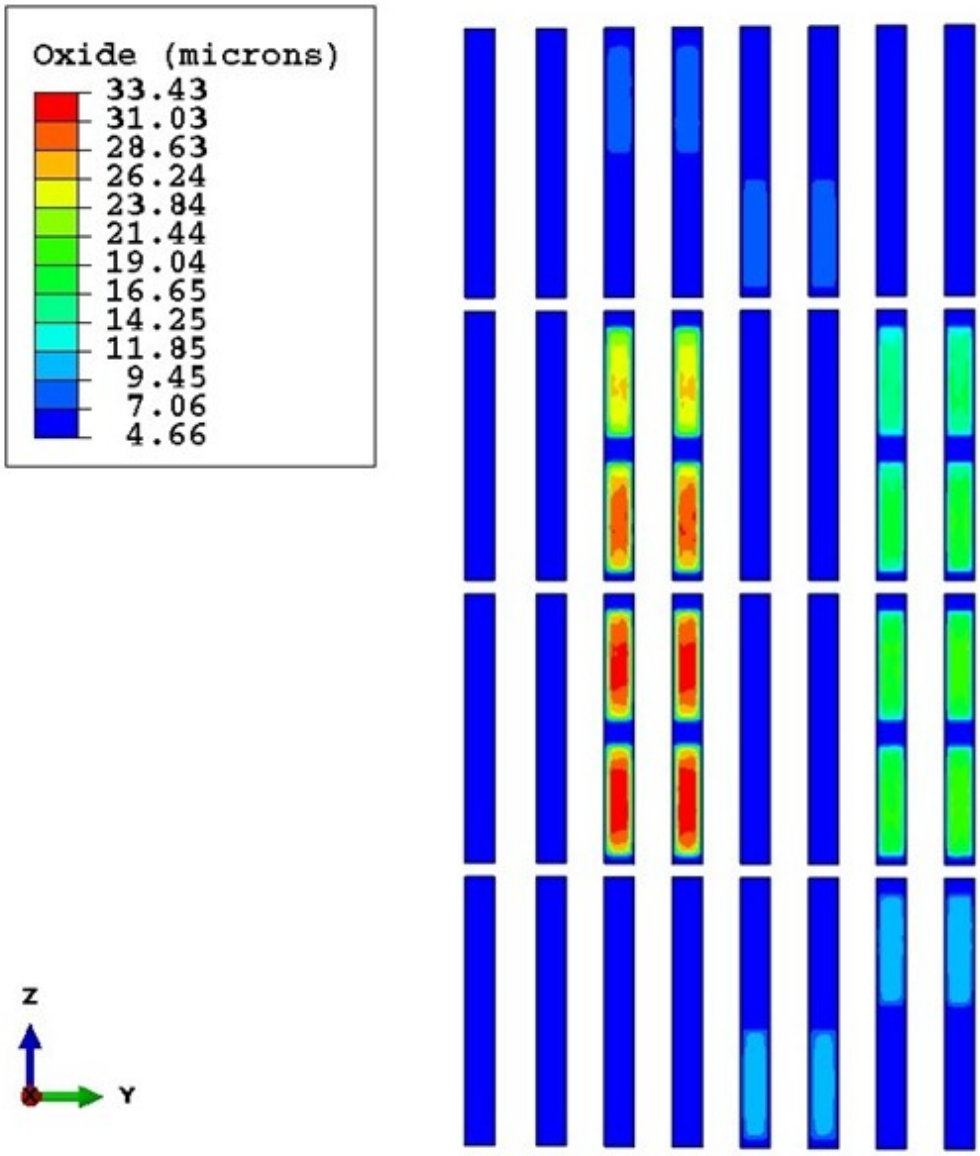


Figure 2: Oxide growth (microns) on MP-2 plates at end of irradiation.

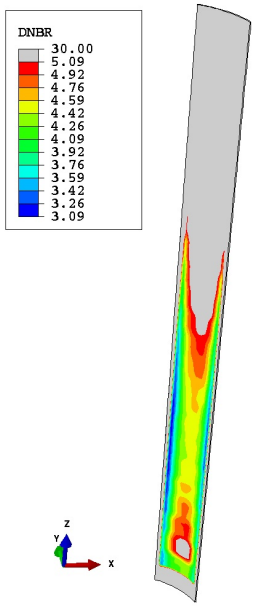


Figure 3: MURR-DDE Plate 4 minimum DNBR during RIA2 transient.

Appendix D Renewable Energy

Table of Contents

D.1 Particle Size and Shape Effect of Crumbler Rotary Shear-Milled Granular Woody Biomass on the Performance of Acrison Screw Feeder: A Computational and Experimental Investigation

Report Participants

Hamed, Ahmed [1], Xia, Yidong [1]
1 Idaho National Laboratory

Scientific Achievement

In this project, Idaho National Laboratory (INL) researchers worked with collaborators from Forest Concepts Inc. to evaluate particle characteristics and operation parameter effects on screw feeding performance for rotary shear-milled Douglas fir by conducting physical experiments and discrete element model (DEM) simulations. For the lignocellulosic biomass, identifying underlying mechanisms controlling its mechanical behavior and determining influential parameters is crucial for optimizing preprocessing and handling unit operations. DEM simulations were utilized to predict the measured AOR values based on the measured material attributes of the biomass. The woody biomass was size-reduced using the Forest Concepts rotary shear mill and tested using a pilot-scale handling unit, the Acrison screw feeder system, consisting of a hopper, an agitator, and a screw conveyor. Three performance metrics are used: mass flow rate, shaft driving torque, and specific energy consumption. The impact of particle size, particle size distribution (PSD), shaft rotational speed (rpm), and hopper dimensions on the performance are investigated. All employed performance metrics revealed the superior flowability of the 2 mm particles in contrast to the larger 6 mm counterpart. Remarkably, a wider PSD resulted in poorer flowability than the two monosize particles, proving the flowability enhancement achieved by a narrower PSD of the woody feedstock. More importantly, DEM simulations unveiled PSD-induced degradation in flowability is attributed to mechanical interlocking and particle segregation effects. Furthermore, a higher shaft rpm caused a higher mass flow rate at the cost of higher specific energy consumption due to viscous dissipation and changes in flow pattern. The researchers considered different DEM approaches varying in model complexity and computational intensity and validated computational results against experimental data to identify the trade-offs between model prediction accuracy and computational efficiency. For this purpose, the LIGGGHTS-INL code, which is an INL capability-extended version of the open-source LIGGGHTS (LAMMPS Improved for General Granular and Granular Heat Transfer Simulations) code was used to perform the DEM simulations on INL high-performance computing (HPC) resources. This work illustrates the utility of computational modeling approaches for predicting granular flow in real material handling units and the importance of careful computational model selection and experimental validation.

Significance

Feeding-related problems represent a grand challenge adversely affecting harnessing the strategic potential of biomass as an abundant, cheap, and renewable energy source that can strategically replace fossil fuel and help achieve net-zero goals. An example of the missed business opportunities is the reported biofuel production rate in 2016, which only achieved 7% of its total active rated capacity due to poor flowability. The study investigated the impact of biomass preprocessing parameters on the feeding performance in a pilot-scale screw conveyor using a state-of-the-art size reduction

technique available at INL BFNUF (the rotary shear system, the Forest Concepts LLC Crumbler). Quantitative metrics are used to investigate the technoeconomic impact of milled woody biomass attributes and operation parameters on the granular flowability, namely, mass throughput, driving torque, and transport cost in terms of specific energy consumption. Experiment and simulation data revealed the superior flowability of the smaller particle size, which can partially compensate for the higher cost required to produce them (as compared to the larger particle size). In addition, the study showed the granular flowability enhancement for dry particles associated with the narrower particle size distribution that characterizes the Crumbler rotary shear system. For critical processing parameters, a higher shaft speed led to a higher mass throughput at the cost of higher specific energy consumption and increased propensity of screw blockage. Simulations aided in identifying key underling mechanisms controlling the transport behavior of the granular biomass system, which are surface-roughness-induced mechanical interlocking, particle segregation, and viscous losses. The study contributes to promoting a fundamental understanding of the characteristic nature of the granular biomass flow behavior and the underlying transport mechanisms to identify critical material attributes and processing parameters and how they impact the biomass feedstock quality attributes. The findings also shed light on the unique characteristics of the lignocellulosic biomass feedstocks and provide a framework to develop dedicated design practices for handling and feeding units beyond the conventional methods based on decades-long accumulated experience from other industries dealing with particulate materials with substantially better flow properties.

Key Publications

" Ahmed Hamed, Yidong Xia, Nepu Saha, Jordan Klinger, David N. Lanning, and Jim Dooley, Particle size and shape effect of Crumbler rotary shear-milled granular woody biomass on the performance of Acrison screw feeder: A computational and experimental investigation , Powder Technology 427 (2023) 118707

Sponsor/Program

This project is supported by the United States Department of Energy (DOE), Office of Energy Efficiency and Renewable Energy, Bioenergy Technologies Office (BETO), the Consortium for Computational Physics and Chemistry (CCPC) and the Feedstock Conversion and Interface Consortium (FCIC), under DOE Idaho Operations Office with Contract No. DE-AC07-05ID14517.

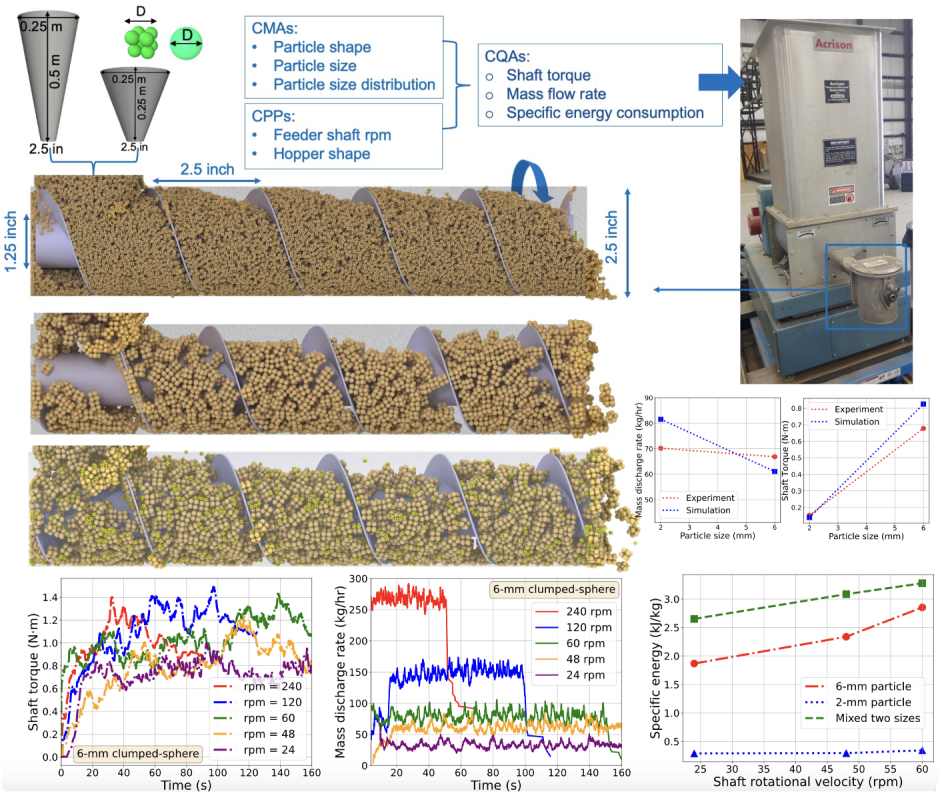


Figure 1: DEM simulation setup of the selected region of interest of the Acrison system: Dimensions of the two conical hoppers used in the DEM screw feeder simulations along with the two considered DEM particle shapes of size D, that is, a single sphere and clumped sphere with cubic shape (top left), the dimensions of the screw shaft while filled with 2 mm clumped-sphere particles (middle left), a snapshot of DEM simulation of the 6 mm clumped-sphere particles (bottom left), a schematic diagram showing the CMAs, CPPs and CQAs considered in the present study (top middle), and the selected region of interest from the Acrison system (right). Computed space-averaged mass discharge rate and rolling average torque versus time using various shaft rotational speeds are also shown for selected cases along with the performance metrics.

D.2 Designing Multimetal Catalyst for Hydrogen Evolution Reaction Using Density Functional Theory and Machine Learning Models

Report Participants

Das, Karmakar, S[1], Li, Meng [1]
1 Idaho National Laboratory

Scientific Achievement

Our current research focus is to develop a cost-effective and sustainable catalyst for hydrogen (H2) production using highly active materials identified on the volcano plot. We have extensively studied the hydrogen evolution reaction activity in Pt, Ni, and Co alloy materials, considering the influence of local environment on hydrogen production. Our methodology combines density functional theory calculations with machine learning models. To explore a wide range of potential catalysts, we have constructed a four-layer Ni (111) slab model and systematically varied the metal composition in the top two layers, generating over 5,000 alloy models with diverse local environments. A crucial step in H2 production is hydrogen atom binding to the catalyst metal surface, occurring at sites like hexagonal close-packed, face-centered cubic, top, and bridge sites. We have systematically calculated H-binding energies for various alloy surfaces at each site. These calculations were performed using the Vienna Ab initio Simulation Package software at the INL's HPC facility. Our next step involves utilizing machine learning models to predict binding energies for additional materials, advancing our knowledge and design capabilities for efficient H2 production catalysts.

Significance

The world is facing an energy shortage, and there is a growing demand for renewable and clean energy sources. Hydrogen (H2) is a crucial green energy source capable of reducing carbon emissions and facilitating a transition to sustainability and efficiency. Presently, the industrial-scale production of H2 relies on platinum (Pt) and C, but the scarcity of Pt presents challenges. We need alternative solutions to address this issue. Our strategy involves combining the most active materials from the third row of the periodic table (Ni and Co) with Pt. This approach aims to comprehend how synergistic effects influence the hydrogen evolution reaction and how we can manipulate the microstructural environment to create a robust catalyst. By doing so, we can pave the way for a sustainable H2 production method that is less reliant on scarce Pt resources.

Key Publications

Karmakar, S and Li, M. Designing Multi-Metal Catalyst for Hydrogen Evolution Reaction Using Density Functional Theory and Machine Learning Models (In progress)

Sponsor/Program

Laboratory Directed Research and Development 23A1070-027FP

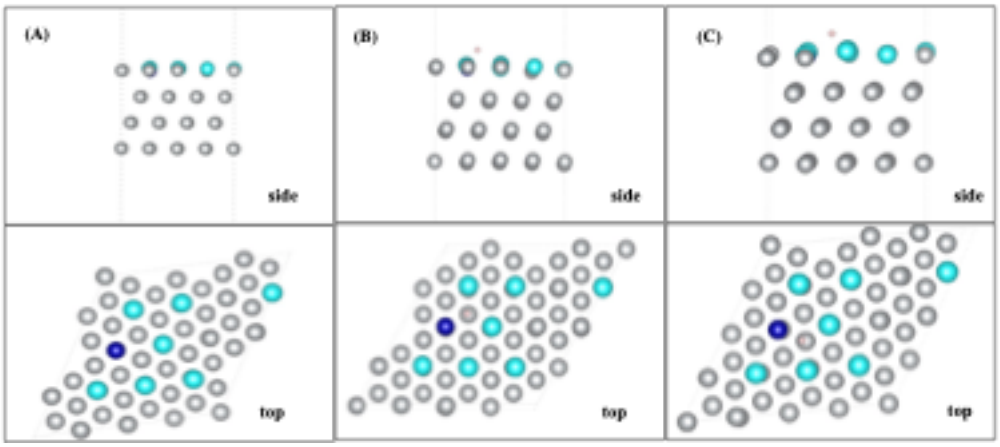


Figure 1: Density functional theory optimized structures (A) alloy structure, (B) H adsorbed at the face-centered cubic site, and (C) H adsorbed at the hexagonal close-packed site. Color codes are Ni: grey, Pt: Cyan, Co: Blue, and H: Pink.

D.3 Center for Thermal Energy Transport under Irradiation Project

Report Participants

Malakkal, Linu [1]
1 Idaho National Laboratory

Scientific Achievement

This work used HPC to perform the atomistic scale modeling of the thermal transport in actinide materials. This work provides insight into the fundamental mechanism of the thermal transport in oxide and nitride fuels. HPC was extensively used in describing the effect of defects on the phonon thermal conductivity of thorium oxide. Also, the role of electron-phonon interactions on the metallic fuels, such as thorium nitride and zirconium nitride, were investigated using software such as Quantum Espresso, the Vienna Ab initio Simulation Package, ShengBTE, Peturbo, and EPW.

Significance

Key findings include the following statements. The scattering due to three phonon process, four phonon process, and the electron-phonon interactions of zirconium nitride and thorium nitride were calculated. The total thermal conductivity, including the phonon and electron thermal conductivity, were predicted, and this computational work provides fundamental insights into the thermal transport of nitride fuels.

Key Publications

Journal publication: (1) Linu Malakkal, Ankita Katre, Shuxiang Zhou, Chao Xiang, David Hurley, Chris Marianetti, and Marat Khafizov. First-principles determination of the phonon-point defect scattering and thermal transport due to fission products in tho2. Submitted to Journal of Physical Review Materials, 2023. Conference presentation: (1) Marat Khafizov, Saqeeb Adnan, Erika Nosal, Miaomioa Jia, Linu Malakkal, Amey Khanolkar, Shuxiang Zhou, Zilong Hua, Kaustubh Bawane, Boopathy Kombaiah, Chao Jiang, Lingfeng He, Michael Manley, and David Hurley. Atomistic understanding of thermal conductivity degradation in irradiated oxide fuels. Oral presentation at the MS&T 23, Columbus, Ohio, 2023. (2) Erika Nosal, Saqeeb Adnan, Miaomiao Jin, Linu Malakkal, and Marat Khafizov. Modeling the effect of point defect scattering on the thermal conductivity of ThO2. Oral presentation at the MS&T 23, Columbus, Ohio, 2023. (3) Linu Malakkal, Marat Khafizov, David Hurley, and Chris Marianetti. Role of electron and phonon interactions in the thermal conductivity of ZrN, ThN and UN. Oral presentation at the TMS, USA, 2024. (4) Linu Malakkal "Invited Speaker at the MS&T 2023, Columbus, Ohio, USA, Oct 2023 on the topic "Irradiation induced structural and thermal conductivity changes in nuclear fuels"

Sponsor/Program

Energy Frontier Research Centers

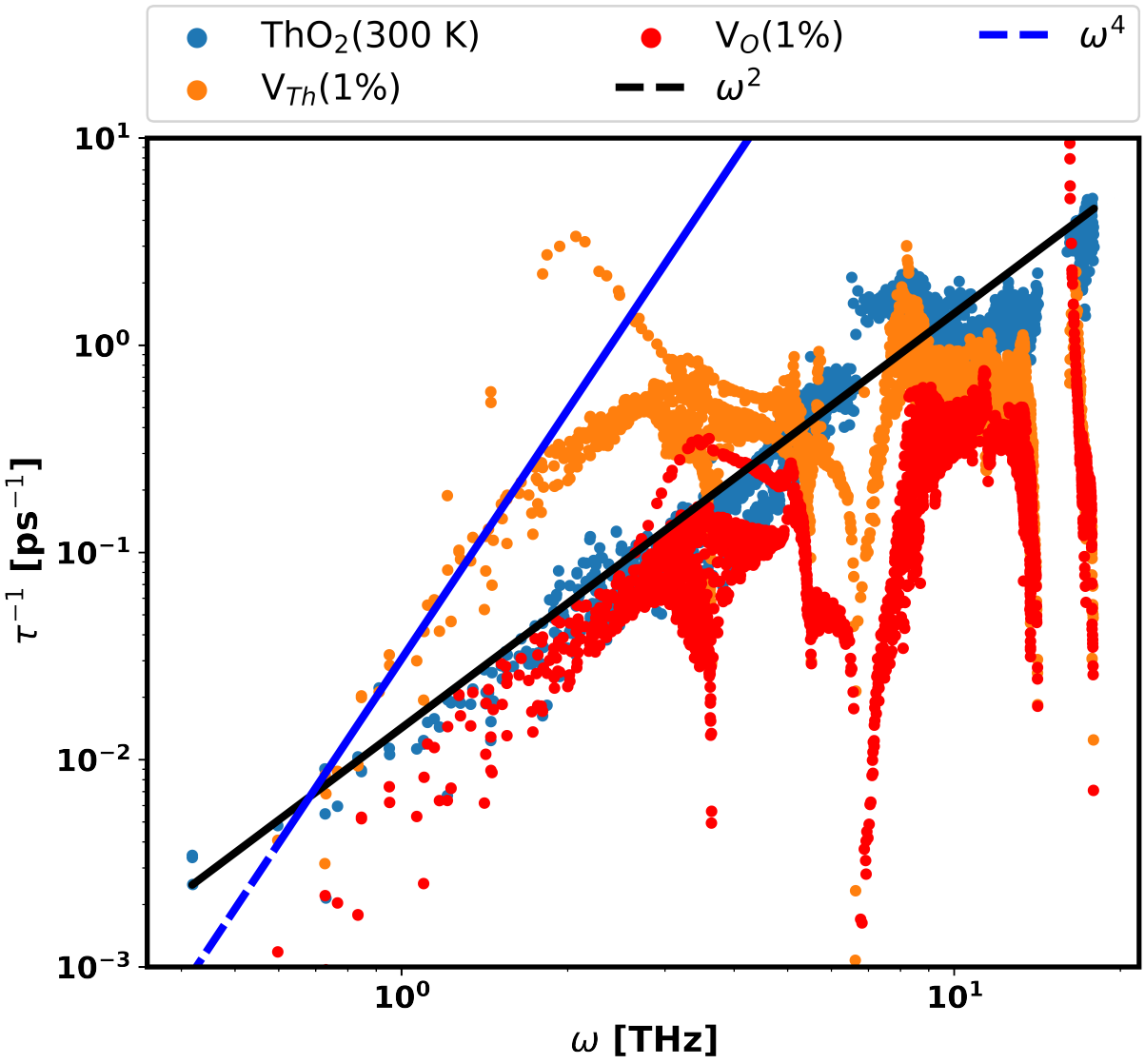


Figure 1: Comparison of the τ^{-1} of the V_{Th} (solid orange dots) and V_O (solid green dots) as a function of phonon frequency (ω) from the Green-function T-matrix method compared to the τ^{-1} predicted by Klemens model (anharmonic scattering [black dashed lines] and the defect scattering [blue dashed lines]) and Born approximation for the V_{Th} (solid cyan dots) and the V_O (solid red dots). Solid blue dots represent the anharmonic scattering of the pristine ThO2 due to three phonon interactions at 300 K.

D.4 Utah Frontier Observatory for Research in Geothermal Energy (FORGE)

Report Participants

Damjanac, Branko N[1]
1 Itasca Consulting Group

Scientific Achievement

The Utah Frontier Observatory for Research in Geothermal Energy (FORGE) is a dedicated underground field laboratory sponsored by DOE for developing, testing, and accelerating breakthroughs in EGS technologies to advance the uptake of geothermal resources around the world. Itasca is a part of the research team. The main role of Itasca's team, in cooperation with the University of Utah and INL, is to numerically simulate the reservoir response to stimulation by fluid injection. The purpose of these simulations is to optimize the development of the field and stimulation strategy. The numerical code, XSite, is used to simulate the hydromechanical response of naturally fractured formation with explicit representation of pre-existing fractures during fluid injection. Last year we conducted extensive parametric study of the reservoir stimulation in Zones 1, 2, and 3 on Well 16A. The comparison of modeling results shows a reasonable match with injection pressure histories and an excellent match with the microseismic data. Modeling results and recorded data are used in selecting the production Well 16B. Long-term fluid circulation between two wells is simulated in XSite. The results are compared with other models.

Significance

The models calibrated using the injection tests at the site (Wells 58–32 and 16A) are used to simulate the response of the reservoir to the proposed stimulation programs for Zones 1, 2, and 3 on Well 16A. Different completion designs, pumping schedules, and fluids are used for three zones. In addition, sensitivity analyses were conducted with respect to some uncertain parameters, including the permeability and strength of the discrete fracture network. The models were used for a forward prediction of the reservoir stimulation, including injection pressures and induced microseismicity. The model results have been used to design the distance to the production Well 16B, which is currently drilled.

Key Publications

Xing, P., B. Damjanac, Z. Radakovic-Guzina, M. Torres, A. Finnila, R. Podgorney, J. Moore and J. McLennan. Comparison of Modeling Results with Data Recorded During Field Stimulations at Utah FORGE Site, PROCEEDINGS, 48th Workshop on Geothermal Reservoir Engineering, Stanford University, Stanford, California, February 6-8, 2023. SGP-TR-224.

Sponsor/Program

Rob Podgorney/FORGE

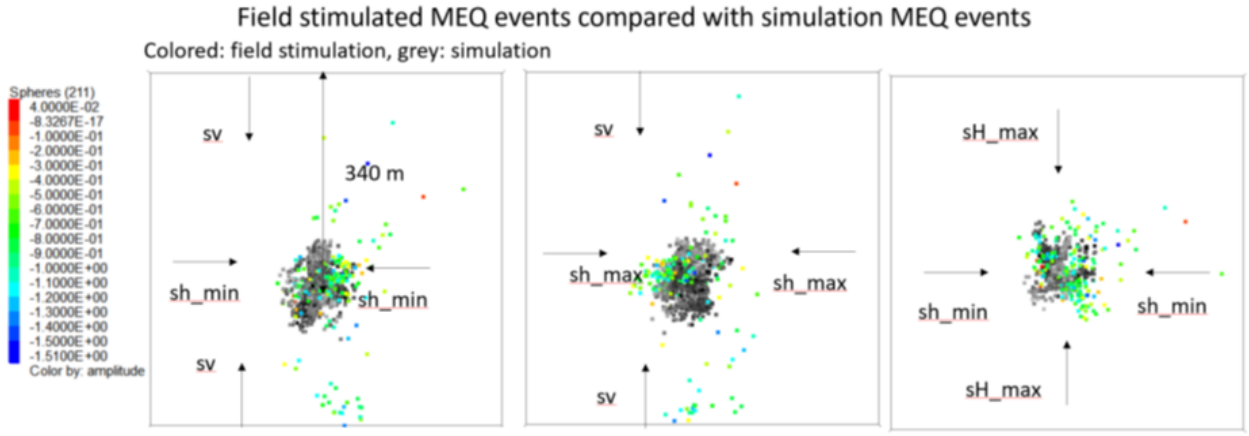


Figure 1: Comparison of the field-detected microseismicity cloud with simulation results for Stage 1. Field detected maximum magnitude is 0.04, and simulation maximum magnitude is 0.03.

D.5 Insights into Waterflooding in Hydrocarbon-Bearing Nanochannels of Varying Cross Sections from Mesoscopic Multiphase Flow Simulations

Report Participants

Diermyer, Zachary R[1], Xia, Yidong [2], Li, Jiaoyan [1]
1 The State University of New York at Buffalo
2 Idaho National Laboratory

Scientific Achievement

Waterflooding is one of the geotechniques used to recover fuel sources from nanoporous geological formations. The scientific understanding of the process that involves the multiphase flow of nanoconfined fluids, however, has lagged, mainly due to the complex nanopore geometries and chemical compositions. This work uses a modified many-body dissipative particle dynamics (mDPD) model implemented using the Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software package. The model has accurately calibrated parameters used to perform parametric flow simulations for studying the influences of waterflooding-driven power, pore shape, surface roughness, and surface wettability on multiphase flow in heptane-saturated silica nanochannels.

Significance

Remarkably, up to an 80% reduction in the effective permeability is found for water-driven heptane flow in a baseline 4.5-nm-wide slit channel when compared with the Hagen "Poiseuille equation. In the 4.5-nm-wide channels with architected surface roughness, the flow rate is found to be either higher or lower than the baseline case, depending on the shape and size of cross sections. A high wettability of the solid surface by water is essential for achieving a high recovery of heptane, regardless of surface roughness. When the solid surface is less wetting or nonwetting to water, the existence of an optimal waterflooding-driven power allows for the highest possible recovery.

Key Publications

Diermyer, Z., Xia, Y., & Li, J. (2023). Insights into Waterflooding in Hydrocarbon-Bearing Nanochannels of Varying Cross Sections from Mesoscopic Multiphase Flow Simulations. Langmuir. Diermyer, Z., Xia, Y., & Li, J. (2022 November 14). Energy Optimization of Nanochannel Fluid Extraction with Various Channel Geometries [Conference presentation]. AIChE Annual Meeting 2022, Phoenix, AZ.

Sponsor/Program

EFRC-MUSE, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under award no. DE-SC0019285

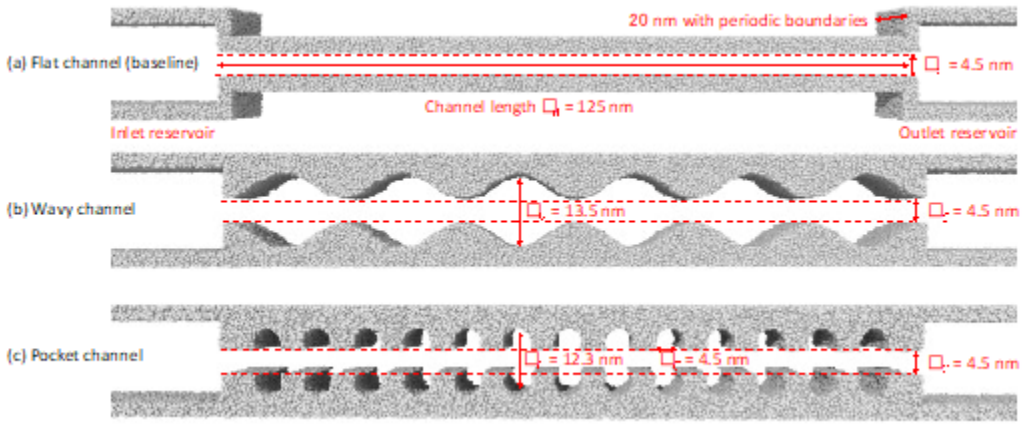


Figure 1: Visualization of the three channel geometries: (a) flat channel, (b) wavy channel, and (c) pocket channel. The full extent of the inlet and outlet reservoirs are not pictured here.

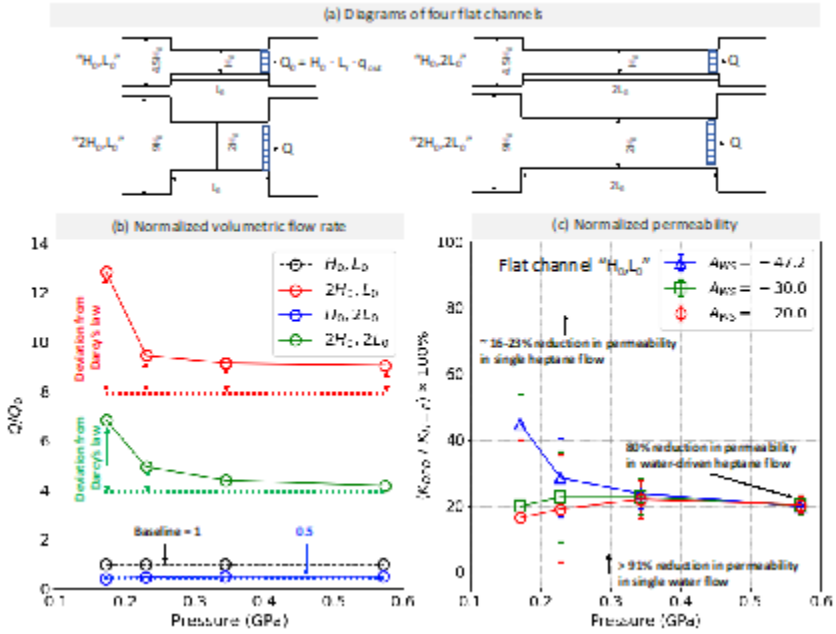


Figure 2: (a) Diagrams of four flat channels with relevant dimensions and the flow rate measurement region. (b) Plot of the normalized volumetric flow rate. (c) Plot of the normalized permeability. H0 = 4.5 nm and L0 = 125 nm are the default flat channel height and length, respectively.

D.6 RELAP5-3D / NUPAC Repository Layout

Report Participants

Duemmler, Kai E[1], Beeler, Benjamin W[1], Woods, Michael [2], Karlsson, Toni [2], Gakhar, Ruchi [2]
1 North Carolina State University
2 Idaho National Laboratory

Scientific Achievement

The transport properties of molten salts are vital for the readiness level of Gen IV molten-salt reactors. This year we conducted an expensive case study on the simulation requirements for calculating the transport properties of LiCl-KCl eutectic salt. Historically, these properties were limited to classical molecular dynamics studies due to computational constraints. We have shown that it is possible to accurately calculate the transport properties of molten salts and some system requirements with these complex salt systems using ab initio molecular dynamics (AIMD).

Significance

With a global push to a carbon-free power grid, there is a need for a consistent baseload power generation that cannot be produced by renewable sources like wind and solar. Nuclear power is capable of filling this role, and there has been a push to raise the readiness level of these Gen IV nuclear reactors, including molten-salt reactors. With any liquid-fueled molten-salt design, plutonium containing salt will form and, for fast spectrum reactors, that will be PuCl3. The literature on the thermophysical properties of NaCl-PuCl3 is very sparse. Figure 1 shows the density of the NaCl-PuCl3 system across the compositional spectrum. What can be observed is that the density increases monotonically with respect to the concentration of PuCl3. The other trend that can be observed is that, as the temperature of the molten salt increases, the density will decrease. Another important thermophysical property of molten salts is the heat capacity. This property is needed to calculate the ability of the salt to extract heat from the core of the reactor. The Isobaric heat capacity for the eutectic NaCl-PuCl3 molten salt can be seen in Figure 2 which shows our work compared to two different experimental values each around the eutectic composition. What can be observed is that the two experimental works disagree by a factor of two. In these cases, AIMD can be used to supplement the experimental work and show that the values reported by Karlsson agree better with computational models. The transport properties of LiCl, KCl, NaCl, MgCl2, eutectic LiCl-KCl, and eutectic NaCl-MgCl2 were calculated via AIMD. We are the first to report the self-diffusion coefficient of MgCl2 and the diffusion coefficient of eutectic NaCl-MgCl2 at these elevated temperatures. The self-diffusion coefficients were calculated via the Einstein relationship. The self-diffusion coefficients are shown in Figure 3. What can be observed is that the eutectic composition has not been studied experimentally, but another AIMD study has been conducted at lower temperatures than what is reported in this work.

Key Publications

In the review process for the First-principles-derived transport properties of molten chloride salts manuscript

Duemmler, K., Woods, M., Karlsson, T., Gakhar, R., & Beeler, B. (2022). An ab initio molecular dynamics investigation of the thermophysical properties of molten NaCl-MgCl2. Journal of

Nuclear Materials, 570, 153916.

Sponsor/Program

LDRD DOE Idaho Operations Office Contract DE-AC07-05ID14517

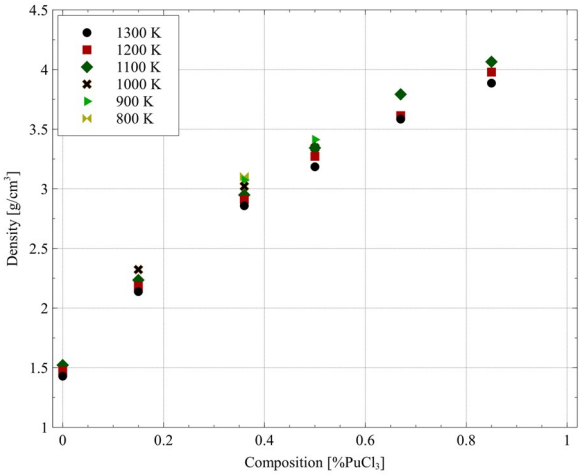


Figure 1: NaCl-PuCl3 density.

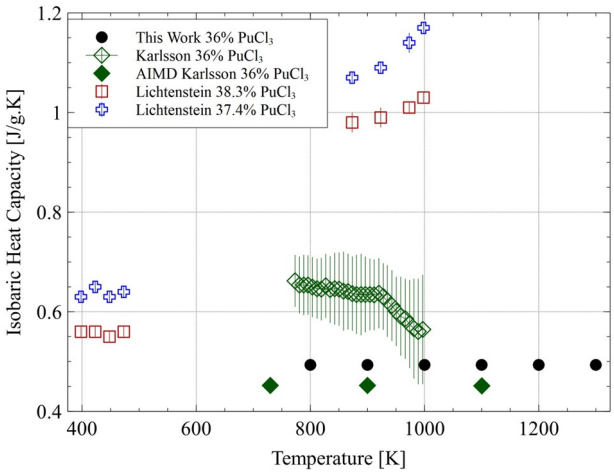


Figure 2: Heat Capacity for eutecitc NaCl-PuCl3.

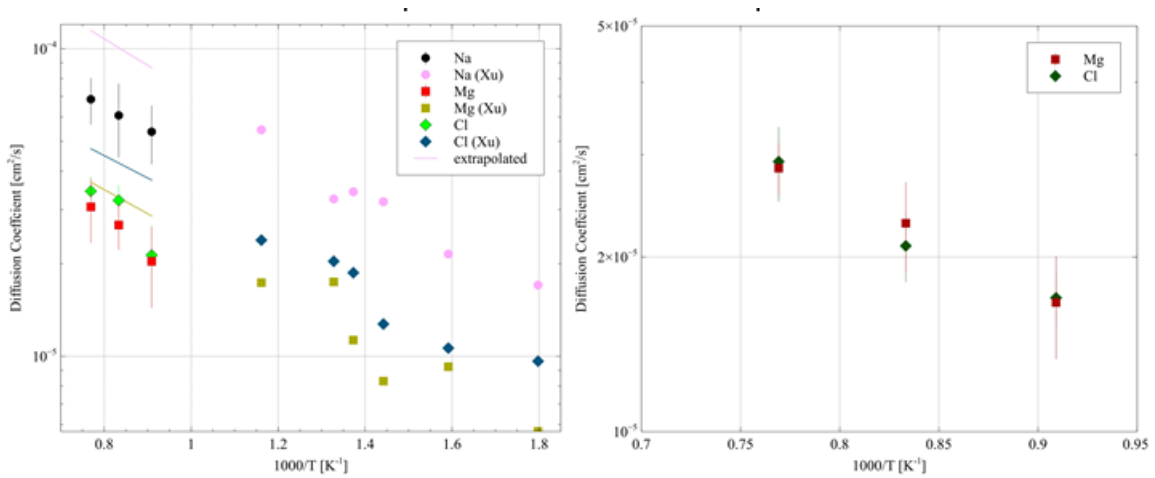


Figure 3: The self-diffusion coefficient for the eutectic NaCl-MgCl2 and MgCl2. What we observed for the eutectic composition is that Na+ ions diffuse the fastest and Mg2+ ions the slowest with chlorine ions falling in the middle. This is the exact same behavior observed by the other AIMD study at lower temperatures.

D.7 Insights into Waterflooding in Hydrocarbon-Bearing Nanochannels of Varying Cross-Sections from Mesoscopic Multiphase Flow Simulations

Report Participants

Diermyer, Zachary R[1], Xia, Yidong [2], Li, Jiaoyan [1]
1 The State University of New York at Buffalo
2 Idaho National Laboratory

Scientific Achievement

In this project, we have used the LAMMPS user-meso package to perform dissipative particle dynamics simulations. The simulations have been performed to study the influences of waterflooding driven power, pore shape, surface roughness, and surface wettability on the multiphase flow in heptane-saturated silica nanochannels. We have found up to an 80% reduction in the effective permeability for water-driven heptane flow in a baseline 4.5-nm-wide slit channel when compared with the Hagen Poiseuille equation. In the 4.5-nm-wide channels with architected surface roughness, the flow rate is either higher or lower than the baseline case, depending on the shape and size of the cross sections. A high wettability of the solid surface to water is essential for achieving a high recovery of heptane, regardless of surface roughness. When the solid surface is less wetting or non-wetting to water, the existence of an optimal waterflooding driven power allows for the highest possible recovery. A detailed analysis on the evolution of the transient water-heptane interface in those nanochannels is presented to elucidate the underlying mechanisms that impact or dictate the multiphase flow behaviors.

Significance

Waterflooding is one of the geotechniques used to recover fuel sources from nanoporous geological formations. The scientific understanding of the process that involves the multiphase flow of nanoconfined fluids, however, has lagged, mainly due to the complex nanopore geometries and chemical compositions. This project is supported by Department of Energy, Office of Science, Energy Frontier Research Center Project. The goal is to bridge the knowledge gap to understand the confinement effects on the hydrocarbon recovery process. Our future work will focus on investigating the multicomponent fluid flow dynamics in realistic nanopore networks.

Key Publications

Zachary Diermyer, Yidong Xia, Jiaoyan Li, Insights into Waterflooding in Hydrocarbon-bearing Nanochannels of Varying Cross-sectins from Mesoscopic Multiphase Flow Simulations , Langmuir, 2023 (accepted).

Sponsor/Program

Energy Frontier Research Centers

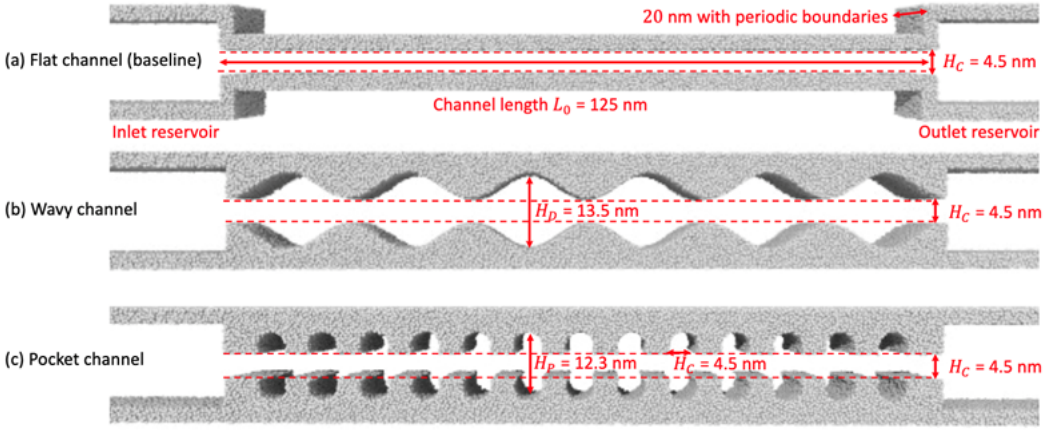


Figure 1: Visualization of the three channel geometries: (a) flat channel, (b) wavy channel, and (c) pocket channel.

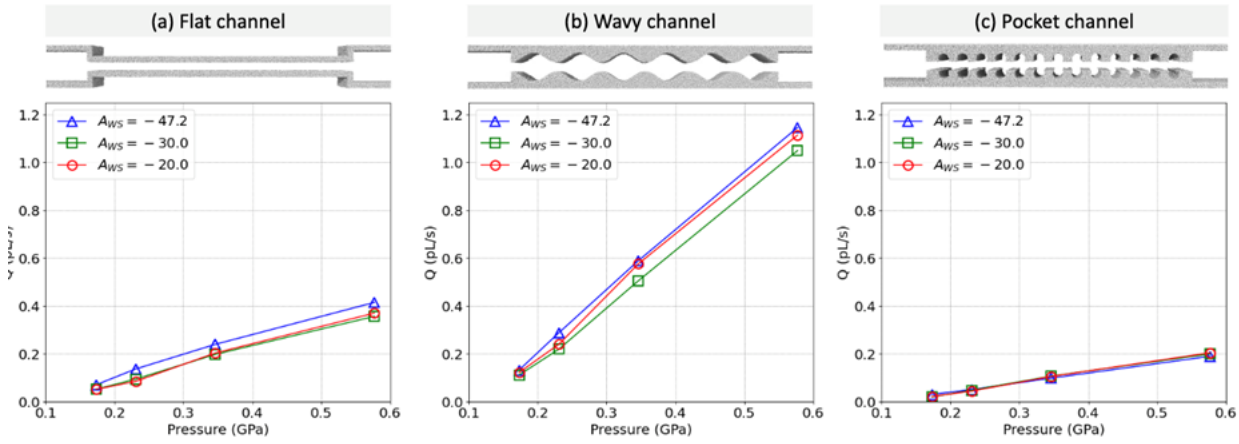


Figure 2: Measured channel outlet volumetric flow rate (picoliter per second) versus inlet pressure: (a) flat channel, (b) wavy channel, and (c) pocket channel. Plotted separately are relatively wetting (triangles), neutral (squares), and relatively non-wetting (circles) silica surface for water.

D.8 SPH Modeling of Granular Biomass Flow Handling

Report Participants

Zhao, Yumeng [1], Jin, Wencheng [2]
1 Georgia Institute of Technology
2 Idaho National Laboratory

Scientific Achievement

In the project, a smoothed particle hydrodynamics (SPH) code was developed to model the granular biomass flow behavior. An open-source software DualSPHysics was used and modified to include a frictional contact and a hypoplastic constitutive model. The model was validated through simulating an elastic block sliding on a slope and a sand column collapse test. The code was then applied to simulate two granular biomass flow cases: an angle of repose and an axial compression test. The simulation results were compared with experiments conducted by colleagues at INL and showed a good match. INL HPC resources were used to perform the simulations.

Significance

The work validated that the developed code is able to simulate granular biomass flow behavior in different loading conditions and matches the experimental cases. It enables us to simulate more complex granular biomass flow behavior, such as hopper flow and auger conveyance. The code provides an economic and quick alternative to the understanding and prediction of the biomass flow process, compared with an experiment. It also helps grasp the physics of complex granular mechanics in the handling process, such as arching and jamming, whose mechanism will be harder to be examined in an experiment. Understanding and predicting the flow behavior in those complex industrial handling processes will benefit the more efficient use of biomass as a renewable energy source. The ongoing work is to simulate those industrial granular biomass flow in real industrial handing scenarios, which requires the use of INL HPC resources.

Key Publications

Zhao, Y., Jin, W., Klinger, J., Dayton, D. C., & Dai, S. (2023). SPH modeling of biomass granular flow: Theoretical implementation and experimental validation. Powder Technology, 426, 118625.

Sponsor/Program

The project is performed for the Feedstock Conversion Interface Consortium (FCIC) with funding graciously provided by the U.S. Department of Energy Bioenergy Technologies Office

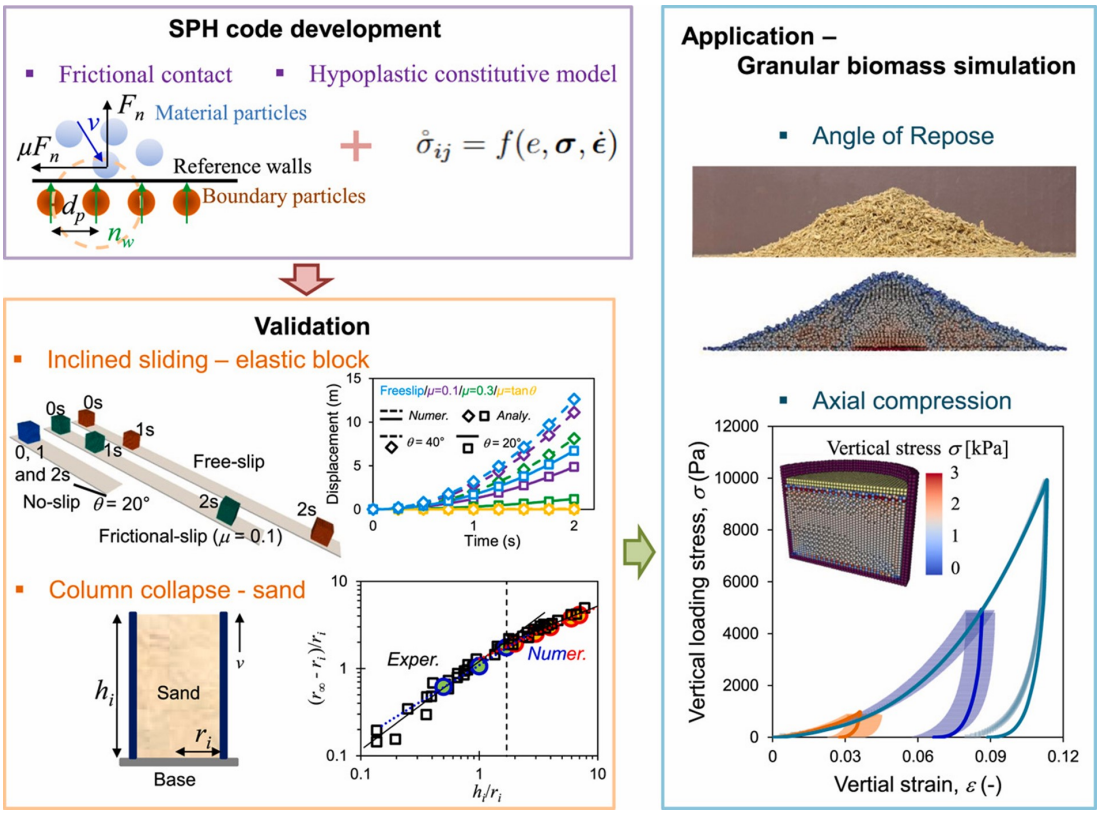


Figure 1: Schematic of the overall workflow. A frictional contact and a hypoplastic constitutive mode is implemented first, then the code is validated using two examples before using to model granular biomass flow through an angle of response and an axial compression test. The granular biomass flow simulation matches the experimental results conducted.

Appendix E Other

Table of Contents

E.1 Particle Fluid Simulation to Model Fluidization of Tungsten Carbide Particles

Report Participants

Schuck, Paul C[1], Stoyer, Benjamin D[1]
1 Idaho National Laboratory

Scientific Achievement

Barracuda and Multiphase Flow with Interphase eXchanges (MFiX) software modeled the fluidization of tungsten carbide particles in a conical bed and compared it with experimental data to validate the software. MFiX software better replicated the experimental data.

Significance

The Department of Defense's Strategic Capabilities Office sponsors the Microreactor Program, which is intended to design, build, and demonstrate a mobile reactor. The reactor will be assembled and initially operated at Idaho National Laboratory (INL). The reactor will be an electricity-generating Generation IV nuclear reactor that uses tristructural isotropic fuel. Tristructural isotropic fuel is processed in a fluidized bed. Understanding the fluidization properties of the bed will help inform processing parameters and improve the fuel's quality.

One step to understanding fluidization properties of the bed is to simulate bed conditions and validate with experimental work. Data were collected for tungsten carbide particles fluidized in room temperature conditions. These data were used as a baseline to validate two software: Barracuda and MFiX.

Both Barracuda and MFiX had challenges predicting some aspects of the bed behavior. In general, MFiX better predicted the downward flow of particles on the edge of the conical bed. In Barracuda, the particles were mostly static on the edge. Additional tuning of MFiX parameters is ongoing to better match the onset of spouting with process flow. Once the bed behavior qualitatively matches the experimental data, the velocities of the particles on the outer edge will be compared to the experimental data. See Figure 1 for a snapshot of an MFiX simulation.

Key Publications

None

Sponsor/Program

INL

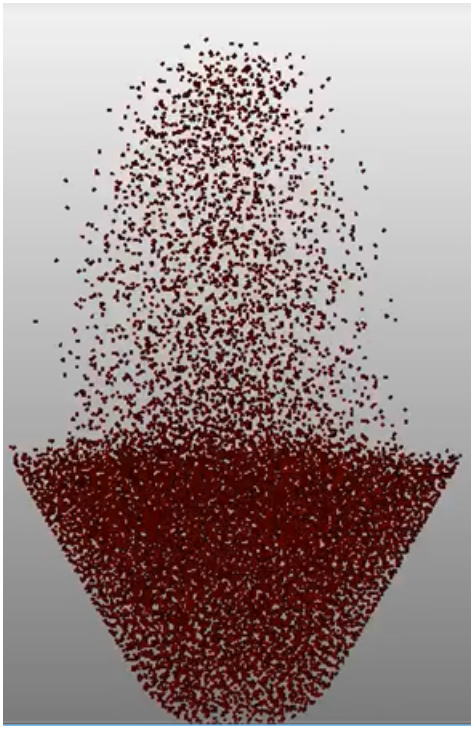


Figure 1: Image of spouted bed simulated in MFiX.

E.2 Bubble Detection and Analysis of a Silicone Oil Experiment

Report Participants

Guillen, Donna P[1], Abboud, Alexander W[1], Noack, Carson [1], Sharapov, Jeremy A[1]
1 Idaho National Laboratory

Scientific Achievement

This research presents two approaches to detect bubbles in a silicone oil experiment and subsequently compare the results with a computational fluid dynamics (CFD) model. The developed bubble detection codes for the silicone oil experiment efficiently extract bubble features, such as size, velocity, and frequency, for various viscosity oils and bubbling rates using image processing techniques. A MATLAB analysis was compared to an artificial intelligence (AI) based approach using Label Studio and YOLOv8. YOLOv8 is a deep learning algorithm used to detect objects in images and videos. The results obtained from the two object detection approaches are compared with the CFD model to validate its accuracy and reliability. This study aims to contribute to the optimization of waste glass melters at the U.S. Department of Energy's Waste Treatment and Immobilization Plant, aiding in the treatment of radioactive tank waste at the Hanford site.

Significance

Legacy radioactive tank waste at the Hanford site in eastern Washington State is slated for vitrification in large Joule-heated, ceramic-lined melters at the Waste Treatment and Immobilization Plant. The project's focus is on supporting the plant through modeling and simulation using CFD. The objective of this study is to characterize the bubbling behavior in highly viscous fluids using a MATLAB approach and compare results obtained by an AI algorithm to that computed by CFD.

Key Publications

1. T. Jin, M.A. Hall, J.D. Vienna, W.C. Eaton, J.W. Amoroso, B.J. Wiersma, W. Li, A.W. Abboud, D. P. Guillen, A.A. Kruger, Glass-contact refractory of the nuclear waste vitrification melters in the United States: a review of corrosion data and melter life, International Materials Reviews, 2023. https://doi.org/10.1080/09506608.2023.2211469 2. A.W Abboud, D.P. Guillen, B. Christensen, Prediction of Melter Cold Cap Topology from Plenum Temperatures with Computational Fluid Dynamics and Machine Learning, International Journal of Ceramic Engineering & Science 4(4), July 2022, 257-269. https://doi.org/10.1002/ces2.10134. 3. P. Ferkl, P. Hrma, A. Abboud, D.P. Guillen, J. Khawand, I. Kopal, M. Kohoutkova, M. Vernerova, J. Klouzek, M. Hall, A.A. Kruger, R. Pokorn, Conversion kinetics during melting of simulated nuclear waste glass feeds measured by dissolution of silica, Journal of Non-Crystalline Solids, 579, 2021, 121363. https://doi.org/10.1016/j.jnoncrysol.2021.121363 4. A.W. Abboud, D.P. Guillen, P. Hrma, A.A. Kruger, J. Klouzek, R. Pokorny, Heat Transfer from Glass Melt to Cold Cap: Computational Fluid Dynamics Study of Cavities Beneath Cold Cap, International Journal of Glass Science, 12(2), 233-244, 2021. https://doi.org/10.1111/ijag.15863 5. A.W. Abboud, D.P. Guillen, R. Pokorny, Effect of Cold Cap Coverage and Emissivity on the Plenum Temperature in a Pilot-Scale Waste Vitrification Melter, International Journal of Applied Glass Science, 11(2), 357-368, 2020. https://doi.org/10.1111/ijag.15031 6. D.P. Guillen, S. Lee, P. Hrma, J. Traverso, R. Pokorny, J.

Klouzek, A.A. Kruger, Evolution of Chromium, Manganese and Iron Oxidation State during Conversion of Nuclear Waste Melter Feed to Molten Glass, Journal of Non-Crystalline Solids, 531, 2020. https://doi.org/ 10.1016/j.jnoncrysol.2019.119860 7. D.P. Guillen and A.W. Abboud, Heat Transfer Effect from Floating Cold Cap Motion in a Waste Glass Melter, Proceedings of the ASME 2022 Power Conference, POWER 2022, July 18-19, 2022, Pittsburgh, PA. 8. A.N. Barron, D.P. Guillen, M. Hall, A.W. Abboud, S. Davidson, A.A. Kruger, A Predictive Model for Offgas Composition in Waste Glass Melters, 14th Pacific Rim Conference on Ceramic and Glass Technology and GOMD 2021, Virtual, December 13-16, 2021. 9. D.P. Guillen, A.W. Abboud, P. Ferkl, M. Hall, S. Lee, P. Hrma, R. Pokorny, W.E. Eaton, D. Dixon, A. A. Kruger, Integration of Generalized Cold Cap into Glass Melter Representation, 14th Pacific Rim Conference on Ceramic and Glass Technology and GOMD 2021, INVITED, Virtual, December 13-16, 2021. 10. D.P. Guillen and A.W. Abboud, Effect of Floating Body Motion on Heat Flux to the Cold Cap in a Waste Glass Melter, Proceedings of the ASME 2021 Power Conference, POWER 2021, July 20-22, 2021, Virtual. 11. D.P. Guillen, A.W. Abboud, P. Hrma, A.A. Kruger, J. Klouzek, R. Pokorny, Using CFD to Understand the Effect of Gas Bubbles Beneath the Cold Cap on Melt Rate during Nuclear Waste Vitrification, GLASS MEETING 2020 on Web with Advances in Fusion and Processing of Glass (AFPG), Virtual, December 7-10 and 16-18, 2020.

Sponsor/Program

U.S. DOE Office of River Protection

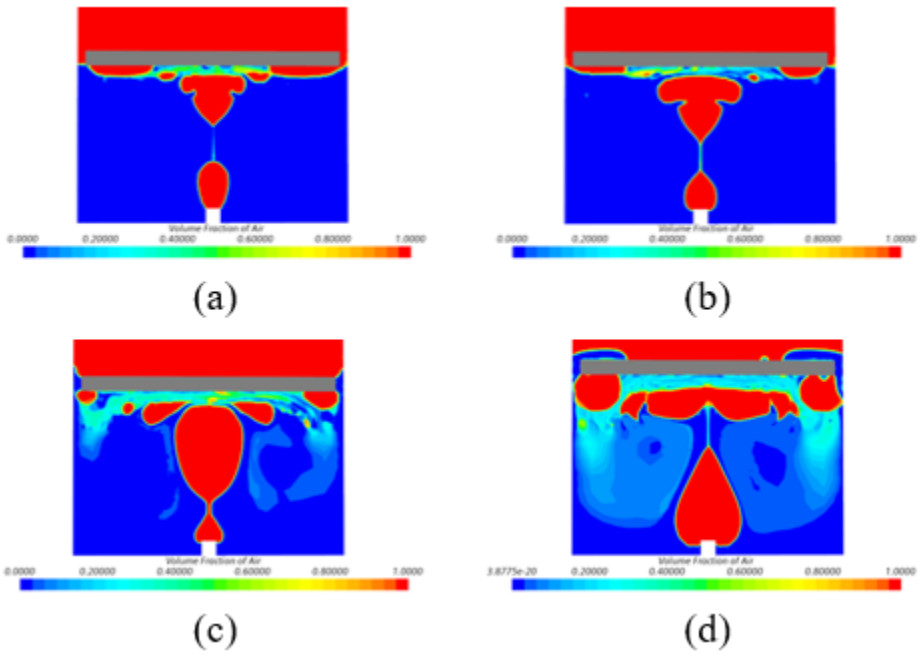


Figure 1: (a) Silicone oil test setup, (b) detection of bubble in image using MATLAB code, (c) AI approach, (d) result from CFD simulation.

E.3 Evaluation of Containers for Distribution of the ALEGRA Hydrocode

Report Participants

Anderson, Matthew W[1], Sgambati, Matthew R[1], Timothy , Fuller J[2], Aydelotte, Brady B[1], Hanson, Kent L[1], Jones, Warren F[1], Merriman, Colin C[1]
1 Idaho National Laboratory
2 Sandia National Laboratory

Scientific Achievement

ALEGRA, an explicit dynamic FEA code developed at Sandia National Laboratories, was built and distributed to INL in an OCI compliant container. On the INL systems, the container was converted to the INL-approved Apptainer format and underwent testing to verify proper function. The container was subsequently successfully installed on a non-internet-connected HPC system, greatly simplifying software deployment on that system, saving time and money.

An example of a shaped charge jet formation problem run with the containerized ALEGRA is shown in Figure 1. Containerized ALEGRA builds were fully capable of running analysis problems with comparable accuracy and speed.

Significance

Software deployment on non-internet-connected HPC systems can be challenging. Software frequently requires numerous third party libraries that can be challenging to fully anticipate and approve in advance. These challenges can result in difficulty in deploying software quickly and smoothly on non-internet-connected HPC systems. Containerized software can be a solution to this problem. Containers provide a toolset that allows software to be built and packaged in what is essentially a lightweight virtual environment. This allows an application to be built with all of its dependencies and then be moved to the desired HPC environment; this greatly speeds software deployment. Containers can be signed and encrypted if needed, providing a convenient way to archive applications for future reference or use. This work followed the approach laid out by Sgambati and Anderson [1]. The ALEGRA containers were developed in a way that lend themselves to software quality assurance for massively parallel applications. Testing found that the containerized ALEGRA builds functioned correctly with a performance similar to non-containerized builds.

Key Publications

[1] Sgambati, Matthew R., and Matthew William Anderson. Software Quality Assurance for High Performance Computing Containers. No. INL/CON-23-71421-Rev000. Idaho National Laboratory (INL), Idaho Falls, ID (United States), 2023.

Sponsor/Program

Department of Defense

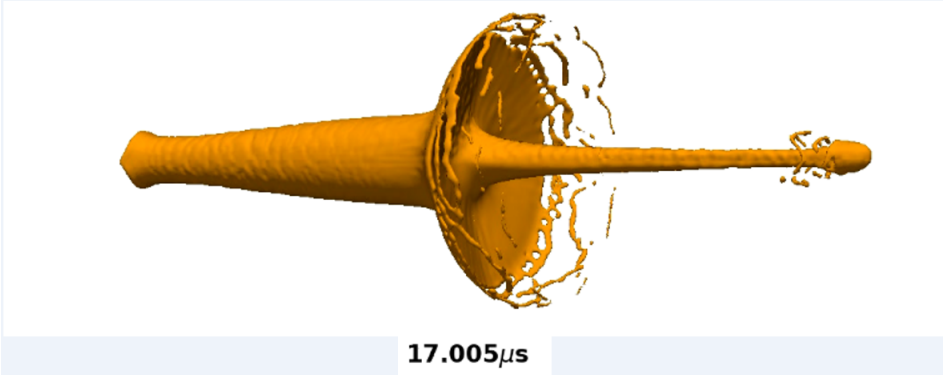


Figure 1: 3D formation model of a shaped charge jet run using ALEGRA deployed in an Apptainer container.

E.4 Artificial-Intelligence-Based Process Control and Optimization for Advanced Manufacturing

Report Participants

Mahmoud, Yaseen T[1]
1 North Carolina State University

Scientific Achievement

Our task is to build a reduced-order models (ROMs) using machine learning algorithms of a MOOSE additive manufacturing model. The goal is testing the effectiveness of ROMs to reduce computational time and produce reliable results.

Significance

The work is still in progress. We are testing multiple data- driven physics-based models to find the best model to approximate the original MOOSE additive manufacturing model.

Key Publications

None

Sponsor/Program

LDRD

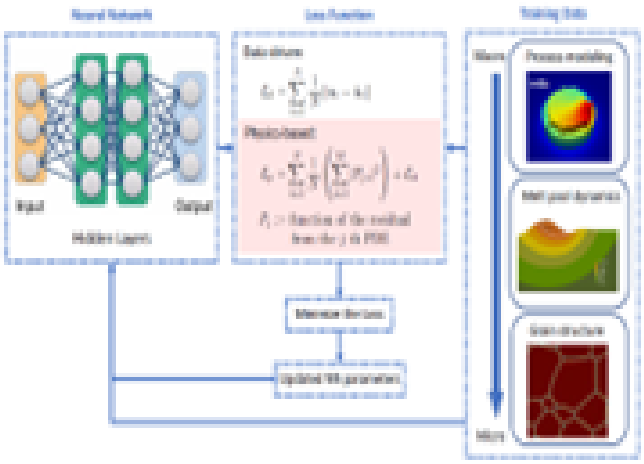


Figure 1: ROMs workflow.

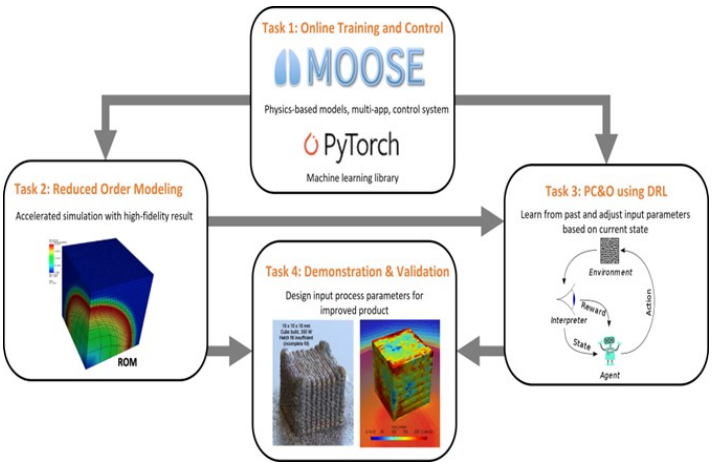


Figure 2: Project tasks.

Appendix F Energy Storage

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F.1 Enhancing Proton Mobility through Improved Hydration

Report Participants

Li, Meng [1], Regalado Vera, Clarita Y[2], Ding, Dong [1]
1 Idaho National Laboratory
2 New Mexico State University

Scientific Achievement

The objective of this work is to understand the effect of enhanced hydration (i.e., higher proton concentration) on the conduction of a proton experiencing proton trapping in perovskite materials by density functional theory (DFT). We performed DFT calculations for Y-doped BaZrO3 and Sc-doped BaZrO3 perovskites with different hydration levels using the Vienna Ab initio Simulation Package implemented on HPC. Of particular importance is identifying how hydration level changes the energy barriers for proton migration. The activation barriers for potential proton diffusion pathways were calculated to study proton mobility in different hydration scenarios. The Gibbs free energy landscape reveals an enhanced proton migration across various levels, attributed to increased hydration levels.

Significance

The proton conductivity of doped ABO3 perovskites is partly dependent on the proton concentration and hence on the level of material hydration. However, how the material hydration ability is affected by differences in doping is not fully understood. DFT calculations without considering differences in hydration ability fail to accurately predict conductivity trends in doped ABO3 perovskites. This work conducted systematic DFT calculations to study the defect characteristics of doped BaZrO3 and to understand how they influence the hydration process and proton mobility under operation conditions. Our work presents a perspective to comprehend how defect interactions and associations affect the hydration ability and proton mobility of proton-conducting oxides.

Key Publications

Clarita Y. Regalado Vera, Hanping Ding, Jagoda Urban-Klaehn, Meng Li, Zeyu Zhao, Frederick Stewart, Hanchen Tian, Xingbo Liu, Yanhao Dong, Ju Li, Meng Zhou, Hongmei Luo, and Dong Ding, Improving Proton Conductivity by Navigating Proton Trapping in High Scandium-Doped Barium Zirconate Electrolytes, Chemistry of Materials, 2023, 35, 5341,5352.

Sponsor/Program

HydroGEN Advanced Water Splitting Materials Consortium

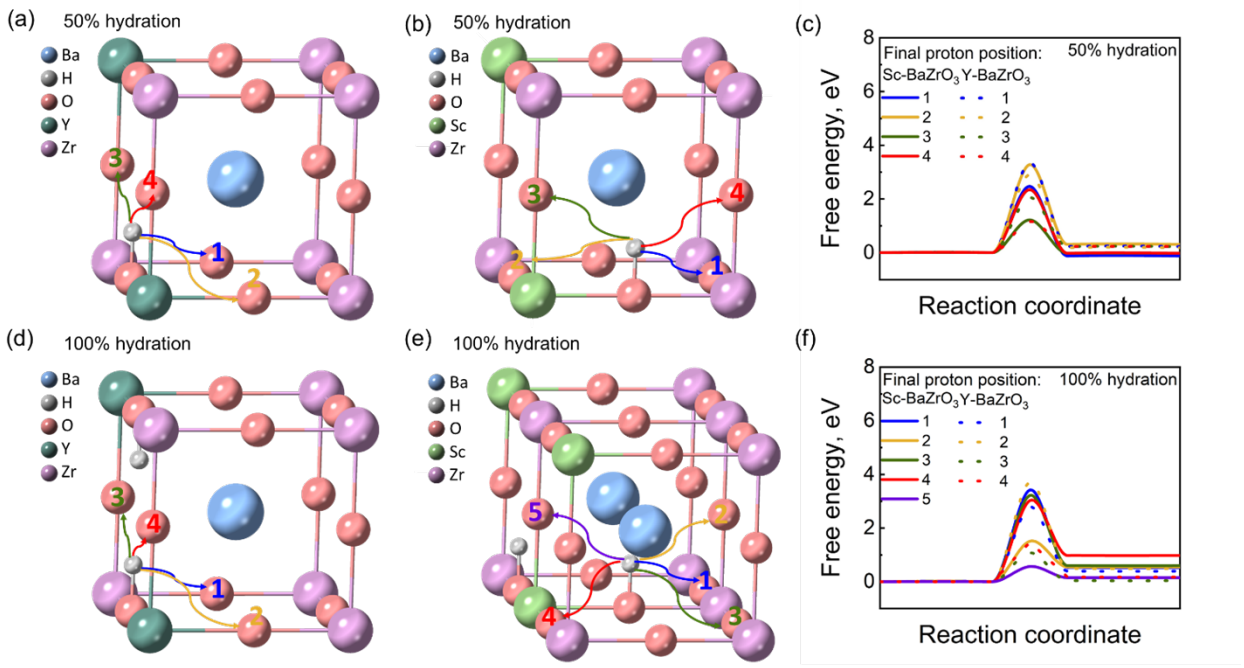

Figure 1: DFT calculation for proton migration of 25 mol% Sc or Y-doped BaZrO3. (a–b) Proton migration paths in the lattice at 50% of hydration. (c) Potential energy profiles for the proton migration paths in (a–b). (d–e) Proton migration paths in the lattice at 100% of hydration. (f) Potential energy profiles for the proton migration paths in (d–e).

F.2 Vacancy-Mediated Transport of Solutes in FCC Nickel under Diffusional Creep: A Density Functional Theory Study

Report Participants

Shousha, Shehabeldin M[1], Kadambi, Sourabh B[2], Kombaiah, Boopathy [2]
1 North Carolina State University
2 Idaho National Laboratory

Scientific Achievement

As part of a Basic Energy Sciences project titled “Fundamental Mechanisms of Newtonian Diffusional Creep in Structural Alloys," we investigated the diffusion of solute atoms, including Cr, Re, and Ta, within face-centered cubic (FCC) nickel-based alloys under conditions of diffusional creep. Our study employed atomistic modeling, utilizing DFT calculations with the Vienna Ab initio Simulation Package software. These calculations determined binding energies, migration barriers, and jump attempt frequencies of solute atoms. Subsequently, we integrated this atomistic data into the KineCluE code to calculate transport coefficients for vacancies and vacancy-solute pairs.

Significance

Nickel-based alloys find wide applications due to their corrosion resistance and high-temperature strength. However, at elevated temperatures, stress-induced vacancy diffusion results in diffusion creep. To understand this, our study calculated vacancy-mediated transport coefficients for various solute atoms (Cr, Re, Ta, W, Mo, and Co) in FCC nickel. We have derived important insights on vacancy drag ratios and solute enrichment and depletion tendencies at point defect sinks. Moreover, we investigated the effect of strain on the transport tendencies and found Cr and Ta, which are the fastest diffusing atoms, to be highly sensitive. For instance, a tensile strain of less than 3% can reverse their segregation behavior from depletion to enrichment at sinks. The calculated coefficients will find utility in parameterizing mesoscale phase field models to further investigate segregation and its effect under diffusional creep.

Key Publications

Shousha, S., Kombaiah, B., Kadambi, S., Vacancy-mediated transport of solute atoms in FCC nickel under diffusional creep: A density functional theory study. (In preparation)

Sponsor/Program

Basic Energy Sciences

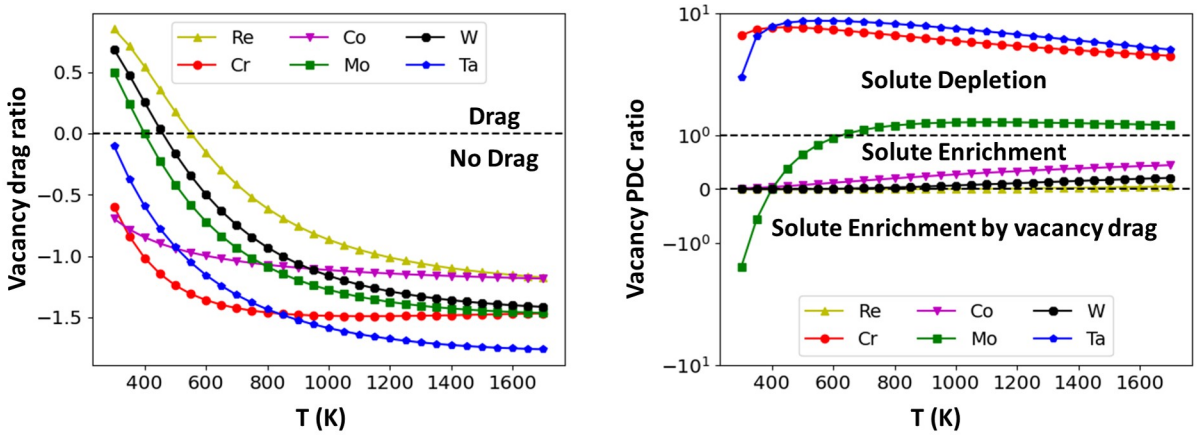

Figure 1: Vacancy drag ratios and partial diffusion coefficient ratios for solute atoms in FCC nickel.

F.3 Shielding and Activation Analysis of the Natrium LMFR

Report Participants

Napolitano, Dominic [1]
1 TerraPower

Scientific Achievement

Investigations will be made on the optimal use of Monte Carlo N-Particle and ADVANTG variance reduction in shielding and activation calculations.

Significance

The project investigates the activation of primary and secondary side sodium and associated radiological impacts as well as radiation damage to core components. Iterations will be made on the placement and shielding of reactor components, such as reactor vessels, intermediate heat exchangers, and fixed in-vessel shielding

Key Publications

In Progress

Sponsor/Program

Natrium/LMFR design and licensing

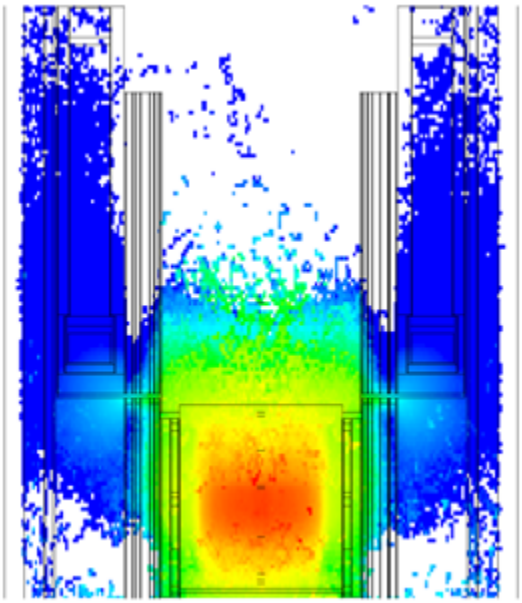

Figure 1: Optimized neutron flux to estimate intermediate heat exchangers sodium activation.

F.4 Molecular Dynamics Simulations of Defect Production in ThO2 under Irradiation

Report Participants

Zhang, Yongfeng [1], Yu, Lin-Chieh [2]
1 University of Wisconsin Madison
2 University of Wisconsin-Madison

Scientific Achievement

We have applied molecular dynamics simulations to simulate electron irradiation for the purpose of investigating the interaction of point defects and the formation of small defect clusters. The LAMMPS code is used for the simulations. The results from the Cooper potential in the literature and the Zhou's potential (internal communication), which is being developed within the Center for Thermal Energy Transport under Irradiation, are compared. These two potentials share the same mathematical expressions but differ in ionic charges and the many-body interaction (i.e., the embedded-atom-method part of the potential). In the simulations, a $20 \times 20 \times 20$ $a0^3$ (with a0 being the lattice constant) simulation cell containing 32,000 Th and 64,000 O ions is utilized. The temperature is controlled at 1500 K, and a zero-pressure, periodic boundary condition is applied. After relaxing the simulation cell, a 100 eV kinetic energy is assigned to a randomly selected primary knock-on atom, either Th or O, by rescaling the velocity along a random direction. This primary knock-on energy is well above the average displacement thresholds for both Th and O reported in the literature. Due to the very short molecular dynamics simulation time, a very high dose rate, 1.0e8 dpa/s, is used, and the total dose is about 0.1 dpa. To identify the defects, the Wigner-Seitz cell algorithm as implemented in the Ovito software is utilized. The concentrations of different types of Frenkel pairs are obtained as functions of time and irradiation dose.

Significance

The calculations identified a substantial discrepancy in the amounts of defects produced predicted by the two potentials adopted, motivating further research to compute the threshold displacement energies and to understand the impact of Coulomb interaction on defect production. The results will improve our understanding on irradiation damage in oxide fuels and its impact on thermal transport. The results will be included in a journal publication soon.

Key Publications

None

Sponsor/Program

Energy Frontier Research Center for Thermal Energy Transport under Irradiation.

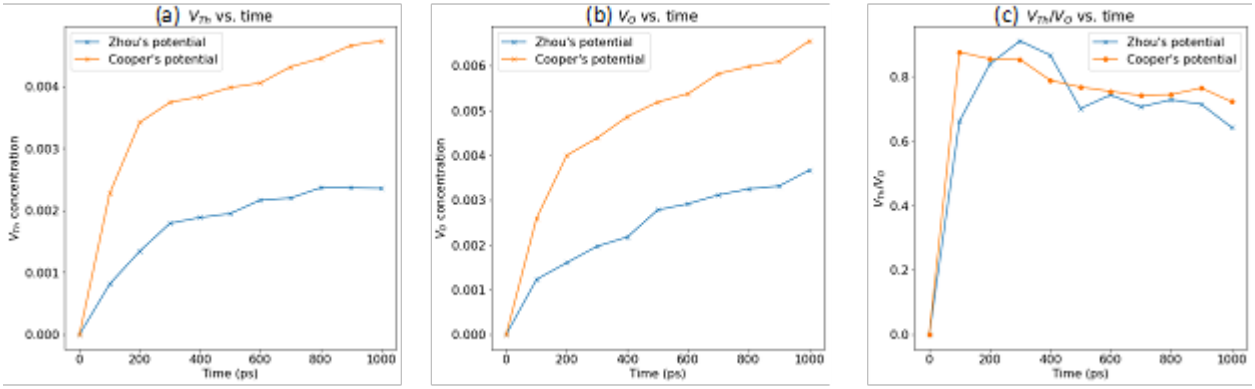

Figure 1: Concentrations of (a) Th vacancy (V_Th) and (b) O vacancy (V_o) and (c) the ratio of V_Th/V_o as functions of time.

Appendix G Operations

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G.1 Reactor Engineering, Advanced Test Reactor

Report Participants

Maile, Andrew D[1], Blight, Derreck S[1], Manwaring, Nathan H[1], Flores, Solmayra [1]
1 Idaho National Laboratory

Scientific Achievement

The Advanced Test Reactor (ATR) MC21 Application was used to perform the core physics analysis (CPA) for Cycle 171B and as-run for Cycle 171A. The CPA is a prediction for the ATR operating cycle and ensures that ATR safety basis requirements will be met for the duration of the cycle while meeting experiment requests. Using the ATR MC21 Application for the 171B CPA allowed for several fuel loadings to be evaluated in a short period of time to ensure the selected fuel met the requirements for the operating cycle. As-run analyses demonstrate model performance versus reality and are used to track ATR fuel element depletion and compositions for future use. The Cycle 171A as-run analysis demonstrated MC21's ability to accurately model critical shim positions and lobe powers. Additionally, MC21 was used to predict the reactivity effects of core changes in the Advanced Test Reactor Critical (ATRC) facility for test plan TP-2023-01. The high fidelity ATRC MC21 model accurately predicted the reactivity worth of core changes.

Significance

For each ATR operating cycle, a CPA must be completed to ensure the reactor is operated within the requirements of the ATR safety basis. The implementation of the ATR MC21 Application allows for several fuel and experiment loadings to be evaluated in a shorter period and with higher fidelity than was possible using previous modeling tools. As additional as-run simulations are modeled using MC21 potential model biases are expected to be accounted for in the CPA predictions which will lead to improved fuel utilization. The benefit of accurately predicting reactivity worth and critical shim positions in the ATRC allows for making large core changes in one step instead of several smaller steps. This reduces the number of core changes and reactivity measurements needed in test plans. Thus, less time is required to complete ATRC test plans and resulting in more availability for additional tests in the ATRC.

Key Publications

None

Sponsor/Program

Idaho National Laboratory

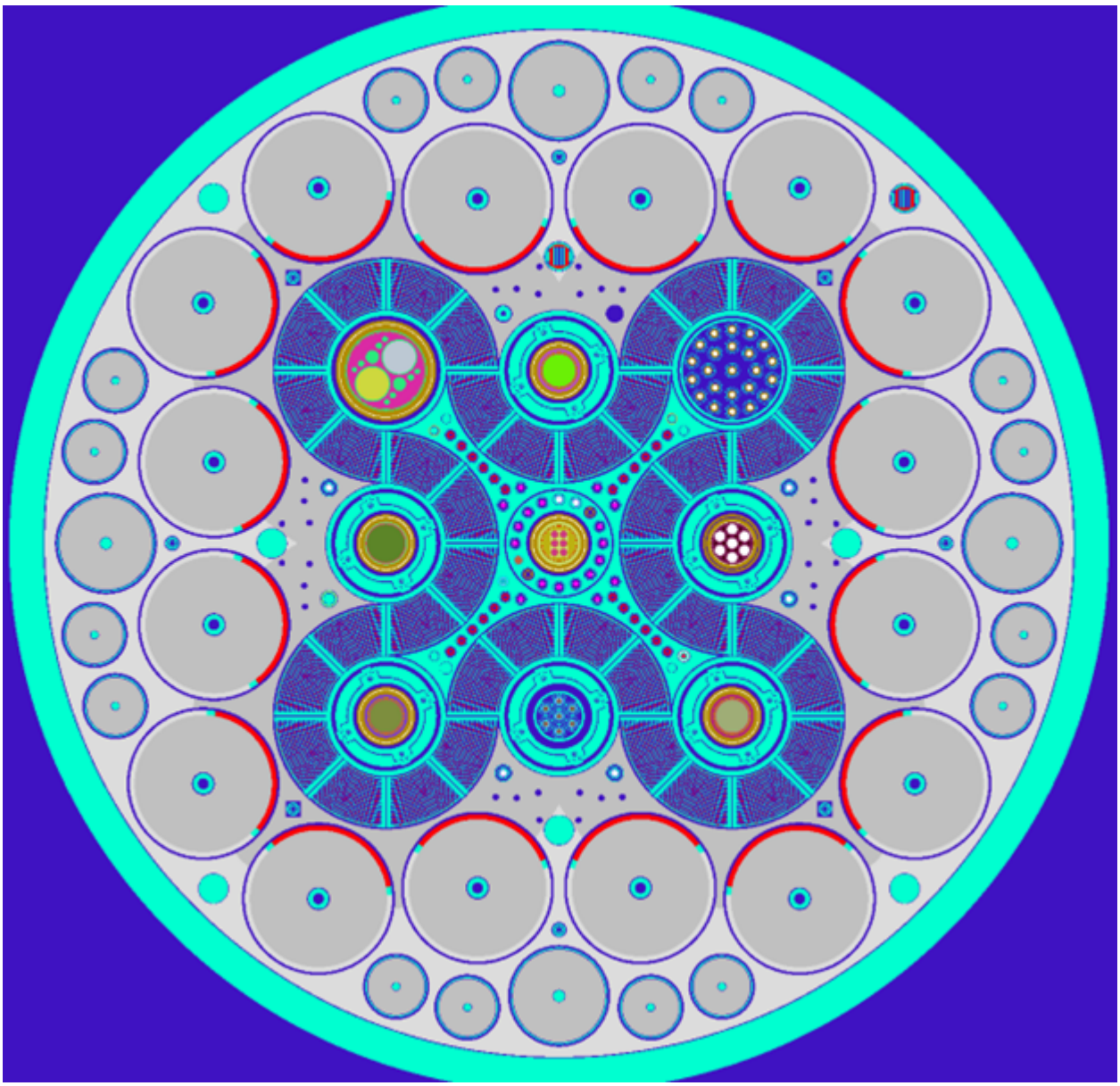

Figure 1: Cross sectional view (x-y plane) of 171A-1 MC21 as-run model.

Appendix H Naval Nuclear Laboratory

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H.1 Training Notebooks for CMCDT Users

Report Participants

Byrne, Stephen A[1], Gill, Daniel F[1], Marinan, Emily J[1], Spychala, Scott J[1], Wegener, Jeffrey J[1]
1 Naval Nuclear Laboratory

Scientific Achievement

A set of Jupyter notebooks are being prepared that guide new users in creating and running models using the Common Monte Carlo Design Tool (CMCDT) suite of codes.

Significance

The completion of this project will result in a set of independent training resources that CMCDT users can reference as they get started with the CMCDT codes. This will benefit new CMCDT users at Idaho National Laboratory (INL) and Naval Nuclear Laboratory (NNL), especially those in the NNL Early Start program.

The work is still in progress, with additional notebooks expected to fill any gaps in the training.

Key Publications

None

Sponsor/Program

NNL

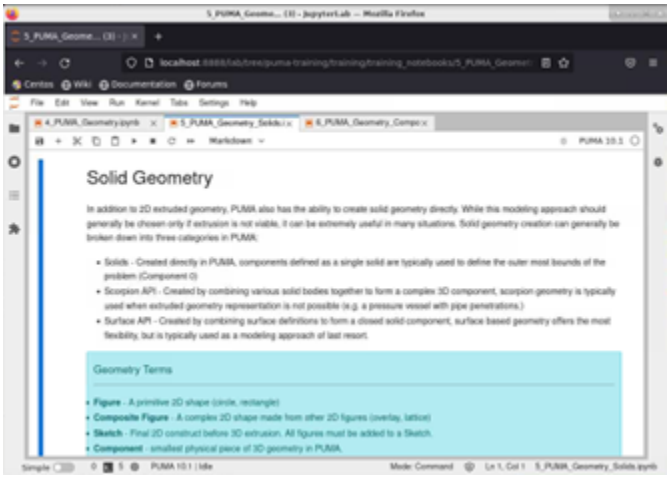

Figure 1: Jupyter notebooks open in Firefox on a Sawtooth terminal.

H.2 Investigation of MOOSE Structural Solver Capabilities

Report Participants

Carter, Jesse J[1]
1 Naval Nuclear Laboratory

Scientific Achievement

NNL is tasked with designing systems to power the U.S. Navy. The Reactor Technology organization within NNL uses the INL Sawtooth High Performance Computing (HPC) cluster to evaluate and test open-source finite-element software for potential inclusion in the structural design workflow. By evaluating codes such as the Multiphysics Object-Oriented Simulation Environment in an open environment, we can more quickly assess the capabilities of available software on production platforms prior to ingressing to NNL systems. Any desired capabilities can be rapidly prototyped and tested on the INL HPC platform.

Significance

By bringing in more options to NNL designers, we can increase flexibility in the design workflow and alleviate bottlenecks that come from licensing and limitations of different software packages. By testing software interoperability on INL HPC systems, we can ensure minimal disruption to NNL users by verifying compatibility with existing software and data infrastructure.

Key Publications

None

Sponsor/Program

NNL

H.3 Overlord API, Bayesian Optimization for Engineering Design Work

Report Participants

Parrish, Kevin D[1], McGovern, Steve [1]
1 Naval Nuclear Laboratory

Scientific Achievement

The objective of this project is to develop a machine learning platform that adaptively learns from physics simulations to efficiently find optimal solutions to engineering design problems with automated workflows. New features have been added, such as built-in convex optimization, more comprehensive benchmarking, Dash based web application for visualization, dimensionality reduction via active subspaces, and discrete optimization including Thompson sampling.

Significance

This project has been shown to reduce the number of high-fidelity calculations of key analyses by an order of magnitude. Moreover, the automation reduces the engineering design work and decreases the walltime to obtain solutions by over 75%. Work is being spent to create derivative programs and integrate Bayesian optimization into existing production tools at NNL.

Key Publications

None

Sponsor/Program

NNL

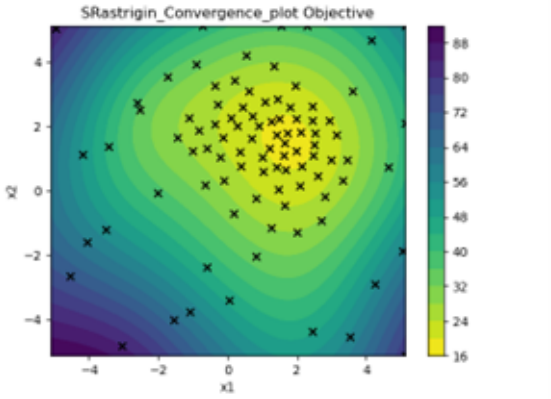

Figure 1: Metamodel objective and trial samples for a 2D Rastrigin benchmark.

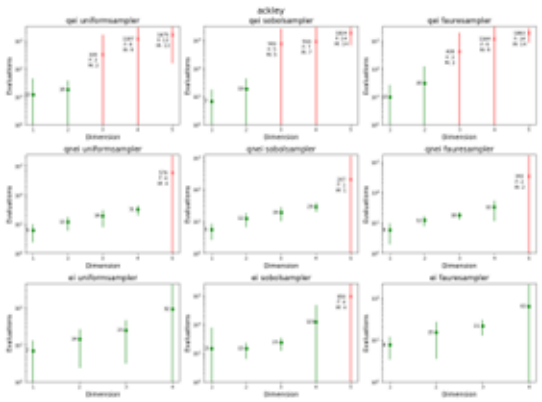

Figure 2: Benchmark results for Ackley function versus dimension over 16 randomized samples with different acquisition functions and initial samplers.

H.4 Atomistic Simulations of ZrO2 Interfaces and Their Effect on Corrosion

Report Participants

Lucking, Michael C[1], Smith, Richard W[1]
1 Naval Nuclear Laboratory

Scientific Achievement

First principles DFT calculations were performed on ZrO2/water interfaces. The (-111) surface of monoclinic ZrO2 was investigated, and nudged elastic band calculations were performed to describe reactions occurring at the surface. A model for the (110)/(-110) grain boundary in monoclinic ZrO2 was also created with DFT calculations. The energetics of oxygen vacancies and their diffusion barriers were calculated with the nudged elastic band method. All calculations were done with the Vienna ab initio Simulation Package simulation package.

Significance

This work is part of a larger effort to develop an in-depth mechanistic understanding of the corrosion process of zirconium alloys. The presence of water molecules adsorbed on the surface changes the location and nature of localized holes at the surface of ZrO2. Surface holes are able to oxidize adsorbed hydroxyl ions on the surface. The resulting hydroxyl radicals are very reactive and will quickly react with the ZrO2 surface in the presence of another hole, forming an oxygen-oxygen bond (Figure 1). These species could lead to the destabilization of the surface and local dissolution of the oxide in addition to changing the local water chemistry, impacting the corrosion process.

Grain boundaries have been proposed to provide fast diffusion paths for oxygen atoms in the oxide scale of corroding zirconium alloys. The diffusion of oxygen atoms through the oxide film is the rate limiting step in the corrosion of zirconium alloys and will determine the rate at which the metal corrodes. They may also be locations where impurities accumulate and boundaries at the surface can provide active sites for chemical reactions. Studying atomistic models of grain boundaries will improve our understanding of corrosion films and enable the development of improved macroscopic models of corrosion with the correct treatment of grain boundary effects. The (110)/(-110) grain boundary in monoclinic ZrO2 (Figure 2) has been chosen as a starting point to study grain boundaries due to its low energy and ability to be modeled with a relatively small number of atoms. The DFT calculations show that oxygen vacancies, both charged and neutral, are found to preferentially reside at grain boundary sites over bulk sites. However, the diffusion barriers of these vacancies at the grain boundary are not significantly different than the diffusion barriers in the bulk. While we can't conclude that none of the grain boundaries in ZrO2 support enhanced oxygen diffusion, we have shown that at least one grain boundary does not lead to enhanced oxygen diffusion rates. Further work on grain boundaries in ZrO2 will be needed to identify which, if any, grain boundaries are responsible for fast oxygen diffusion and which grain boundaries do not enhance the oxygen diffusion of the corrosion film.

Key Publications

None

Sponsor/Program

NNL

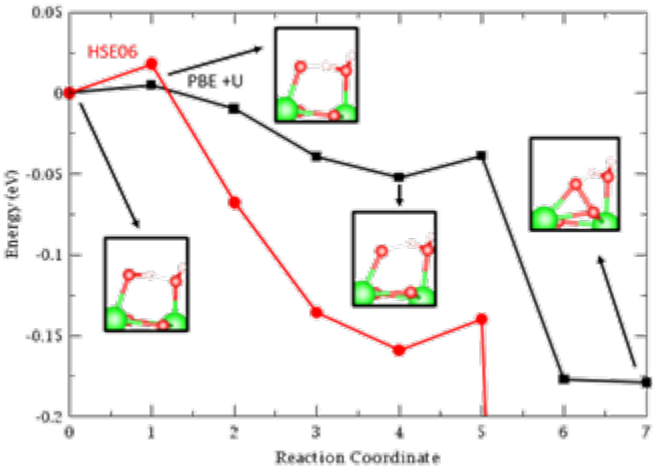

Figure 1: Calculated reaction barrier for the reaction of a hydroxyl radical with a localized hole on a lattice oxygen on the ZrO2 surface. PBE +U and HSE06 results are shown in black and red, respectively. Insets show the local atomic structure at various points along the reaction path, with Zr atoms in green, oxygen atoms in red, and hydrogen atoms in pink.

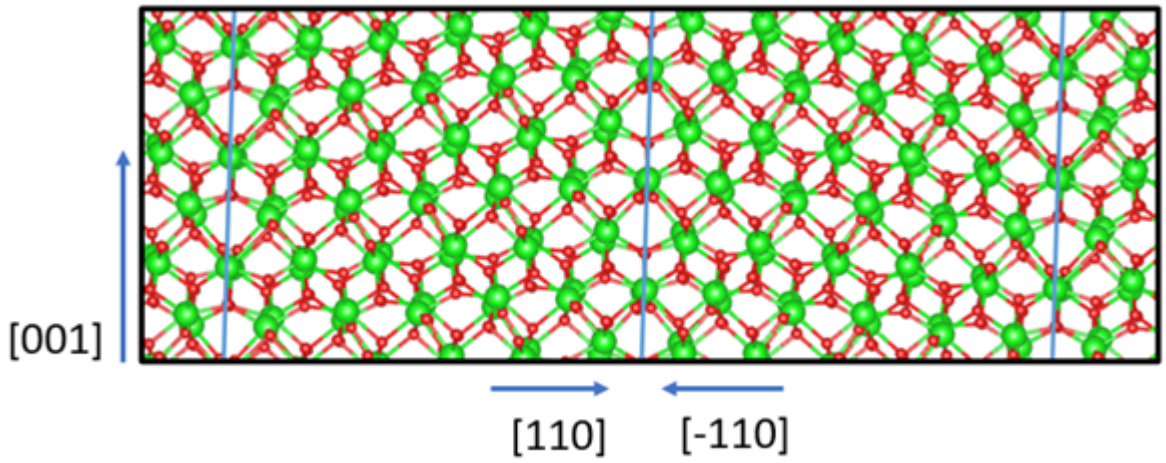

Figure 2: (110)/(-110) grain boundary model in monoclinic ZrO2. Locations of the grain boundaries are identified with blue vertical lines. The supercell used in the calculations has periodic boundary conditions. Crystal directions are shown next to the atomic structure. Zr atoms are in green, and oxygen atoms are in red.

H.5 Machine-Learned Interatomic Potential Development

Report Participants

Wormald, Jonathan L[1], Chamberlain, Eric S[1], March-Rico, Jose F[1], Najafabadi, Reza N[1]
1 Naval Nuclear Laboratory

Scientific Achievement

Machine-learned interatomic potentials (MLPs) are being developed with the MLP generator available in the MedeA atomistic simulation environment (Materials Design Inc.). The MLP generator was developed through the NNL- sponsored Advanced Materials Simulation Engineering Tool Project. MLPs are currently being evaluated for Zr metal, the Zr-H system, and the Zr-O system with applications in radiation damage, thermodynamic processes, and corrosion. Testing through LAMMPS molecular dynamics (MD) simulations includes but is not limited to defect energetics, phase transitions, phonons, and diffusion. Validation of MLPs includes a comparison to training set entries to determine accuracy to quantum mechanical calculations and a comparison to experiment data to determine the accuracy of the quantum mechanical methods for predicting key phenomena related to environmental degradation.

Significance

In Zr alloys the HCP and BCC phases are of technological significance to fabrication and service, but the face-centered cubic (FCC) phase is also important as it relates to the formation of zirconium hydride (ZrHx). A set of Zr-H spectral neighbor analysis potential type MLPs have been used in LAMMPS to simulate the heating and cooling of Zr models to assess the phase transition behavior. Figure 1 plots the potential energies of HCP, FCC, and BCC cells taken through temperature ramps. The HCP and FCC runs ramp up in time, whereas the BCC run ramps down. As expected, HCP is the stable phase at low temperatures, and BCC takes over at high temperatures. Upon heating, a prompt transition from HCP to BCC takes place at about 1400 K, which is higher than the experimental value of 1135 K, but given the inclusion of ZrHx structures in the MLP development, the result is encouraging. Significant undercooling occurs in the return phase transition from BCC to HCP; moreover, BCC is unstable at low temperatures and will collapse to FCC or HCP with small perturbations to the MD simulation box. Figure 2 illustrates the crystal structure during the HCP ! BCC phase transition. Although FCC is the least preferred state of Zr for all temperatures, the spectral neighbor analysis potential predicts that it is metastable such that sufficient thermal agitation is required to cause an FCC to HCP transition.

Key Publications

N/A

Sponsor/Program

NNL

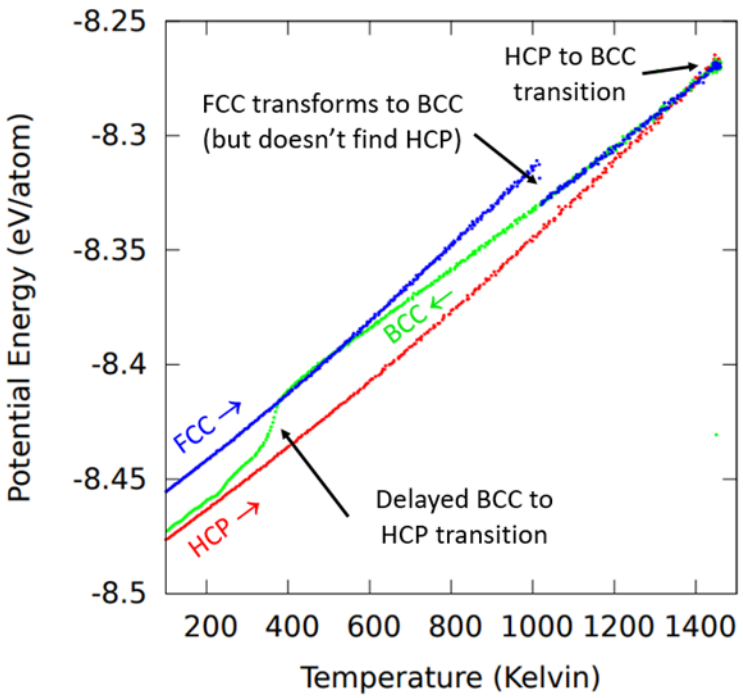

Figure 1: Potential energy trends for phase changes from heating and cooling simulations. HCP transforms to BCC when heated above 1400 K. Significant undercooling is required to observe the BCC ! HCP transition for the ramp rates of this MD study. Upon heating, FCC transforms to BCC near 1000 K bypassing any transition to HCP.

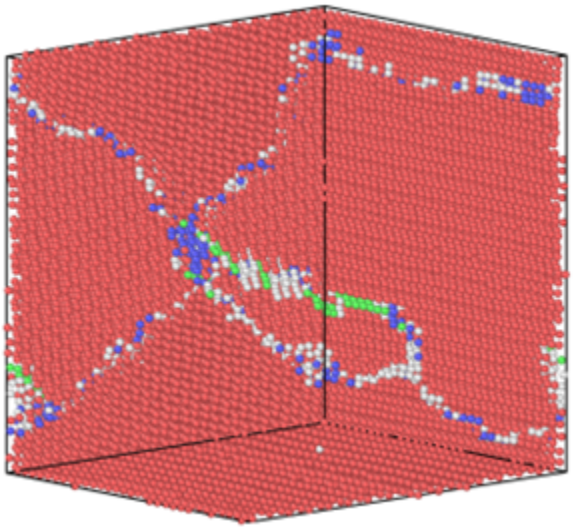

Figure 2: Partially transformed cell in the transition from BCC (blue atoms) to HCP (red atoms). White or green coloring reflects twin or misaligned HCP crystallites as derived from common neighbor analysis in Ovito.

H.6 Multiscale Modeling of Environmental Degradation in Structural Materials

Report Participants

Anglin, Benjamin S[1]
1 Naval Nuclear Laboratory

Scientific Achievement

NNL is developing environment-sensitive, physically based plasticity models at various length scales across many orders of magnitudes, as shown in Figure 1. Results obtained from one length scale are readily passed to another length scale owing to the unified set of physics and understanding of underlying mechanisms built into each of these models. INL HPC supports both electronic structure calculations and novel fast Fourier transform (FFT) driven crystal plasticity simulations. These results are integrated with a multiscale physically based model for oxidation to simulate stress corrosion cracking on an explicit 3D microstructure.

Significance

Environmental cracking is a localized pheomenon in structural materials where only the conditions near the crack tip are of importance. In the case of stress corrosion cracking in aqueous environments, these conditions include local chemistry, stress, and material microstructure. Conventional empirical models used to predict stress corrosion cracking rely on large datasets to offer model accuracy whereas physically based models developed in this project use an understanding of underlying operative physical mechanisms to build accuracy, thereby promoting confidence in model accuracy outside the available dataset. Simulations over a wide range of time and length scales, such as electronic structure theory to capture the atomic-level environment and chemistry, are used to construct and inform a crystal plasticity model that explicitly accounts for mechanical deformation in the material microstructure. Stress corrosion cracking simulations of explicit microstructures quickly become intractable in finite-element methods owing to the large domains required to emulate significant explicit microstructures. An alternative approach, employed here, is to use FFTs to solve the micromechanical equations throughout a large (104 grains) microstructure. Thus, realistic simulations of stress corrosion cracking can be achieved, as shown in Figure 2.

Key Publications

Anglin, B. S. & Webb, T. W., Modeling Stress Corrosion Cracking with Explicit Three-Dimensional Grain Microstructures, Proceedings of the 20th International Conference on Environmental Degradation of Materials in Nuclear Power Systems, Snowmass Village, CO, 2022

Sponsor/Program

NNL

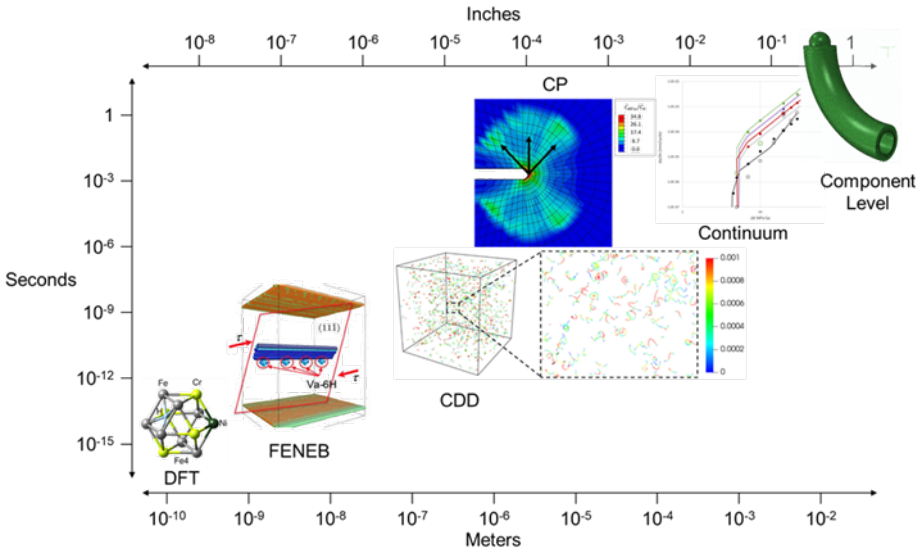

Figure 1: A schematic of the range of length scales, in both meters and inches, and time scales, in seconds, spanned in the multiscale modeling approach employed in the EICEM program. Legend: DFT = density functional theory; FENEB = free end nudged elastic band; CDD = continuum dislocation dynamics; CP = crystal plasticity.

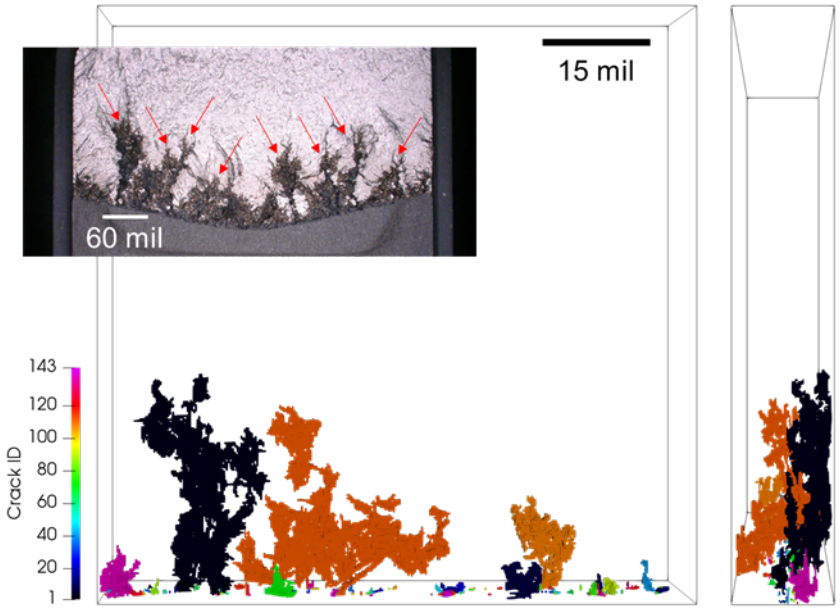

Figure 2: (Top left) Light optical image of SCC fingers in specimen MG5-027 (Heat D2739) developed in a 12.2% cold worked 304 stainless-steel specimen loaded in the LT orientation. Red arrows indicate the fingers. (Bottom) A simulated SCC crack that resembles SCC fingers after 15% cold rolling visualized from the top-down (left) and side views (right) colored by individual crack identification number. The bounding boxes indicate the microstructural volume.

H.7 Investigation of Cross-Slip Mechanisms in Zirconium

Report Participants

Baker, Kristopher L[1]
1 Naval Nuclear Laboratory

Scientific Achievement

This project extends the open-source molecular dynamics software package LAMMPS to predict defect reaction pathways in a model zirconium material. Starting from a zero-temperature reaction path discovery tool, the atomic-scale reaction mechanisms are being explored. This will pave the way for more advanced finite-temperature reaction path exploration methods to reveal temperature and stress effects on the reaction rate.

Significance

The activation of cross-slip of screw dislocations in zirconium alloys is a rate-controlling deformation mechanism that is still poorly understood. This work seeks to predict the minimum energy reaction paths for cross-slip in zirconium to inform continuum-scale finite-element deformation models. Currently, the methodology is being used to probe the possible reactions using a simple methodology. Once the simulation framework is optimized for these types of reactions, further studies will investigate temperature and stress effects on the reaction rate. Preliminary data on two possible cross-slip reactions are presented in Figure 1. Figure 2 shows the miscoordinated atoms undergoing the double cross slip transition, where the center of the dislocation line can be observed to change orientation to an inclined slip plane.

Key Publications

N/A

Sponsor/Program

NNL

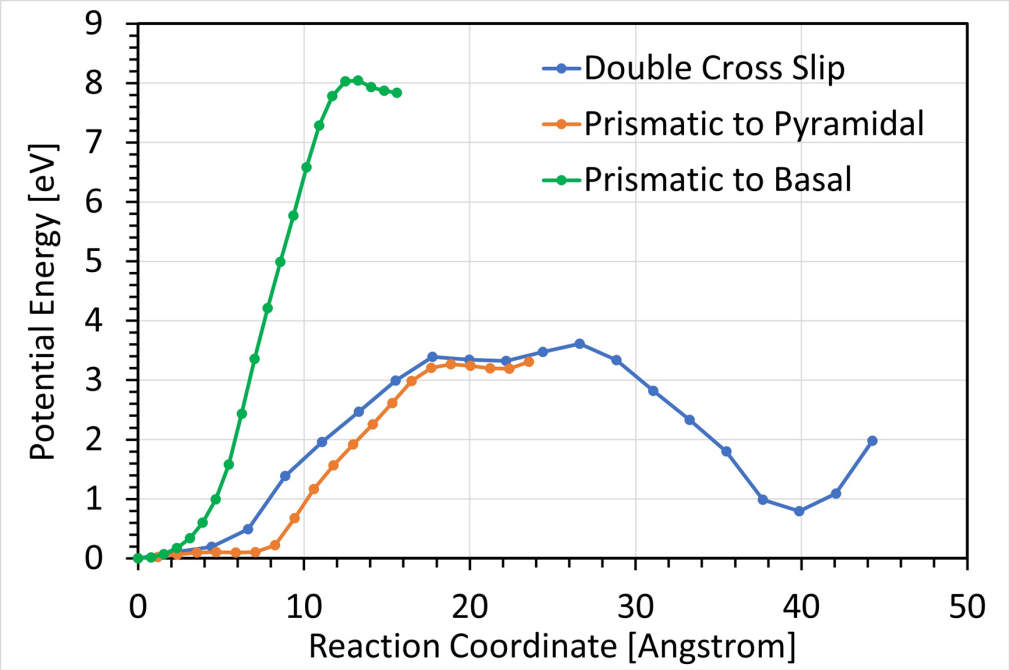

Figure 1: Preliminary plot of various cross-slip reaction path energies.

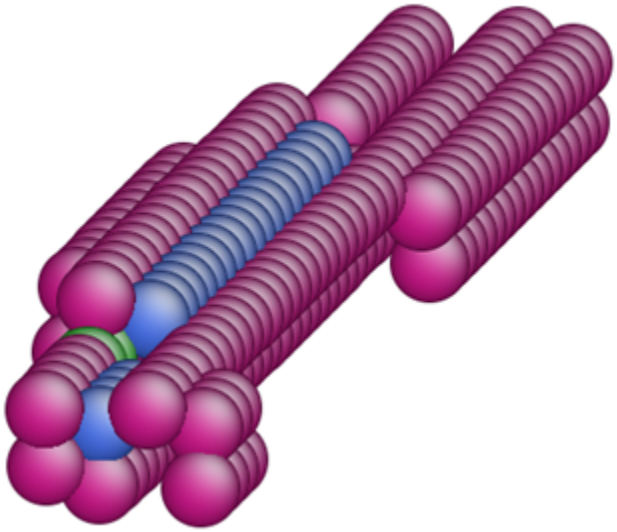

Figure 2: Atomic configuration of the double cross-slip transition. The miscoordinated atoms are shown, and the center of the dislocation line has rotated to rest on an inclined slip plane.

H.8 Explore Collaboration Opportunities with RELAP5-3D

Report Participants

Andress, Spencer W[1], Berkenpas, Michael B[1], Buschman, Francis X[1], Meholic, Michael J[1], Steere, Ryan P[1]
1 Naval Nuclear Laboratory

Scientific Achievement

This work on the INL HPC thus far has been focused primarily in two areas. The first is related to evaluating our capability to establish a more collaborative development relationship with the RELAP5-3D team at INL. The second is related to developing and running models of open literature experimental facilities or canonical problems using RELAP5-3D. This team has been working with INL to identify software limitations and availability on the INL HPC system that can be targeted to make this a more effective collaboration environment. Through current contracts with INL, some of these limitations are being addressed that could make this a more viable workspace for RELAP5-3D development and use in the near future.

Significance

Understanding the capabilities and limitations of performing collaborative development and assessment of RELAP5-3D, between NNL and INL, on the INL HPC environment is important in shaping the strategic direction of RELAP5-3D use and development at NNL.

Key Publications

None

Sponsor/Program

NNL

H.9 Reduced-Order Modeling of Neutron Transport by Proper Orthogonal Decomposition in Energy

Report Participants

Dominesey, Kurt A[1]
1 Naval Nuclear Laboratory

Scientific Achievement

This project aims to develop reduced-order models (ROMs) of neutron transport achieved by Galerkin or balanced proper orthogonal decomposition (POD) in energy. This approach enables a high-fidelity energy treatment to be directly embedded in a reduced-order representation of the transport equation, providing increased accuracy without the excessive computational cost generally associated with high-fidelity energy methods. Achievements over the past year include a derivation of coarse-group, Petrov-Galerkin ROMs; implementation in C++ using the deal.II finite-element library; and characterization of model accuracy in prototypical light-water reactor pin-cell benchmarks. These results will inform the development of similar capabilities in the NNL's Advanced Deterministic Transport (ADT) suite of reactor physics applications

Significance

High-fidelity yet computationally affordable models of reactor physics are essential to designing and analyzing nuclear reactors. Using POD, such a model can be created by extracting the dominant features from a set of high-fidelity reference solutions, as visualized in Figure 1. Accordingly, these POD ROMs may offer a comparable level of fidelity at a substantially reduced computational effort, making them eminently useful analysis tools. Moreover, as a means of model approximation, POD may prove superior to the predominant methods practiced in reactor physics, such as cross-section condensation and associated techniques.

Key Publications

None

Sponsor/Program

NNL

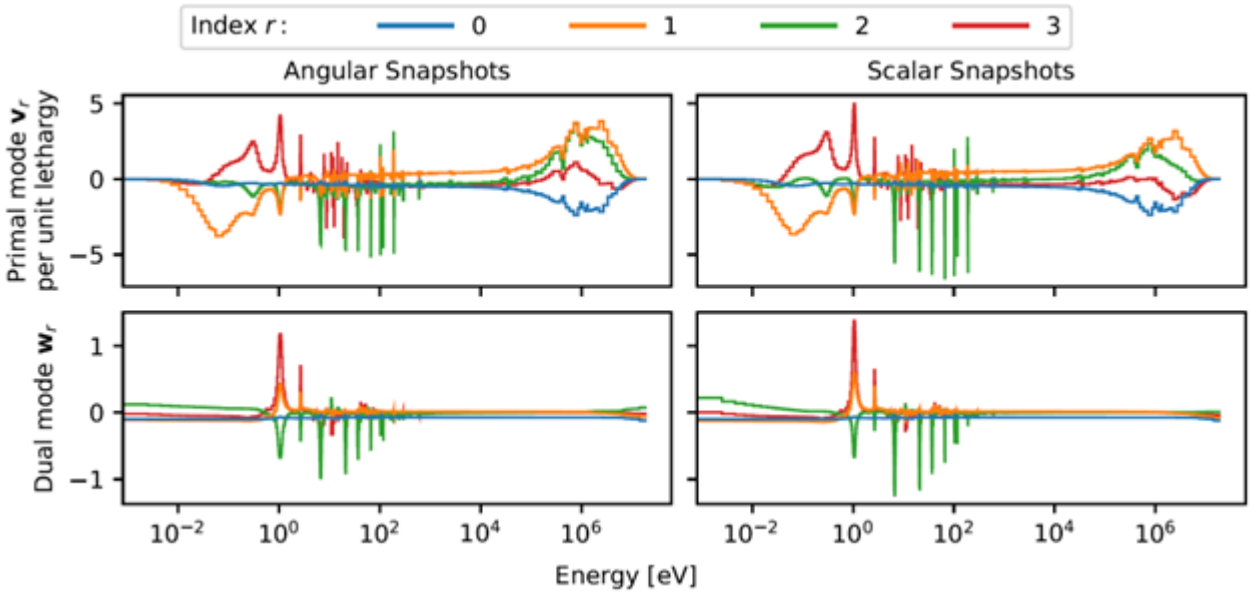

Figure 1: Balanced energy modes computed from light-water reactor pin-cell reference solutions.

H.10 DFT Calculations to Predict Physical Properties and Diffusion Parameters for Interstitial and Vacancy Mechanisms in U_3–0Si–0_2

Report Participants

Abdalla, Yassir G[1], Ougouag, Abderrafi M[2], Ivanov, Kostadin [3]
1 Naval Nuclear Laboratory
2 Idaho National Laboratory
3 North Carolina State University

Scientific Achievement

Modeling of microstructural development of fuel under neutron irradiation poses a significant challenge, especially for new fuel types that lack experimental data. In this research, calculations to predict physical properties and diffusion parameters for interstitial and vacancy mechanisms were based on DFT and done using MedeA (Vienna ab initio Simulation Package, PHONON, LAMMPS, etc.).

Significance

U_3 0Si 0_2 fuel has potential for usage in future power reactors due to its higher reactivity loading, longer fuel cycles, and high uranium density. Exploring the possibility of using the fuel (U3Si2) pellets in advanced reactors is important in studying the accident-tolerant nature of the fuel. Activation energies, jump frequencies, diffusion coefficients, and relaxation volumes for migration through interstitial and vacancy mechanisms are predicted using advanced DFT calculations, while elastic constants, such as shear modulus and poison ratio, are calculated using the MT-Elastic Properties module, which accounts for the isotropic behavior of U_3 0Si 0_2. Dislocation climb speed, di-interstitial climbing speed, and interstitial recombination rate can all be computed using these values. This work is still in progress.

Key Publications

The following research article is in progress: DFT Calculations to predict physical Properties and Diffusion parameters for interstitial and vacancy mechanisms in U_3 0Si 0_2.

Sponsor/Program

ATR
NNL
Research towards a PhD with NCSU

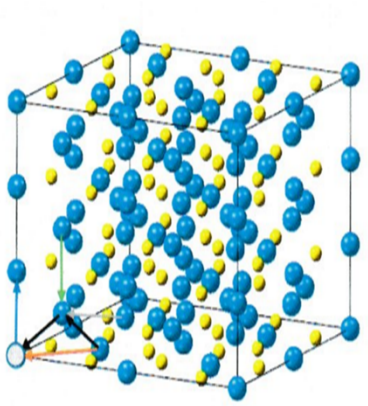

Figure 1: Vacancy diffusion mechanisms for U atoms.

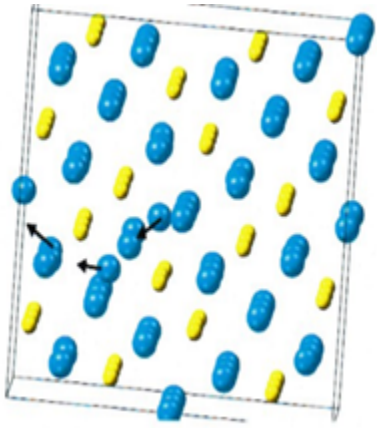

Figure 2: Interstitial diffusion mechanism.

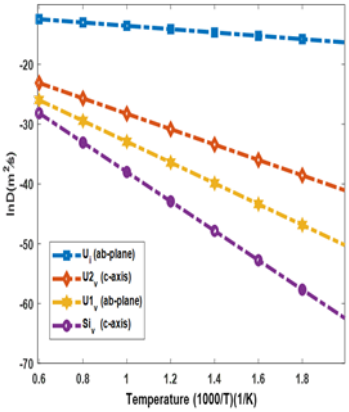

Figure 3: Diffusion coefficients as a function of temperature.

H.11 Development of 3D Polyhedral Meshing Utility Corona

Report Participants

Becker, Troy L[1], Dominesey, Kurt A[1]
1 Naval Nuclear Laboratory

Scientific Achievement

Corona is a new NNL meshing utility for the ADT project (which includes the neutral-particle deterministic transport solver Jaguar). It is a C++ program that accepts a custom hierarchical YAML description of 3D geometry and meshes it for the transport solver Jaguar. Achievements over the past year include completing most of the computational geometry functionality to mesh the 3D volumes with bricks, while ensuring convex mesh cells.

Significance

This development effort is to support an ADT workflow that expands capability from 2D-extruded geometry to true 3D geometry.

Key Publications

None

Sponsor/Program

NNL

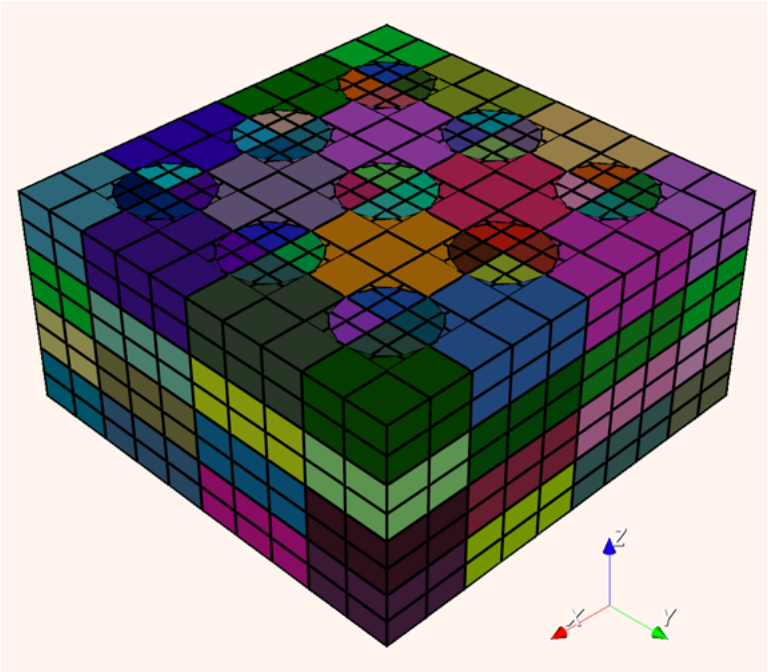

Figure 1: Meshed 3 × 3 assembly with a thermal grid.

H.12 Arc-dpa Parameterization of Defect Production in -Zirconium

Report Participants

March-Rico, Jose F[1], Wormald, Jonathan L[1], Zerkle, Michael L[1], Smith, Richard W[1]
1 Naval Nuclear Laboratory

Scientific Achievement

Damage accumulation in irradiated materials has historically been quantified using the Norgett-Robinson-Torrens displacements per atom (NRT-dpa) formula. The athermal recombination corrected dpa (arc-dpa) method has been recommended to modify the traditional NRT-dpa with the incorporation of in-cascade athermal recombination of defects. The resources at the INL HPC Enclave have been utilized to run displacement cascades in -zirconium to quantify the extent of athermal recombination and provide parameters to calculate the arc-dpa damage efficiency function. Arc-dpa parameters have been calculated using traditional embedded-atom method potentials in addition to a new MLP developed as part of the Advanced Materials Simulation Engineering Tool project (Figure 1).

Significance

Arc-dpa calculations are more physically realistic than NRT-dpa calculations. The arc-dpa also results in unique damage rates for different materials exposed to the same neutron energy spectrum, as well as for the same materials exposed to different neutron energy spectra. By providing arc-dpa parameters for -zirconium, calculations of damage rates in higher-order engineering codes can be greatly improved. Additionally, this work compares and contrasts differences in simulation predictions between traditional embedded-atom method potentials and modern MLPs. Cascade characteristics were found to be nearly equivalent for simulations performed with both interatomic potential types, but the MLP predicts a factor of two greater defect production (Figure 2). This is expected to be driven by the relatively lower interstitial mobility predicted by the MLP. The work performed here marks the first time that displacement cascades have been performed in -zirconium using a modern MLP developed by Materials Design Inc. in collaboration with NNL. It is worth highlighting that the interstitial mobility predicted by these potentials appears to have a significant effect on damage production rates from cascade simulations. As such, it is recommended to consider and report diffusion-related properties when possible to assist in discussions of future displacement cascade simulations.

Key Publications

N/A

Sponsor/Program

NNL

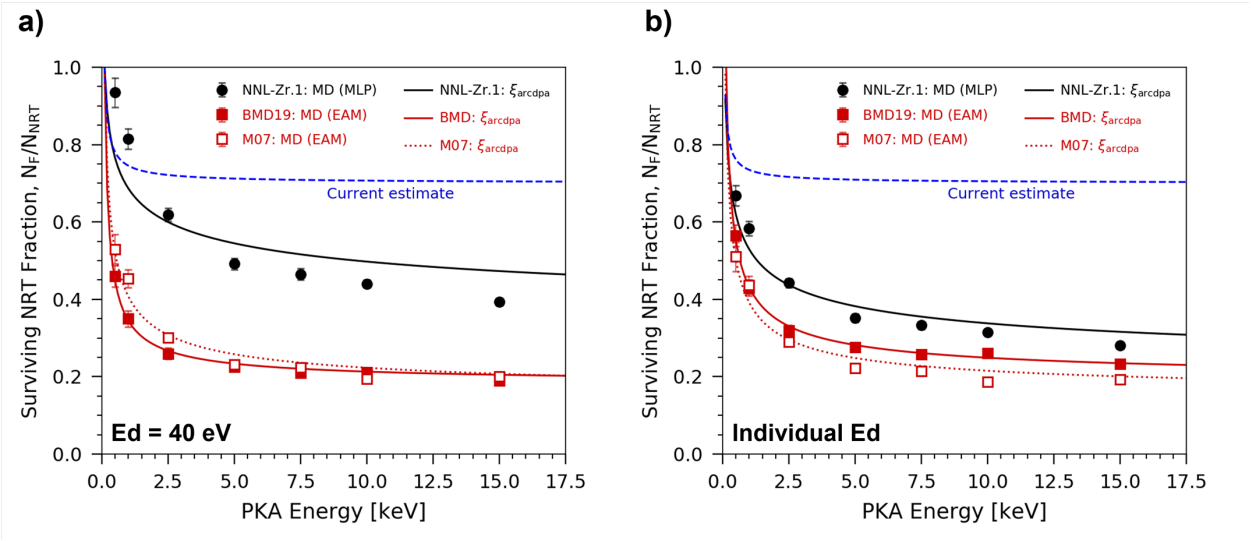

Figure 1: The surviving fraction of Frenkel pairs that survive post-cascade at T = 8 K compared to the NRT-predicted number of stable defects when calculated with: a) the standard E_d= 40 eV for each potential or b) the individual (E_d) values calculated for each potential. The arc-dpa damage efficiency function, arcdpa, is fit to the averaged MD results. Error bars represent the standard error of the mean.

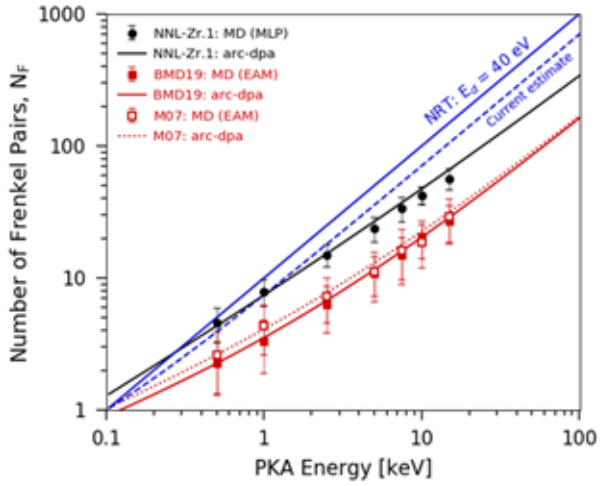

Figure 2: The surviving number of Frenkel pairs that survive post-cascade at T = 8 K for the BMD19.3, M07 #3, and NNL-Zr.1 potentials. Markers indicate MD data averaged over 50 simulations (error bars represent standard deviation) while the solid lines are calculated with based on the arc-dpa damage efficiency curves fitted in Figure 1. The NRT-predicted number of defects (Ed = 40 eV) and the arc-dpa model based on parameters estimated by experimental values are plotted for comparison.

H.13 MFEM for Simulations at Scale- Developing GPU-Capable Structural and Fluids Solvers Using the MFEM Library

Report Participants

Mattis, Steven A[1], DeCaria, Victor P[1], Schneier, Michael H[1]
1 Naval Nuclear Laboratory

Scientific Achievement

Solvers for structural engineering and computational fluid dynamics are being prototyped using MFEM, a C++ based finite-element method library created by Lawrence Livermore National Laboratory that contains state-of the-art functionality, including arbitrary high-order elements, adaptive mesh refinement schemes, and graphics processing unit (GPU) accelerated solvers. This project involves evaluating methods for using MFEM for general applications in single-phase computational fluid dynamics and structural mechanics. Models, discretizations, and geometries used will be common in the open literature (e.g., Reynolds-Averaged Navier-Stokes with k-epsilon and Large Eddy Simulation turbulence models, linear and nonlinear elasticity on rectangular beams). In particular, this project is interested in code portability and flexibility to be run on a variety of hardware architectures including GPUs. The scalability of these solvers and finite-element discretization are being analyzed in the strong and weak sense. This scalability, especially in regards to high-order and discontinuous Galerkin methods will likely be novel for some of these classes of problems.

Significance

There is currently a paradigm shift occurring within the HPC community towards GPU-accelerated machines due to their higher performance and improved efficiencies. Although there is no silver-bullet solution that will meet all needs, it is essential to leverage existing software solutions to manage the generic software tasks outside of numerics, modeling, and acceptability measures while being flexible enough to serve multiple engineering domains. To this end, MFEM provides one such solution. The MFEM project has an annual budget of over 10 million dollars with 15 full time developers at Lawrence Livermore National Laboratory, as well as many others spread throughout the Department of Energy (DOE) national laboratories, academia, and industry. The DOE has made a massive investment in the development of modular and flexible open-source libraries that can be used as building blocks for computational methods. These component libraries are designed to provide exascale performance with markedly reduced developer time. Their large reach and diverse developer communities ensure that they are kept up to date with the newest hardware and software technologies.

It is uncertain how feasible it is to procure GPU-enabled versions of existing proprietary solvers, and how long it will take to acquire them if we can. No single open-source or commercial off-the-shelf software solution exists that can sufficiently model the large-scale problems of the future. A software library like MFEM can, however, be used as a set of building blocks to develop our own versions of GPU-enabled solvers designed with GPU capability in mind. MFEM is very lightweight and flexible and has been used to develop several DOE solvers that have shown impressive scalability on a variety of architectures.

Key Publications

N/A

Sponsor/Program

NNL

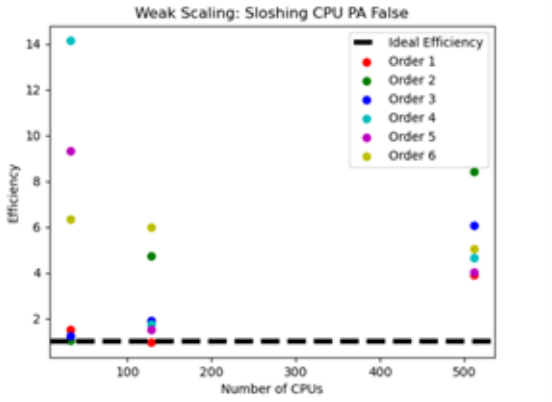

Figure 1: Weak scaling of a two-phase flow model on central processing units.

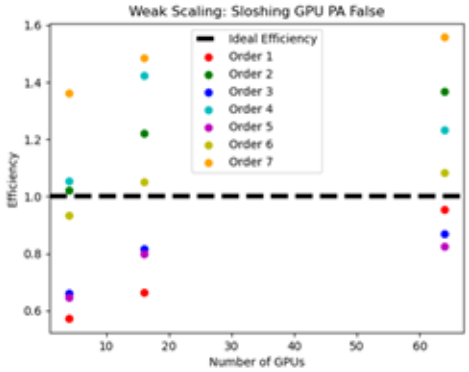

Figure 2: Weak scaling of a two-phase flow model on GPUs.

H.14 PWR-1 Depletion Feedback Model Validation and Use for Spent Fuel Packaging Decisions

Report Participants

Neumann, Kyle V[1], Spychala, Scott J[1], Jaber, Amir E[1]
1 Naval Nuclear Laboratory

Scientific Achievement

A spent fuel criticality safety analysis is performed to ensure that fuel removed from the reactor can be transported and stored safely while minimizing the impact to people and the environment. Some PWR-1 fuel from the Shippingport Atomic Power Station is in storage today. This project extends previous development and validation of a PWR-1 depletion feedback model to provide technical expertise to safely package the PWR-1 nuclear fuel. The depletion feedback model provides input to the safety analysis by characterizing the remaining inventory for criticality calculations and providing irradiation data for use in structural analyses.

Significance

This project finalizes the validation of a depletion feedback PWR-1 model and applies it for use in spent fuel criticality analyses for processing and packaging decisions. Some blanket fuel assemblies from the PWR-1 core remain in storage today. A detailed nuclear model was developed to determine the amount of fuel remaining to support safely packaging the assemblies. As a part of the process, meticulous checks and comparisons are performed to ensure any bias or uncertainties in the models are accounted for. Figure 1 illustrates the neutron flux distribution in the core and shows the expected behavior. Final results demonstrate the ability of the model to predict local actinide masses in good agreement with experimentally measured values from each core refueling. Cumulative fluence irradiation data is provided to simplify structural analysis for equipment design and show acceptable performance under abnormal conditions. The project demonstrates that PWR-1 blanket fuel is subcritical and maintains structural integrity during packaging and transportation.

Key Publications

N/A

Sponsor/Program

NNL

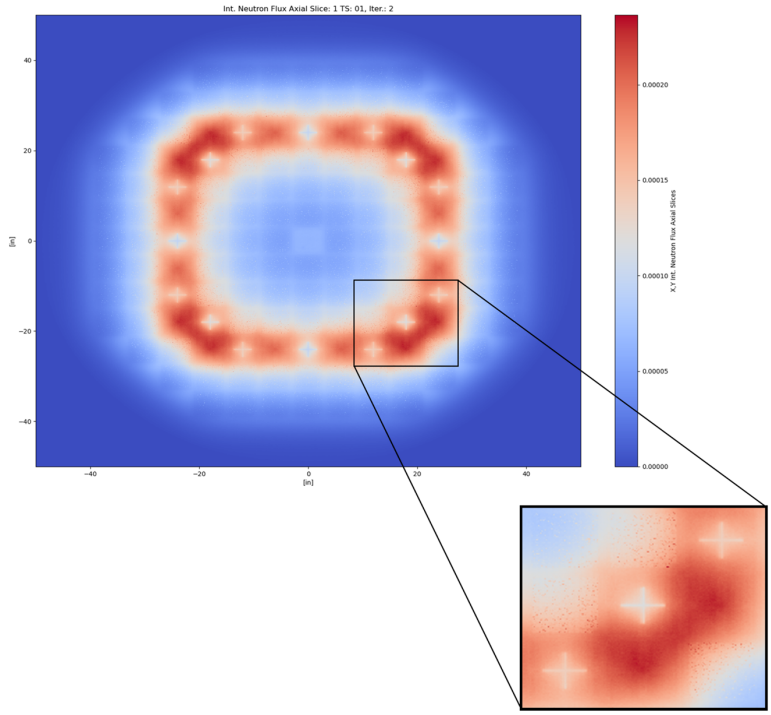

Figure 1: Neutron flux distribution in the PWR-1 core.

H.15 Physics-Informed Generative Adversarial Networks

Report Participants

Schneier, Michael H[1], Buchanan, John R[1]
1 Naval Nuclear Laboratory

Scientific Achievement

This project has successfully created physics-informed neural networks for the Boussinesq and incompressible Navier-Stokes equation using the machine-learning framework PyTorch.

Significance

ROM through physics-informed neural networks allows for high-fidelity simulation solutions to be achieved in near real time. This will enable design optimizations, as well as uncertainty quantification for problems where this was not previously feasible.

Key Publications

N/A

Sponsor/Program

NNL

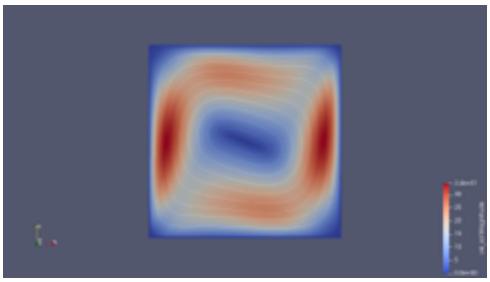

Figure 1: Neural-network-generated velocity field.

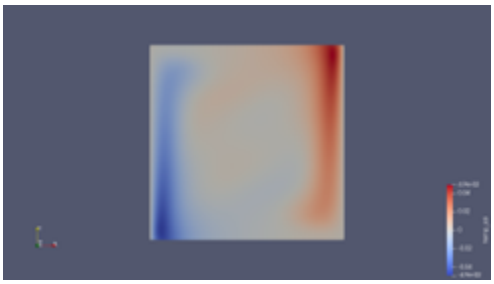

Figure 2: Neural-network-generated temperature field.

H.16 Thermal Neutron Scattering Law Development

Report Participants

Wormald, Jonathan L[1], Holmes, Jesse [1], Trainer, Amelia J[1], Zerkle, Michael L[1]
1 Naval Nuclear Laboratory

Scientific Achievement

Thermal neutron scattering laws (TSLs) are nuclear data that capture the effects of interatomic binding in solids and molecules on neutron thermalization. TSLs are generated as Evaluated Nuclear Data File (ENDF) materials with the FLASSH code using vibrational spectra computed with ab initio methods in the MedeA atomistic simulation environment (Materials Design, Inc.). Current TSL development projects include new or revised TSL evaluations from ab initio methods and the development of new TSL generation methods. Modern ENDF TSL evaluations are commonly prepared with ab initio lattice dynamics or ab initio molecular dynamics. MLPs are being developed for next generation TSL evaluations. An FFT method has been developed to improve TSL evaluations.

Significance

TSLs of moderator and reflector materials are essential nuclear data for predicting criticality and the power distribution of fission systems operating with a thermal neutron spectra. TSL evaluations for several moderator materials being considered for use in advanced reactor concepts have been generated with ab initio methods, tabulated in ENDF-6 format, and submitted for inclusion in the next release of the U.S. national ENDF/B nuclear data library by NNL. ZrC and ZrHx TSL evaluations submitted for inclusion in the ENDF/B-VIII.1 nuclear data library are illustrated in Figure 1. The TSL for C(ZrC), generated with ab initio lattice dynamics, has been shown to exhibit quantum oscillations characteristic of metal hydride moderators (see Key Publications). Additionally, a phonon band gap in ZrC can impact criticality and impart quantum driven neutron thermalizating behaviors with analogs to electronic semiconductor physics. MLPs are being applied to capture large anharmonicities in ZrHx and YHx neglected with current ab initio techniques. Anharmonic effects in the H(YHx) phonon spectrum are demonstrated in Figure 2. An FFT method for TSLs of quantum oscillators, such as metal-hydrides and ZrC, has the potential to reduce biases in processed libraries for neutron transport simulations, thereby helping to isolate the impact of TSL physics on these calculations.

Key Publications

" Wormald, J.L, J.C. Holmes, M.L. and Zerkle. 2023. Influence of Quantum Oscillations in the Thermal Scattering Law of Zirconium Carbide on Neutron Thermalization and Criticality, Nuclear Science and Engineering. https://doi.org/10.1080/00295639.2022.2138063. " Wormald, J.L., M.L. Zerkle. 2023 Thermal Neutron Scattering Law of UBe13 and PuBe13, Proc. Of ICNC 2023. 12th International Conference on Nuclear Criticality Safety, Miyagi, Japan, Oct. 1-6, 2023.

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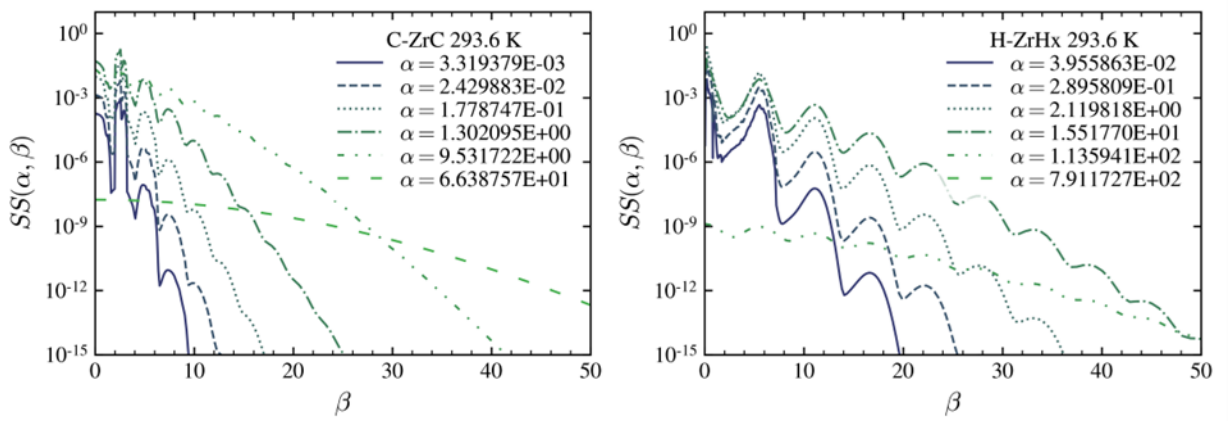

Figure 1: Symmetric TSL of C(ZrC) and H(ZrHx) evaluated with the FLASSH code and phonon spectra from ab initio lattice dynamics and ab initio molecular dynamics methods, respectively. These TSL evaluations have been submitted for inclusion in the ENDF/B-VIII.1 nuclear data library. Both materials exhibit quantized oscillations as a function of unitless energy transfer.

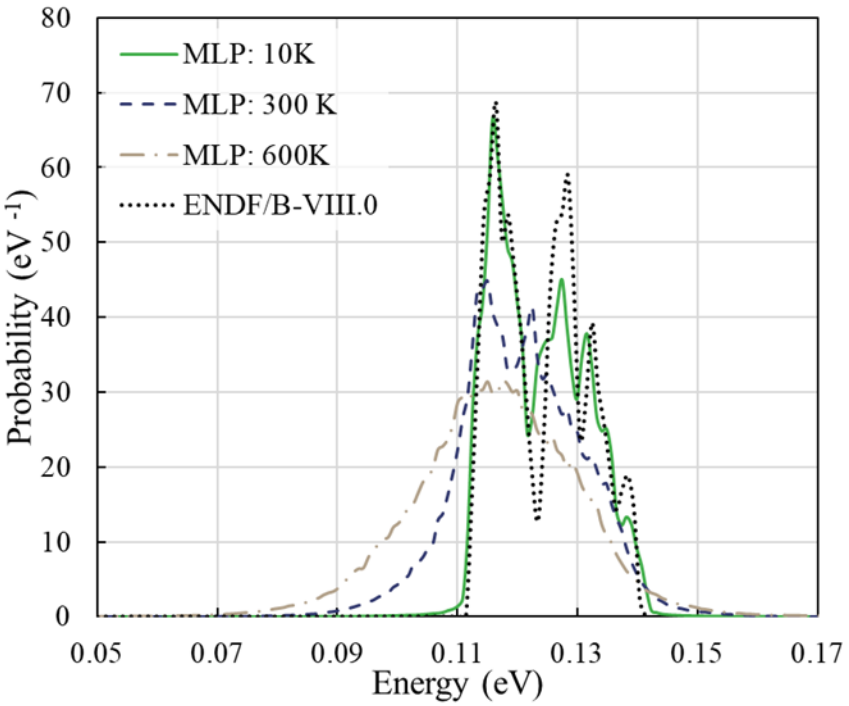

Figure 2: Phonon spectra of H(YH2) predict from molecular dynamics with a YH2 MLP compared to the ENDF/B-VIII.0 ab initio lattice dynamics spectrum. The 10 K MLP is in good agreement with ab initio, which neglects anharmonicity; however, the MLP captures anharmonic spectral shifts and broadening at higher temperatures.


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