

# Laboratory Directed Research and Development

# 2017 ANNUAL SUMMARY REPORT

National Needs  
Current and Future Missions  
Research Highlights  
Building Talent and Leadership  
Building Scientific Excellence  
Ideas to Impact  
Building Partnerships



Energy Challenges  
Advanced Design and Manufacturing

Security Challenges  
Cybercore Integration Center



On the cover:

Energy Challenges: Research scientist **Dong Ding** to enable clean energy at INL's Energy Innovation Laboratory. In one project, he develops direct carbon fuel cells that could transform how the nation uses coal. In another, he has worked to reduce the energy cost of chemical conversions to create petrochemical precursors from currently abundant natural gas.

Security Challenges: INL cybersecurity experts **May Chaffin and Jonathan Chugg** address security challenges related to automotive control systems and charging stations to better define requirements for a long-term solution that would eliminate future vulnerabilities and threats.

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## ACRONYMS

3SBD	safety, security, and safeguards by design
AEM	advanced electrolyte model
AKUFVE	apparatus for continuous measurement of distribution factors in solvent extraction (translation of Swedish abbreviation to English)
AMI	acoustic measurement infrastructure
AMS	accelerator mass spectrometer
ANE	advanced nuclear energy
ANI	active neutron interrogation
ARTIST	Advanced Reactor Technology Integral System Test
ASTM	American Society of Testing Materials
ATF	accident-tolerant fuel
ATR	Advanced Test Reactor
CAES	Center for Advanced Energy Studies
CAN	controller area network
CCE	consequence-driven, cyber-informed engineering
CD	cluster dynamics
CDS	change detection systems
CEA	French Alternative Energies and Atomic Energy Commission
CED	clean energy deployment
CFD	computational fluid dynamics
CI	critical infrastructure
CIP	critical infrastructure
CIVET	continuous integration, verification, enhancement, and testing
CNT	carbon nanotube
CO <sub>2</sub>	carbon dioxide
CZM	cohesive zone model
DCFC	direct current fast charger
DER	distributed energy resource
DFM	drift-flux model
DFT	density functional theory
DOE	U.S. Department of Energy
DOE-NE	U.S. Department of Energy Office of Nuclear Energy

DTF	density functional theory or distributed test facility
DTPA	diethylenetriaminepentaacetic acid
EMImFHF	1-ethyl-3-methylimidazolium fluorohydrogenate
ESS	energy storage system
EXAFS	extended x-ray fine structure
FIB	focused-ion beam
FO	forward osmosis
FY	fiscal year
GB	grain boundary
HES	hybrid energy system
HEU	highly enriched uranium
HIL	hardware in the loop
ICS	industrial control system
IHTL	intermediate heat transport loop
IL	ionic liquids
INL	Idaho National Laboratory
IPWR	integral pressurized water reactor
IR	infrared
IRMPD	infrared multi-photon dissociation
L/D	length-to-diameter
LDRD	laboratory-directed research and development
LIB	Li-ion batteries
LN	lanthanide
LOCA	loss-of-coolant accident
LVDT	linear variable differential transformer
LWR	light-water reactor
MA	minor actinide
MASLWR	multi-application light water reactor
MCP	micro-channel plate
MIT	Massachusetts Institute of Technology
MOOSE	Multi-Physics Object-Oriented Simulation Environment
MTR	material and test reactor
NCSU	North Carolina State University



NGAS	next generation armor steel
NRAD	neutron radiography reactor
NREL	National Renewable Energy Laboratory
NUC	National University Consortium
OBR	optical backscatter reflectometer
ODH	oxidative dehydrogenation
ODS	oxide-dispersion-strengthened
OSU	Ohio State University
PA	phosphoranimine
PB-FHR	pebble-bed, fluoride-salt-cooled, high-temperature reactor
PCHE	printed circuit heat exchanger
PCP	primary coolant pumps
PLC	programmable logic controller
PRA	probabilistic risk analysis
QD	quantum dots
R&D	research and development
rDG	reconstructed discontinuous Galerkin
ROM	reduced order models
RTDS	Real-Time Digital Simulator
RTE	radiation transport equation
RTIL	room-temperature ionic liquid
RTS	real-time simulation
RTPS	real-time process simulator
SEM	scanning electron microscopy
SHADE	scintillation hydro-gel for antineutrino detection
SHINE	scintillation hydro-gel for isotopic neutron emitters
SME	subject matter expert
SNM	special nuclear material
SPP	Strategic Partnership Projects
SPS	spark plasma sintering
TAP	temporal analysis of product
TEM	transmission electron microscopy
TREAT	Transient Reactor Test

UN	uranium mononitride
UNM	University of New Mexico
UT	ultrasonic thermometers
WiFIRE	wireless radiofrequency signal identification and protocol reverse engineering
XFEM	extended finite element method



# Introduction



## INTRODUCTION

The Laboratory-Directed Research and Development (LDRD) Program at Idaho National Laboratory (INL) reports its status to the U.S. Department of Energy (DOE) by March of each year. The program operates under the authority of DOE Order 413.2C, “Laboratory Directed Research and Development” (April 19, 2006), which establishes DOE’s requirements for the program while providing the laboratory director broad flexibility for program implementation. LDRD funds are obtained through a charge to all INL programs. This report includes summaries of all INL LDRD research activities supported during Fiscal Year (FY) 2017.

INL is the lead laboratory for the DOE Office of Nuclear Energy (DOE-NE). The INL mission is to discover, demonstrate, and secure innovative nuclear energy solutions, other clean energy options, and critical infrastructure with a vision to change the world’s energy future and secure our critical infrastructure. Operating since 1949, INL is the nation’s leading research, development, and demonstration center for nuclear energy, including nuclear nonproliferation and physical and cyber-based protection of energy systems and critical infrastructure, as well as integrated energy systems research, development, demonstration, and deployment. Since 2005, INL has been managed and operated for DOE by Battelle Energy Alliance, LLC, a wholly owned company of Battelle. Battelle Energy Alliance, LLC, is a partnership between Battelle, BWX Technologies, Inc., AECOM, the Electric Power Research Institute, the National University Consortium (or NUC, comprising Massachusetts Institute of Technology, Ohio State University, North Carolina State University, University of New Mexico, and Oregon State University), and the Idaho university collaborators (i.e., University of Idaho, Idaho State University, and Boise State University).

Since its creation, INL’s research and development (R&D) portfolio has broadened with targeted programs supporting national missions to advance nuclear energy, enable clean energy deployment, and secure and modernize critical infrastructure. INL’s research, development, and demonstration capabilities, its resources, and its unique geography enable integration of scientific discovery, innovation, engineering, operations, and controls into complex large-scale testbeds for discovery, innovation, and demonstration of transformational clean energy and security concepts. These attributes strengthen INL’s leadership as a demonstration laboratory. As a national resource, INL also applies its capabilities and skills to the specific needs of other federal agencies and customers through DOE’s Strategic Partnership Program.

LDRD is a relatively small, but vital DOE program that allows INL and other DOE laboratories to select a limited number of R&D projects for the following purposes:

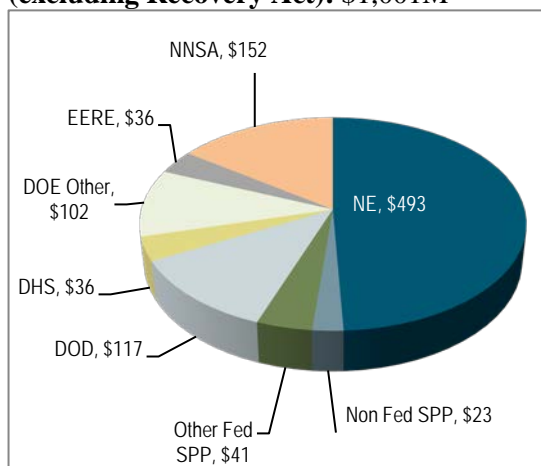
- Maintaining the scientific and technical vitality of INL
- Enhancing INL’s ability to address future DOE missions
- Fostering creativity and stimulating exploration of vanguard science and technology
- Serving as a proving ground for new research
- Supporting high-risk, potentially high-value R&D.

Through LDRD, INL is able to improve and accelerate its mission-critical outcomes, build or advance its core capabilities, and enhance its ability to conduct cutting-edge R&D for its DOE, National Nuclear Security Administration, and Strategic Partnership Program sponsors.

## INL LDRD AT A GLANCE

**Location:** Idaho Falls, Idaho  
**Type:** Multi-Program Laboratory  
**Contractor:** Battelle Energy Alliance, LLC  
**Lead Program Secretarial Office:** DOE-NE  
**Responsible DOE Site Office:** DOE Idaho Operations Office  
**Website:** <http://www.inl.gov/>

### FY 2017 Total Laboratory Operating Costs (excluding Recovery Act): \$1,001M



**FY 2017 LDRD Program Cost**     **FY 2017 Funding Cap:** \$32M

### FY 2017 LDRD Investments: 2.3% of Business Volume

	Projects		Funding (total cost)		Total	
	Continue	New	Continue	New	Projects	Funding
ANE	25	18	\$6,589,124	\$4,948,511	43	\$11,537,635
CED	10	6	\$4,462,786	\$1,347,167	16	\$5,809,953
CIP	11	14	\$2,142,219	\$2,478,400	25	\$4,620,619
<b>Total</b>	<b>46</b>	<b>38</b>	<b>\$13,194,130</b>	<b>\$8,774,077</b>	<b>84</b>	<b>\$21,968,302</b>

ANE = advanced nuclear energy    CED = clean energy deployment    CIP = critical infrastructure

**FY 2016 LDRD Program Cost**     **FY 2016 Funding Cap:** \$30M

### FY 2016 LDRD Investments: 1.9% of Business Volume

	Projects		Funding (total cost)		Total	
	Continue	New	Continue	New	Projects	Funding
ANE	22	22	\$5,886,019	\$5,109,994	44	\$10,996,014
CED	11	4	\$3,161,781	\$1,059,345	15	\$4,221,130
CIP	7	5	\$1,392,006	\$706,126	12	\$2,098,132
<b>Total</b>	<b>40</b>	<b>31</b>	<b>\$10,439,809</b>	<b>\$6,875,466</b>	<b>71</b>	<b>\$17,313,311</b>

ANE = advanced nuclear energy    CED = clean energy deployment    CIP = critical infrastructure

**FY 2015 LDRD Program Cost**     **FY 2015 Funding Cap:** \$28M

### FY-14 LDRD Investment: 2.0% of Business Volume

	Projects		Funding		Total	
	Continue	New	Continue	New	Projects	Funding
ANE	30	17	\$7,666,500	\$3,167,400	47	\$10,833,900
CED	12	6	\$2,874,800	\$1,683,800	18	\$4,558,600
CIP	7	9	\$1,122,800	\$1,266,100	16	\$2,388,900
<b>Total</b>	<b>49</b>	<b>32</b>	<b>\$11,664,100</b>	<b>\$6,117,300</b>	<b>81</b>	<b>\$17,781,400</b>

ANE = advanced nuclear energy    CED = clean energy deployment    CIP = critical infrastructure

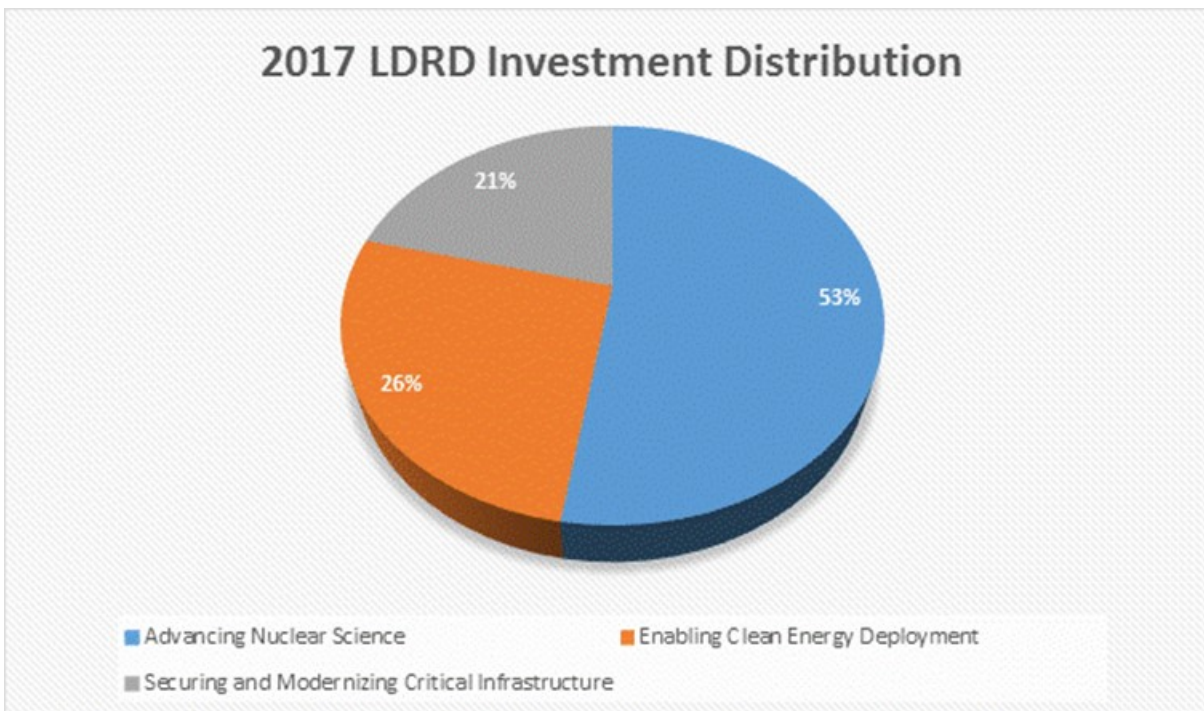
## LDRD SELECTION PROCESS

Each year, projects are selected for inclusion in the LDRD Program through a proposal process. To select the best and most strategic ideas submitted, the associate laboratory directors responsible for the various mission areas establish committees for the focus area and for transformational funds to review new proposals and ongoing projects. The committees are staffed by senior research and technical managers who are subject-matter experts and have no conflict of interest regarding the proposed projects.

Project funding proposals for the Strategic Initiatives R&D Fund, the Transformational R&D Fund, and University Partnership Fund undergo two rounds of review. During the first round, the committees evaluate short preliminary proposals and select the most promising for development into full proposals. During the second round, the committees review the full proposals and those ongoing projects that request second or third-year funding. After reviews are completed, the committees provide funding recommendations to the associate laboratory directors who, in turn, present the recommendations and their input to the deputy laboratory director for science and technology. The deputy laboratory director develops an overall funding strategy and provides approvals for the investments. All projects selected for funding must also receive concurrence from the DOE Idaho Operations Office.

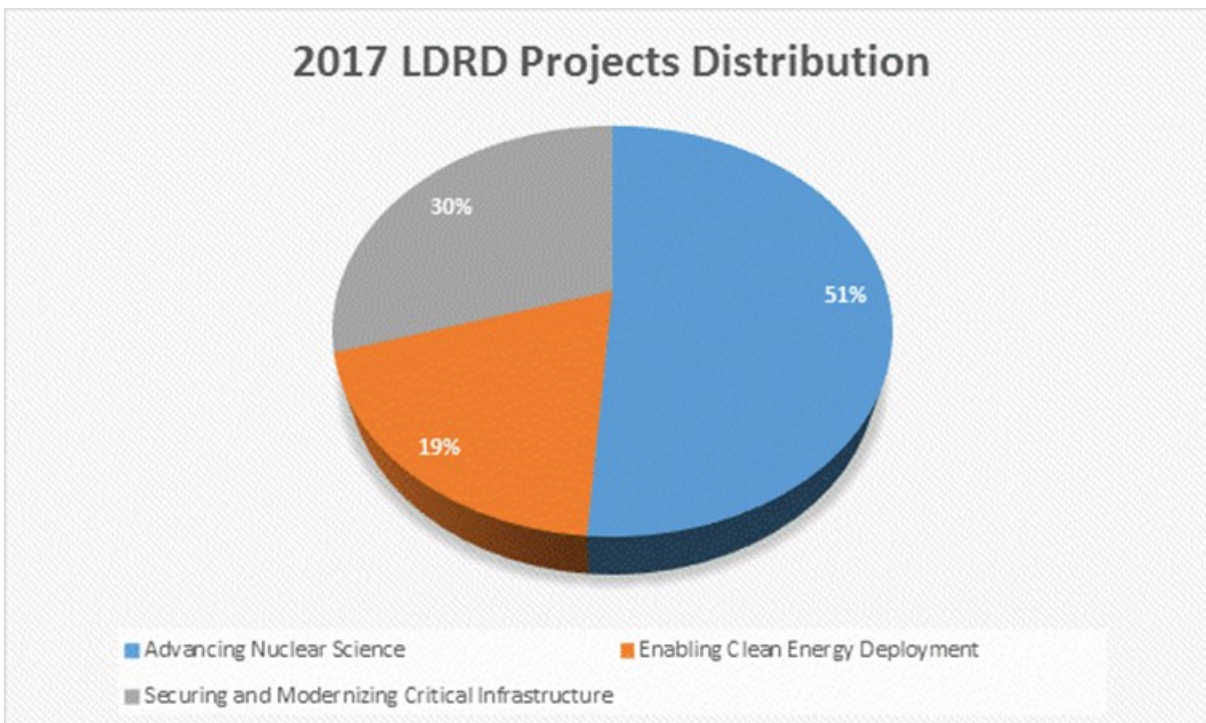
## LDRD Investment Focus Areas

During FY 2017, \$21.97M was allocated to the INL LDRD Program (Figure 1). This funding supported 84 projects, 38 of which were new starts (Figure 2).



*Figure 1. Level of LDRD fund investment by INL mission focus area for FY 2016.*





*Figure 2. LDRD projects by INL mission areas for FY 2016.*

To meet the LDRD objectives and fulfill the particular needs of INL, a Strategic Initiatives R&D Fund and Russell Heath Postdoctoral Fellowship Fund were established (Table 1). The Strategic Initiatives R&D Fund helps develop new capabilities in support of INL strategic objectives. Russell Heath Postdoctoral Fellowship Fund Program investments provides a funding source to enhance INL's Science and Engineer talent pipeline. University collaborations are encouraged within all funding areas to help build and sustain university collaboration.

The Strategic Initiatives R&D Fund is the strategic component of the INL LDRD Program and the key tool for addressing the R&D needs of the INL-mission priority areas. This Russell Heath Postdoctoral Fellowship investment supports outstanding early-career scientists and engineers in nuclear, engineering, computational, physical, and biological fields of study with an interest in energy-, environment-, and security-related science and technology challenges. This LDRD program component help build S&T pipeline for INL.

*Table 1. Overview of the strategic initiative R&D and Russell Heath Postdoc Fellowship funds.*

	<b>Strategic Initiatives R&amp;D Fund</b>	<b>Russell Heath Postdoc Fellowship Fund</b>
Purpose	Address research priorities of the INL strategic initiative areas	Investigator-driven ideas aligned with INL mission areas
Reviewers	Initiative review committees composed of senior technical managers and subject-matter experts	Russell Heath review committee composed of senior technical managers and subject-matter experts
Review Process	Preliminary and full-proposal review, which may include a presentation to the review committee	Full-proposal review, which may include a presentation to the review committee
Review Cycle	Annual	Bi-Annual
Average Project Budget	Typically about \$262 K/year	Typically about \$100 K/year
Project Duration	12 to 36 months	24 months
LDRD Outlay	\$15.60M (90% of program)	\$500K (less than 1% of the program, could support up to 5 postdoc fellows)

## FY 2017 Call Focus Areas

Some of the strategy's success depends to a large extent on INL's ability to identify and nurture cutting-edge science and technology on which enduring capabilities can be built; these are called focus areas. INL uses the resources of the Strategic Initiatives R&D to encourage research staff to submit proposals aimed at addressing mission-focus-area research goals. In spring, the laboratory issued an integrated annual call for proposals. The call emphasized specific research initiatives that are critical to accomplishing INL's strategic laboratory-agenda critical outcomes and advancing INL's core capabilities. For the sake of simplicity in this report, each LDRD project has been assigned to a single initiative area; however, LDRD projects may have applicability to develop core capabilities that support multiple initiative. See also the appendix to this report for project relevance to various agencies and DOE offices.

### Advancing Nuclear Energy

During FY 2017, INL invested \$11.54M in 43 LDRD projects (including one Russell Heath Postdoc fellowship project) in support of Advancing Nuclear Energy initiative areas covering the topics listed below. Proposal PIs were also encouraged to foster and develop regional and national partnerships with industry and academic institutions (including Center for Advanced Energy Studies [CAES] and NUC institutions).

- **Advancing reactor analysis, safety, and simulation:** The objective of projects in this focus area is to continue to advance INL's nuclear energy leadership in the area of nuclear reactor engineering (design,

analysis, and evaluation, including methodologies and tools for reactor and safety analysis) to ensure safe, reliable, and higher economic performance of the existing and future fleet of nuclear power plants and to enable rapid deployment of advanced systems. Proposals focused on advanced reactor designs to improve the commercial viability of nuclear power plants including small modular reactors and MW-class reactors. Research topics focused on new reactor concepts, enhancements to existing concepts and designs, adaptation to grid dynamics, load-following and hybrid energy systems, and new approaches to dealing with the various sources of investment risk and other potential risk-reducing strategies.

- **Advancing fuels and materials irradiation, post-irradiation examination, and testing capabilities:** The objective of this part of the call was to seek research proposals that would support development of advanced instrumentation for both in-reactor and out-of-reactor fuels and materials performance as well as innovative post-irradiation examination (PIE) capabilities that address challenges associated with testing of large numbers of highly irradiated samples are requested.
- **Transient testing:** This part of the call sought research proposals that would support development of testing platforms with the ability to support variable-scale and highly instrumented experiments and development of technologies for real-time in situ monitoring to support transient testing.
- **Fuel cycle materials recovery:** Research proposal ideas were sought to focus on development of new material-recovery R&D capabilities (an example is development of technology that allows the use of EBR-II spent-fuel treatment product to fuel a future test or demonstration reactor).
- **Advanced manufacturing techniques:** Research proposal ideas were sought to reduce cost of reactors and provide more consistent products and improving safety. Proposals were sought for research in the area of advanced manufacturing techniques, including fuels and fuel-assembly components.
- **Probabilistic risk assessment and related methods:** Proposals were sought for R&D in the areas of probabilistic risk assessment (PRA) and risk management, human-factors and human-reliability analysis (HRA), and the supporting functions of data analysis, computer tools and computing power, and statistical analysis in support of advancing nuclear safety and regulations.
- **Methods, tools, and concepts for utilization of existing INL reactors and other experimental facilities:** Innovative research proposals were invited on topics that would encourage novel use and leveraging of INL reactors and major experimental facilities (including the Neutron Radiography Facility [NRAD], Transient Reactor Test Facility [TREAT], Advanced Test Reactor [ATR], Advanced Test Reactor Critical [ATRC] facility, Science and Technology Application Research [STAR] center).

### Enabling Clean Energy Deployment

During FY 2017, INL invested \$5.81M in sixteen LDRD projects in support of Enabling Clean Energy Deployment initiative areas. The strategic intent is to advance development and deployment of clean energy innovation that accelerates regional clean energy transitions and also contributes to enhancing the development of regional innovation centers. Proposals submitted were required to advance clean energy technologies directed towards impactful regional solutions, associated with (1) advanced transportation, (2) clean energy integration, (3) advanced manufacturing, and (4) energy and environment (including energy-water). Proposal PIs were also encouraged to foster and develop regional and national partnerships with industry and academic institutions (including CAES and NUC institutions).

### Securing and Modernizing Critical Infrastructure

During FY 2017, INL invested \$4.62M in 25 LDRD projects in support of DOE's Securing and Modernizing Critical Infrastructure initiative areas that would help advance (1) control-systems cyber security, (2) design of resilient critical infrastructure, (3) nuclear non-proliferation solutions, (4) future defense intelligence systems, (5) materials technologies that overcome physical barriers or kinetic threats, and (5) threat analysis. Proposal PIs

were also encouraged to foster and develop regional and national partnerships with industry and academic institutions (including CAES and NUC institutions).

## PROJECT AND INVESTMENT RELEVANCY TO PROGRAM OFFICES

In support of the objectives of the various DOE programs, FY 2017 projects had relevancy to the program offices shown in Table 2.

*Table 2. Primary relevancy and investments by program office.*

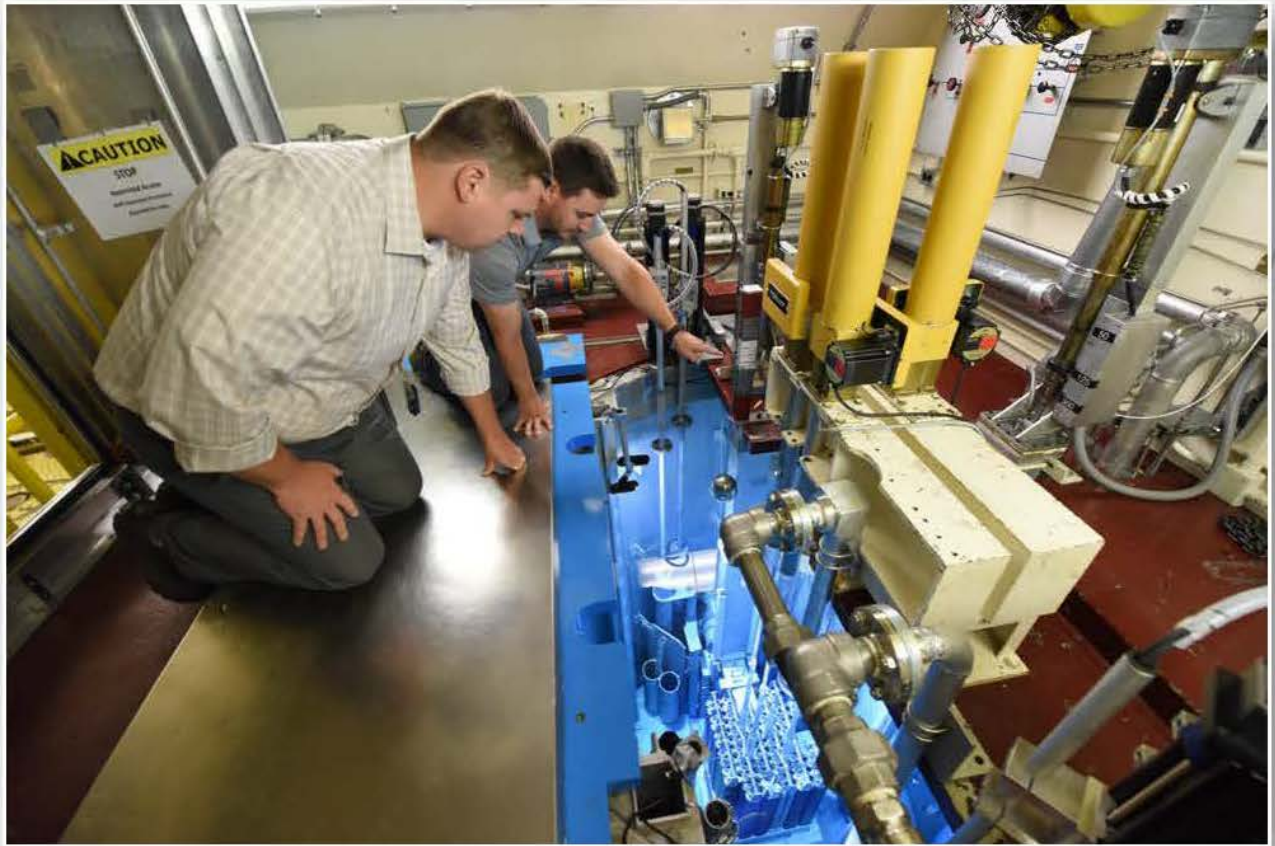
Program Office	Projects	Investment(\$K)
DOE-NE	61	\$15,641
Energy Efficiency and Renewable Energy	24	\$8,263
National Nuclear Security Administration	22	\$4,785
Fossil Energy	13	\$5,523
Electricity Delivery and Energy Reliability	21	\$4,369
Science	35	\$10,002
Department of Homeland Security	23	\$4,163
Environmental Management	9	\$2,707
Naval Reactor	9	\$2,156

As reported in DOE's FY 2017 LDRD *Report to Congress*, indirect funding from DOE-NE programs contributed approximately \$9.85M to the LDRD Program at INL, which supported nuclear-energy-related LDRD projects worth \$15.64M (61 projects).

## REPORT ORGANIZATION

The remainder of this report is divided into three main sections, one for each of the three mission focus areas discussed above. These sections contain project write-ups that are arranged by project number. Each write-up contains (a) a description of the project, including its objectives and purpose; (b) a summary of the project's scientific or technical progress; (c) a statement of the benefits the project has provided to DOE's national security missions and, if applicable, the missions of other federal agencies; (d) a list of publications, presentations, invention disclosures, patents, and copyrights resulting from a project; (e) list of postdocs and interns who were supported through the project and who participated in delivering project outcomes; and (f) where applicable, a list of university, industry, and national-laboratory collaborators. Project summaries are categorized based on the three strategic areas. Appendixes follow the individual project summaries. Appendix A lists agencies benefiting from INL's LDRD investments. Appendix B provides a summary list of all publications in FYs 2016 and 2017, along with impact factors. Appendix C provides a summary list of university, industry, and national-laboratory collaborations through LDRD projects and a summary of the scope of those collaborations. Appendix D provides a list of interns and postdocs and their university affiliations. Finally, Appendix E provides a list of patents for FYs 2016 and 2017, as well as a brief description of these patents.





# Advancing Nuclear Energy



- 15-002: Experimental Scenarios of Adversity and Recovery in Aqueous Separations
- 15-013: Simulation Based Analysis of Procedures and Accident Management Guidelines
- 15-023: Development of Stochastic Three-Dimensional Soil Response Capability in MOOSE to Provide Design and Beyond Design Basis Seismic Motions for Nuclear Facilities
- 15-032: Development of New Method for High Temperature Thermal Conductivity Measurements of Nuclear Materials
- 15-040: Acoustic Telemetry Infrastructure for In-Pile ATR and TREAT Monitoring
- 15-060: Development of Efficient TREAT Modeling Capabilities with Graphite Data Improvement
- 15-141: Interfacing MOOSE Components to Enhance Capability
- 15-142: New In-Core Neutron Diagnostics
- 15-144: Investigation of Sonication Assisted Electrolytic Reduction of Used Oxide Fuel in Molten Salt
- 15-145: Advanced Neutron and X-Ray Imaging at TREAT
- 16-003: Recycling of Tantalum-Containing Waste Materials to Recover Tantalum Metal
- 16-010: Development of a Fully Coupled Radiation Damage Production and Evolution Simulation Capability
- 16-013: Micromechanistic Approach and Critical Experiments for Quantitative Predictions of Delayed Hydride Cracking in Zirconium Alloys
- 16-026: Computationally Efficient Prediction of Containment Thermal Hydraulics Using Multi-Scale Simulation: Feasibility Study
- 16-036: Neutron Microscope to Enable High-Resolution Neutron Tomography at INL
- 16-040: Integration of Prognostic Techniques and Probabilistic Safety Assessment for Online Risk Monitoring
- 16-046: Development of a Synergistic Approach to Study Irradiated Materials Using Coupled Experiments and Simulation
- 16-050: Stress Corrosion Cracking Testing in Supercritical Carbon Dioxide
- 16-055: Capability Extension for Multiscale, Multi-Application development within the Multiphysics Object-Oriented Simulation Environment
- 16-058: Predicting Radiation-Induced Microstructural Change via Implementation and Validation of Multiscale Cluster Dynamics in MOOSE
- 16-070: Characterization of Neutron Beamlines at the Neutron Radiography Reactor
- 16-071: Evaluation of Advanced Digital Neutron Imaging Systems for PIE of Nuclear Fuel
- 16-096: Supporting Operator Performance and Situation Awareness in Highly Automated Nuclear Power Plants

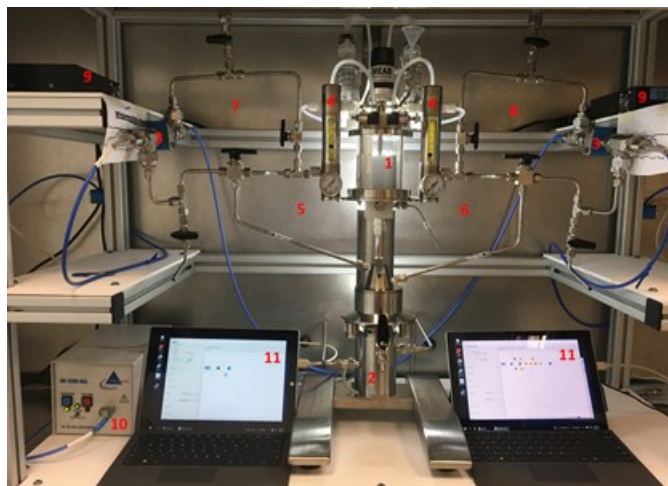
- 16-149: In-core Qualification of Developmental Instrumentation
- 16P6-003FP: Phenomena Identification and Ranking Table Technique Applied to the MEGA-POWER Heat Pipe Reactor Concept
- 17A1-024FP: Design to Enable Narrow Pulse Width in Transient Tests
- 17A1-070FP: Multi-Purpose Non-Destructive Examination Station in the ATR Canal
- 17A1-086FP: Development of a Complete Kinetic Model for Free-Radical-Induced Degradation of Formic and Oxalic Acids
- 17A1-093FP: Digital Neutron Imaging of Irradiated Nuclear Fuel Using a Gamma-Discriminating Scintillation System
- 17A1-105FP: Safety Margin Evaluation for Experiment Irradiation in ATR
- 17A1-111FP: Design of Low Activation Retrievable Sample Holder for TREAT Irradiation of Science-Based Specimens
- 17A1-124FP: Systematic Error Control in Cross Section Library Generation for Novel Reactors
- 17A1-150FP: Advanced Manufacturing of Metallic Fuels and Cladding by Equal-Channel Angular Pressing
- 17A1-164: Application of Traditional Risk Assessment Methods to Cyber Manipulation Scenarios
- 17A1-201FP: Human Reliability Analysis for Advanced Reactor Technologies and Systems
- 17A1-223FP: New Approach for PIE Using Modular Transportable Instrumentation
- 17A1-227FP: Multi-Physics, Multi-Scale Coupled Simulation of Power Impulse Experiments
- 17P10-003FP: In-Situ Small-Scale Mechanical Testing of Neutron Irradiated Ferritic Steels
- 17P11-007FP: Coupling of Modeling and Experiment to Develop Predictive Models of the Mechanical Behavior of Nuclear Fuels and Materials
- 17P11-014FP: The Influence of Irradiation on the Corrosion Kinetics and Hydrogen Pickup of Zirconium Alloys
- 17P11-018FP: Advanced Manufacturing of UO<sub>2</sub> Fuel Pellets with Radially and Axially Zoned Burnable Poisons and Hour-Glassing Control Features
- 17P11-022FP: Development of Nonlinear Eigenvalue Solvers in the Multiphysics Object Oriented Simulation Environment (MOOSE)
- 17P11-032FP: Production, Encapsulation and Process Optimization of Energy Producing Isotopes

## 15-002: Experimental Scenarios of Adversity and Recovery in Aqueous Separations

Peter Zalupski,<sup>1</sup> Colt Heathman,<sup>1</sup> and Rocklan McDowell<sup>1</sup>

### General Project Description

The AKUFVE apparatus [1–3] is an instrument for rapid and accurate measurements of distribution coefficients, designed with a specific aim to streamline the ability to continuously monitor movement of materials in re-circulating immiscible liquid phases. This flow system can be directly connected to various detectors, enabling radiometric, spectrophotometric, atomic absorption, pH, temperature measurements, while liquid delivery is supported by attached burettes. This configuration offers a unique opportunity to dynamically study aqueous separations as conditions are intentionally varied to monitor either beneficial or detrimental effects. The main objective of this research project is the incorporation of online monitoring tools around the AKUFVE re-circulating unit. The demonstration of this experimental capability has been the focus of this project, building a monitoring tool for a variety of hydrometallurgic streams.



*Figure 1. Design of online monitoring re-circulating liquid-liquid distribution unit based on AKUFVE apparatus. 1) mixer, 2) H-centrifuge, 3) flow-through uv-vis cells, 4) flow gauges, 5) heavy-phase recirculating loop, 6) light phase recirculating loop, 7) heavy phase monitoring loop, 8) light phase monitoring loop, 9) QEPro spectrophotometers, 10) light source, 11) data acquisition.*

<sup>1</sup> Idaho National Laboratory

## Summary of Scientific, Technical and Programmatic Progress

Re-circulating online monitoring capability has been installed, allowing for continuous tracking of the partitioning of chromophoric species between two immiscible liquid mixtures. Figure 1 shows the re-circulating operation of the unit, where two immiscible phases are mixed (1), and two clean phases are being recirculated into the mixing chamber after H-centrifuge separation (2). At this particular stage, as the separated liquids are directed through the flow-through spectrophotometric cells of 20 cm path length (3) following a return to the mixing chamber. The movement of solutes across the liquid-liquid boundary may be probed spectrophotometrically in this configuration by monitoring optical absorption features of a chromophore in aqueous and non-aqueous environments. This experimental capability offers opportunities to study the cause/effect features for variety of liquid-liquid distribution equilibria, where perturbation yields a vast spectrum of information in search for efficient methodologies for recovery of valuable resources via hydrometallurgical means. This is a unique experimental capability, which focuses on studying equilibrium changes using detectors installed in-line, performing measurements on clear, separated phases returning to the mixing stage.

To demonstrate, liquid-liquid partitioning of neodymium ion was monitored as pH of the aqueous environment was increased from 2.36 to 4.61. In the light (non-aqueous) phase a strong cation exchanger bis(di-2-ethylhexyl)phosphoric acid was employed. The heavy phase (aqueous) contained diethylenetriaminepentaacetic acid (DTPA) buffered by 1 M lactate, representing the TALSPEAK process [4]. An adverse, unpredictable response to decreasing acidity is typically observed for the partitioning of trivalent *f*-elements in such liquid-liquid systems [5]. Figure 2 illustrates the evolution of optical absorption characteristics of  $[\text{Nd}(\text{DTPA})]^{2-}$  as the aqueous acidity decreases. The increasing absorption indicates that evolving pH progressively forces neodymium out of non-aqueous environment back to the aqueous mixture, as quantified by the decreasing liquid-liquid distribution trend shown in Figure 3.

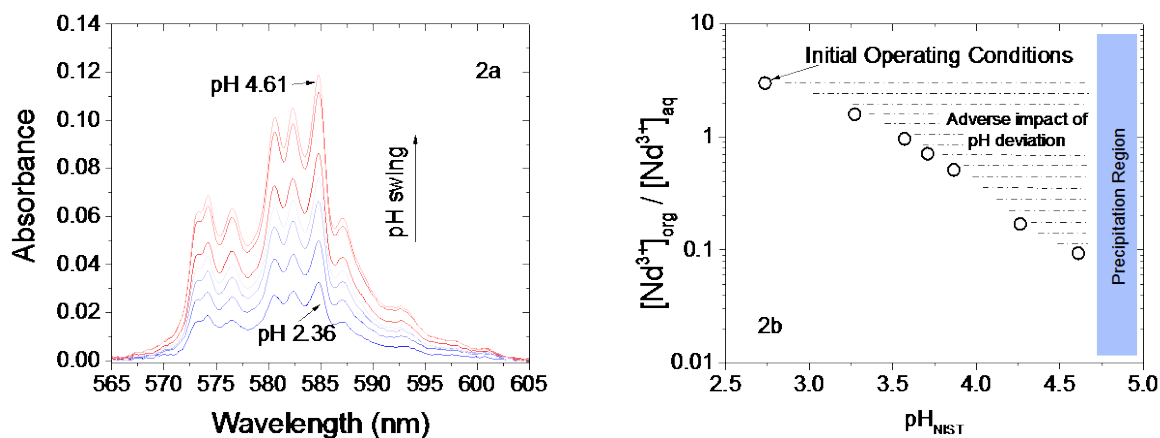


Figure 2. (a) Optical absorption of  $[\text{Nd}(\text{DTPA})]^{2-}$  complex as monitored in the aqueous phase of liquid-liquid distribution system containing (org) 0.2 M bis(di-2-ethylhexyl)phosphoric acid in *n*-dodecane, (aq) 0.05 M diethylenetriamine pentaacetic acid, 1 M lactate, 0.5 mM neodymium,  $2.36 < \text{pH} < 4.61$ ; (b) Calculated liquid-liquid distribution of neodymium during the pH swing experiment.

In conclusion, the online monitoring tool for tracking material balance in liquid-liquid distribution systems has been built and successfully tested using spectrophotometric measurements. This new experimental capability offers a continuously re-circulating, dynamic means of studying physical and chemical properties of liquid mixtures in aqueous separations.

### Benefits to DOE

Demonstration of this new online monitoring tool for tracking movements of valuable materials in mixtures designed for their recovery and purification may attract multiple new customers and collaborative relations. Demonstrations will target interest in this experimental capability from a variety of partners, both domestic and international. Potential sources of follow-on funding will include partners interested in reprocessing of spent fuels (e.g., JAEA or the FCRD program [An/Ln]), those working with critical materials like rare earths (Critical Materials Institute), and others working in remediation (Environmental Management).

### References

- [1] Rydberg, *J. Acta Chem. Scand.* 23 (1969), pp. 647–659.
- [2] Andersson, C., Andersson, S.O., Liljenzin, J.O., Reinhardt, H., Rydberg, *J. Acta Chem. Scand.* 23 (1969), p. 2796.
- [3] Johansson, H., Rydberg, *J. Acta Chem. Scand.* 23 (1969), pp. 2797–2807.
- [4] Weaver, B., Kappleman, F.A. J. *Inorg. Nucl. Chem.* 30 (1968), pp 263–272.
- [5] Nilsson, M., Nash, K.L. *Solvent Extr. Ion Exch.* 27 (2009), pp. 354–377.

## 15-013: Simulation Based Analysis of Procedures and Accident Management Guidelines

Curtis Smith,<sup>1</sup> Ronald Boring<sup>1</sup> and Diego Mandelli<sup>1</sup>

### General Project Description

This project seeks to improve the state-of-the-art of probabilistic risk analysis (PRA) by modeling plant logic, procedures, and accident-management guidelines in a unified way. Existing fault-tree/event-tree risk models address human performance in a largely ad hoc way; thus, incorporating a complete set of procedures and guidelines into a simulation model of plant risk is well beyond the state-of-practice. Despite decades of work on human reliability methods for PRA, procedurally mandated actions still surprise observers (e.g., shutting off high-pressure injection at Three Mile Island or shutting off systems at Fukushima), partly because of the ad hoc and generally incomplete treatment of human performance in state-of-practice PRA. The work is novel in that it includes a comprehensive set of procedures and accident-management guidelines in this simulation model of plant performance. Because nuclear power plants are not fully automated, accounting for the human operation of the plant is essential to high-fidelity simulation. For example, the timeliness and reliability of operator response can determine the ultimate success or failure of various plant processes and affect safety outcomes. To create accurate models of plant performance, it is essential to include operator simulation of procedure-based activities. For this reason, dynamic human reliability analysis (HRA) has been the focus of this LDRD.

### Summary

Initially, this research investigated a computerized online decision support system for risk-informed management of beyond design basis accidents. Using RAVEN, we forecast decision support options (for plant operators) from a large spectrum of simulation-based scenarios. The novel aspect of this work was inclusion of a comprehensive set of procedures and accident management guidelines in a simulation model of plant performance.

The LDRD team next developed an approach to represent operator actions while implementing mitigating procedures for initiating events. The Human Unimodel of Nuclear Technology to Enhance Reliability (HUNTER; see Figure 1) serves as the approach for gathering HRA methods and models to interface dynamically with thermo-hydraulic simulations. The complexity of a completely rendered dynamic HRA model, which requires modeling human cognition and decision making, can verge on the intricacies of artificial intelligence. These approaches may require long-term research efforts to reach fruition. In an effort to meet immediate modeling needs, the HUNTER framework was developed as a simplified approach to dynamic HRA. In fact, the term unimodel—the U in HUNTER—refers to a simplified model of cognition or decision making. HUNTER uses simplified approaches to dynamic HRA as a stepping stone to richer modeling. The outcome of this research is the realization of dynamic operator models (in terms of timing and reliability quantification) that can augment dynamic PRA approaches.

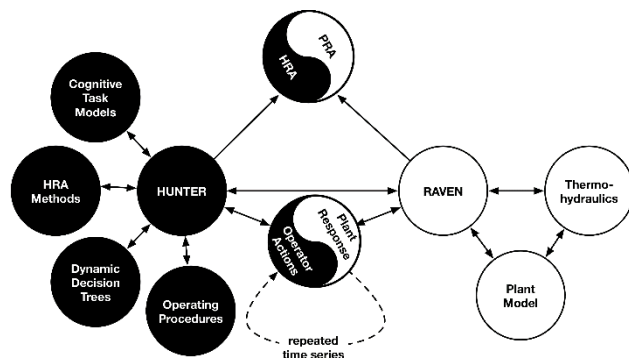


Figure 1. The HUNTER framework used for HRA modeling.

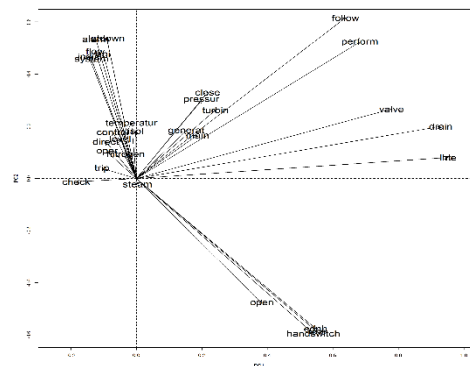


Figure 2. A principle components analysis resulting from text mining of procedure word stems.

In the HUNTER approach, operating procedure steps are mapped to task level primitives, which contain information about nominal human-error probabilities, timing of operator actions, and characteristics of possible error outcomes. A novel approach was developed to map operating procedure steps to a set of task level primitives, including the extraction of procedure steps using automated text mining (see Figure 2). In this manner, it is possible to create a dynamic representation of operator actions. An example multi-unit station blackout example at a nuclear power plant was modeled with the approach.

### Benefits to DOE

The capability has the potential to materially improve the state-of-practice of PRA, affecting facilities at INL and elsewhere and promoting work for INL staff. INL will benefit by the latest developments in PRA that may also be applied to other DOE facilities. The HUNTER framework, developed and refined as part of this LDRD, has the potential to support future activities under DOE’s Light Water Reactor Sustainability Program’s Risk-informed Safety Margins Characterization. By pairing simulated operator action with thermal-hydraulics, the HUNTER approach enables complex yet automated modeling of operator performance in PRA. Additional interest has been expressed by the Electric Power Research Institute (EPRI), which is looking for simplified dynamic modeling tools for HRA to support severe-accident modeling of commercial nuclear power plants.

### Publications

Boring, R., R. Rasmussen, T. Ulrich, S. Ewing, and D. Mandelli, (2017). “Task and procedure level primitives for modeling human error.” In R. Boring (ed.), *Advances in Human Error, Reliability, Resilience, and Performance (Advances in Intelligent Systems and Computing)*, pp. 30–40. Heidelberg: Springer Verlag.

Boring, R., M. Rasmussen, C. Smith, D. Mandelli, and S. Ewing, (In press, 2017). “Dynamicizing the SPAR-H method: A simplified approach to computation-based human reliability analysis,” *Proceedings of the 2017 Probabilistic Safety Assessment Conference*.

Ewing, S.M., R. Boring, D. Mandelli, and K. Savchenko, (2017). “Determination of a generic human error probability distribution, part 2: A dynamic SPAR-H example application,” *Transactions of the American Nuclear Society*, 116, pp. 295–298.



- Ewing, S., R. Boring, M. Rasmussen, and T. Ulrich, (2017). “Text mining for procedure-level primitives in human reliability analysis,” In R. Boring (ed.), *Advances in Human Error, Reliability, Resilience, and Performance (Advances in Intelligent Systems and Computing)*, pp. 239–249. Heidelberg: Springer Verlag.
- Ewing, S.M., K. Savchenko, D. Mandelli, and R. Boring, (In press, 2017).” Determination of a generic human error probability distribution, part 1: A dynamic formulation of SPAR-H.” *Transactions of the American Nuclear Society*, 116, pp. 299–302.
- Rasmussen, M. and R. Boring, (In review). “Auto-calculation of complexity in computation-based human reliability analysis,” *EURO Journal on Decision Processes*.
- Rasmussen, M., R. Boring, T. Ulrich, and S. Ewing, (2017). “The virtual human reliability analysis,” In R. Boring (ed.), *Advances in Human Error, Reliability, Resilience, and Performance (Advances in Intelligent Systems and Computing)*, pp. 250–260. Heidelberg: Springer Verlag.
- Ulrich, T., R. Boring, S. Ewing, and M. Rasmussen, (2017). “Operator timing of task level primitives for use in computation-based human reliability analysis,” In R. Boring (ed.), *Advances in Human Error, Reliability, Resilience, and Performance (Advances in Intelligent Systems and Computing)*. Heidelberg: Springer Verlag, pp. 41–49.

## Interns and Postdocs

Interns: Thomas Ulrich and Kateryna Savchenko

Postdoc: Dr. Martin Rasmussen

## Collaborations

Universities: University of Idaho, and Norwegian University of Science and Technology

## 15-023: Development of Stochastic Three-Dimensional Soil Response Capability in MOOSE to Provide Design and Beyond Design Basis Seismic Motions for Nuclear Facilities

Justin Coleman<sup>1</sup> and Swetha Veeraraghavan<sup>1</sup>

### General Project Description

Attenuation of earthquake energy through soil media is a phenomenon that depends on many factors. Numerical modeling of the effects of earthquake wave passage on both the soil and structure make simplifying assumptions. Typically, the nuclear industry takes deterministic approaches to calculate seismic demands in designs for nuclear structures. These deterministic approaches generally do not account for two main aspects of seismic wave propagation: (1) the seismic wave field is three-dimensional in space and time, including both body and surface waves (currently the nuclear industry uses equivalent linear codes assuming vertically propagating shear waves), and (2) the variability in a soil’s material properties are not captured; rather, a deterministic approach is used to bound the problem by using lower-bound, best-estimate, and upper-bound soil material properties.

This LDRD addresses both failings by implementing the capability to perform source-to-site simulations—including earthquake fault rupture—and to quantify soil material variability by implementing risk calculations into MASTODON.

### Summary of Scientific, Technical, and Programmatic Progress

The software, Multi-hazard Analysis for STOchastic time-DOMaiN phenomena (MASTODON), is a MOOSE based, finite element application that analyses the response of 3-D soil-structure systems. MASTODON is being developed to be a dynamic probabilistic risk assessment framework that enables analysts not only to perform deterministic analyses, but also probabilistic or stochastic simulations for the purpose of risk assessment. A theory manual for MASTODON was produced this year using and MASTODON was open sourced on September 18, 2017.

LDRD funding allowed researchers to implement the ability to calculate three-dimensional wave passage and quantify material property variability. The researchers developed pre-processing tools for Monte-Carlo and developed a numerical procedure for modeling earthquake fault rupture source to site and post-processing risk calculations

The following capabilities were developed in MASTODON over the three-year LDRD:

- Implemented a computationally efficient method for solving large soil domains called domain reduction method (DRM). This method takes a large problem containing an earthquake fault and a nuclear facility and divides it into two problems: (i) Earthquake fault rupture and wave propagation in large soil domain with no structure and (ii) simulation of soil-structure interaction in a smaller soil domain (Figure 1). This capability allows the analyst to generate earthquake ground motion from a fault rupture in the large domain and use this ground motion as input to the smaller domain. The analyst can then run probabilistic simulations on the local model accounting for variability in the local soil and structure.

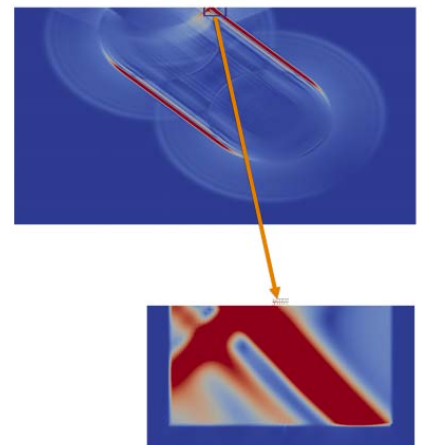


Figure 1. Earthquake wave passage using DRM

- Developed earthquake-energy release and fault dislocations methods to simulate rupture of complicated earthquake faults using a combination of point sources (Figure 2). Using this capability the analyst can generate a number of earthquake scenarios and calculate wave passage from source to site. This allows the analyst to estimate scenarios that cause adverse structural response and propose design solutions for the structure.
- Produced a demonstration problem showing the response of a nuclear containment building, with a reactor pressure vessel and fuel rod, to earthquake ground motion from an inclined fault rupture. The response of the pressure vessel was coupled to the fuel-rod model created in BISON to simulate the thermal and mechanical response of the fuel rod when a scram is triggered due to the earthquake.

Boundary conditions were added to absorb spurious wave energy at the edges of the model and to automate input of stress conversion to approximate wave propagation in an infinite soil domain. This capability allows the user to approximate an infinite domain in a finite space and to input ground motion at the appropriate location in the model.

## Benefits to DOE

MASTODON had a software quality assurance assessment on August 3, 2017, and received an effective rating. The effective rating means that code development is meeting the intent of ASME NQA-1 and in the future will allow for quality level 1 calculations. MASTODON received laboratory approval to proceed with open source on September 13, 2017. This allows for the global seismic R&D community to contribute to the project. The seismic research team was recently awarded a technology commercialization funding to work with Southern Company, X-energy, and TerraPower to optimize advanced reactors using seismic isolation systems. Additionally, the team is working on a CRADA with the Bureau of Reclamation to perform seismic analysis of dams using MASTODON. These collaborations with end users will allow the seismic research group to “test drive” the added MASTODON capabilities. Collaboration with Professor Jacobo Bielak of the the Southern California Earthquake Center (SCEC) has yielded an opportunity to work with SCEC, leaders in numerical earthquake-wave propagation research.

## Publications

Veeraraghavan, S., Spears, B., Coleman, J. (2017), “High Frequency Content in Nonlinear Soil Response – A Numerical Artifact or a Reality?,” *Soil Dynamics and Earthquake Engineering*, Manuscript Submitted June 2017.

Veeraraghavan, S., Bielak, J., Coleman, J. (2017), “Effect of Inclined Waves on Deeply Embedded Nuclear Facilities,” *Structural Mechanics in Reactor Technology (SMiRT)* Conference, Busan, South Korea, August 2017.

Coleman, J. L., Slaughter, A., Veeraghavan, S., Bolisetti, C., Spears, R., Hoffman, W., Kurt, E. (2017). *"MASTODON theory manual."* INL/EXT-17-41930, Idaho National Laboratory, Idaho Fall, ID.

## Presentations

Coleman, J. “Developments in Nonlinear Soil-Structure Interaction Analysis,” Presented at *Structural Mechanics in Reactor Technology (SMiRT)* Conference, Panel Session on Nonlinear Soil-Structure Interaction Analysis, Busan, South Korea, August 2017.

Veeraraghavan, S. and J. Coleman, 2016, “Development of MASTODON and Applications,” *DOE Natural Phenomena and Hazards* DOE Headquarters Working Meeting, October 18, 2016.

Veeraraghavan, S., J. Coleman, B. Spencer, 2016, “Effect of Soil Heterogeneity on Nuclear Facility Soil Foundation Interaction,” *Engineering Mechanics Institute Conference* 2016, Nashville, Tennessee, May 2016.

Veeraraghavan, S., 2016, “Development of MASTODON,” *INL Seismic R&D Advisory Panel*, June 28, 2016.

Coleman, J. and S. Veeraraghavan, 2016, “Seismic Research and Development Initiative,” *DOE Headquarters to DOE-NE 2*, February 24, 2016.

### **Interns and Postdocs**

Interns: Ozgun Numanoglu and Dhruv Datta

Postdocs: Swetha Veeraraghavan

Professor: Jacobo Bielak,

### **Collaborations**

Universities: University of Illinois Urbana-Champaign, Purdue, and Carnegie Mellon University

## 15-032: Development of New Method for High Temperature Thermal Conductivity Measurements of Nuclear Materials

Krzysztof Gofryk,<sup>1</sup> Robert Mariani,<sup>1</sup> and Michael Tonks<sup>2</sup>

### General Project Description

Thermal transport is an important property in reactor design and safety because thermal conductivity of nuclear fuels governs the conversion of heat produced from fission events into electricity. Different scattering processes (such as grain boundary, defects, and phonon-phonon interactions) affect thermal conductivity at different temperatures. In order to fully understand and reliably model this property, it is crucial to study the thermal conductivity in a broad temperature range. Our objective is to develop a new method for measurement of thermal conductivity in nuclear materials using the  $3\omega$  method. This ac technique is considered to be the best pseudo-contact method available; it enables direct measurement of thermal conductivity of very small samples. In addition, this technique has intrinsically the lowest possible error caused by infrared radiation. The error-term arising from radiation is estimated to be less than 2% even at 1000 K. Adaptation of this method will be novel for nuclear materials. The new experimental setup will allow study of the thermal conductivity of small samples of nuclear materials in exceptionally broad temperature range (between 2 and 800 K), and the data obtained will help to advance theoretical understanding and modeling of reactor fuel and, consequently, future fuel development.

### Summary

During the third year of the project we have installed and tested ARS cryocooler. This instrument, together with the rest of the experimental setup, allows us to measure the electrical resistivity, heat capacity and thermal conductivity of various materials (metals and insulators) in wide temperature range (7–800 K).

Figure 1 shows the complete experimental setup and its schematic diagram. - performed several tests on metallic (Pt, Cu, Alumel, UN) and insulating samples ( $\text{UO}_2$ ,  $\text{SiO}_2$ ). All tests met our expectations (see Figure 2) and therefore the new and complete measurement capability for thermal and transport properties (measured in wide temperature range) of nuclear materials is now available at INL (see more detail in K. Shrestha and K. Gofryk, *Review of Scientific Instruments*, submitted).

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<sup>2</sup> University of Florida

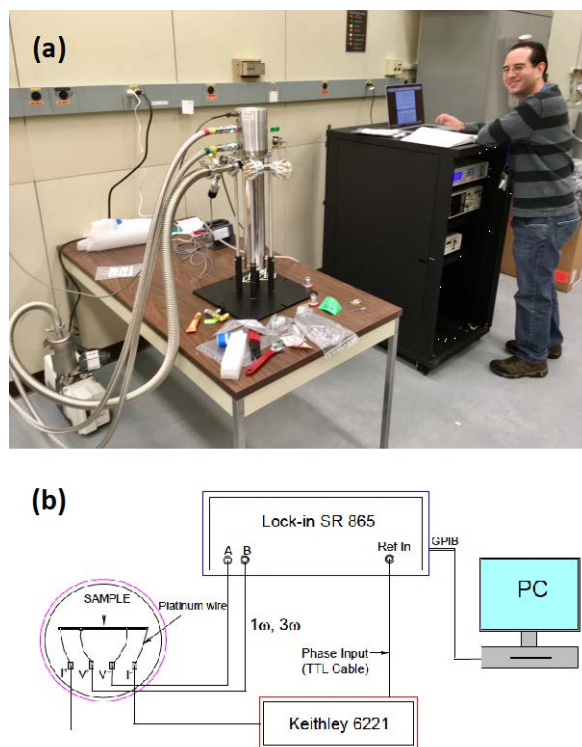


Figure 1. The complete experimental setup developed for the thermal conductivity measurements using  $3\omega$ -method and installed in IF-603, lab C6; (a) Experimental setup together with ARS cryocooler, electronics, and PC, all controlled by specially developed LabView software; (b) schematic diagram of the instrumental setup.

## Benefits to DOE

Thermal conductivity is a key engineering parameter in the conversion of heat produced by fission events to electricity. New, reliable methods for thermal conductivity determinations of nuclear materials, such as  $3\omega$  technique, together with advanced modeling are key parameters in understanding and developing new nuclear fuels, leading to more efficient energy production. While developed for small bulk samples, this method may also be applied for micro-size and thin-film materials, which is unique and can be extended in the future to active materials such as Np-, Pu-, and Am-based phases. In addition, this ac thermal conductivity method could be also modified to measure ac Seebeck coefficient ( $2\omega$ -method) and heat capacity. Altogether, this cutting edge research will help INL to maintain a leading position in nuclear fuel research.

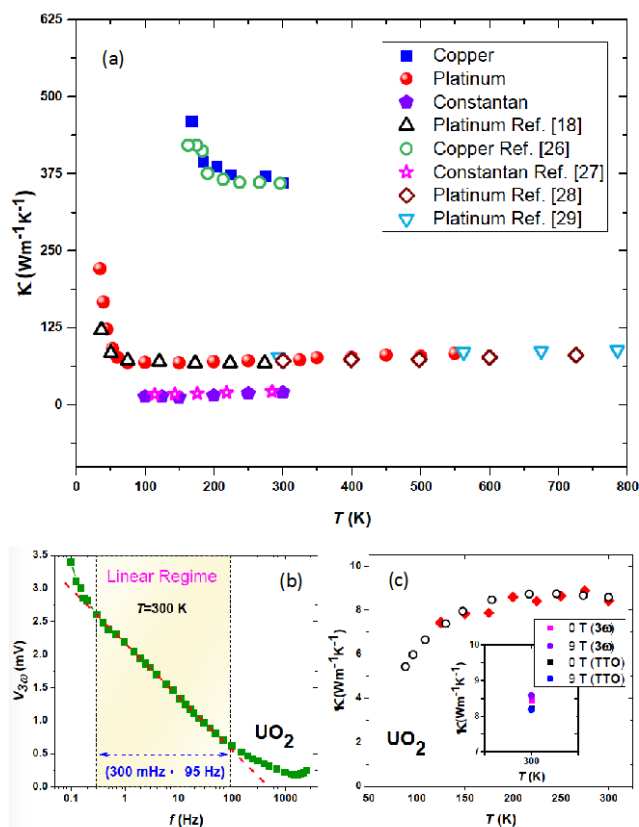


Figure 2. (a) The temperature dependence of the thermal conductivity of copper, platinum, and constantan. The open symbols represent the data taken from the previous reports while the solid symbols refer to the experimental data obtained by the  $3\omega$  method (see the K. Shrestha and K. Gofryk, *Review of Scientific Instruments*, in more detail); (b) The frequency dependence of third harmonic voltage of  $UO_2$  single crystal; (c) Thermal conductivity of  $UO_2$  at different temperatures. The open circles are the data taken from K. Gofryk et al., *Nature Comm.* 2014. Inset: the thermal conductivity measured by the  $3\omega$  method and TTO option in PPMS under 0 and 9 T of applied magnetic field.

## Publications

K. Shrestha and K. Gofryk, "A new experimental setup for the thermal conductivity measurements of actinide materials based on  $3\omega$  approach," under review with *Review of Scientific Instruments*.



## **Presentations**

Shrestha K., and K. Gofryk American Physical Society, March 2017

Gofryk, K., LDRD review meeting (DOE HQ), March 2017

Shrestha, K., and K. Gofryk: poster at Material Research Society, April 2017

Shrestha, K., and K. Gofryk: 33rd International Thermal Conductivity Conference (ITCC) and the 21st International Thermal Expansion Symposium (ITES), May 2017

## **Interns and Postdocs**

Interns: Michael Tonks, Junwei Meng, Daniel Mast, and Howard Yanxon

Postdocs: Dr. Keshav Shrestha and Dr. Daniel Antonio

## **Collaborations**

University: University of Florida

## 15-040: Acoustic Telemetry Infrastructure for In-Pile ATR and TREAT Monitoring

Vivek Agarwal,<sup>1</sup> James A. Smith,<sup>1</sup> James Lee,<sup>1</sup> and James K. Jewell<sup>1</sup>

### General Project Description

The research project developed an acoustic measurement infrastructure (AMI) to obtain an acoustic baseline of the Advanced Test Reactor (ATR) reactor under different operating conditions. This presents an opportunity to (1) identify quiescent frequency ranges that would aid in the design of the carrier frequency of acoustically telemetered sensors, (2) enhance or tune the acoustically-telemetered-sensor design prior to fabrication and installation inside the reactor core; and (3) understand and characterize the salient measurement parameters of an actual thermoacoustic sensor signal: frequency, amplitude and phase. Additionally, AMI can be adapted for Transient Reactor Test Facility. The current implementation of AMI includes (i) ATR; (ii) acoustic sources from primary coolant pumps (PCPs); (iii) acoustic transducers installed on the surface of the reactor vessel; and (iv) signal processing algorithms to develop the first-ever ATR acoustic baseline signatures as shown in Figure 1.

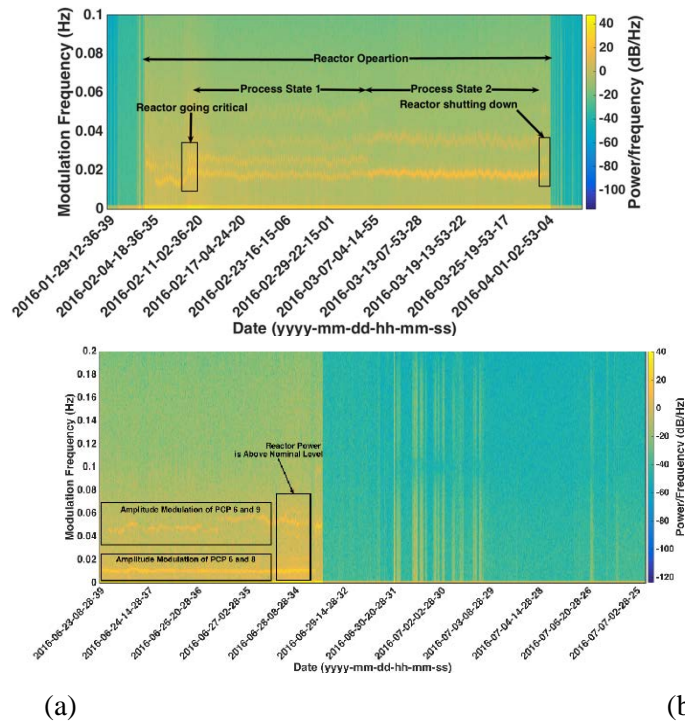


Figure 1. Acoustic baseline signature of ATR recorded during (a) normal operation and (b) powered axial locator mechanism.

### Summary

A novel and innovative premise behind AMI for ATR provided and laid the foundation for (1) *wireless communication* of key in-pile parameters through reactor structures under different operating conditions; (2) *real-time non-intrusive* in-pile measurements to understand fuel/material behavior while reactor is

operational; (3) *structural health monitoring* of structures inside and outside the reactor vessels. Emergency coolant pump seal break (see Figure 2) and rabbit-tube removal had a significant frequency change (high frequency vibration of rabbit tube could have fatigued a beryllium block, see Figure 3); (4) Understanding and characterizing the *salient measurement parameters* (frequency, amplitude, and phase) of acoustically telemetered sensor; (5) *Process improvement* to ATR operation by cross verifying ATR operational logs; (6) *Advanced data analytics and visualization* of ATR process states; (7) identification of presence of *electric power sources* (commercial UPS versus diesel generators), see Figure 2.

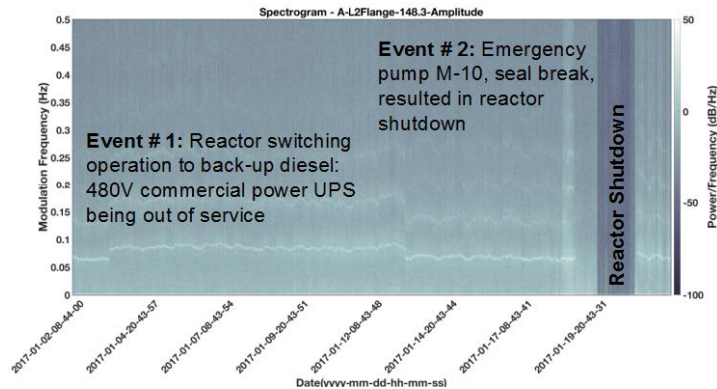


Figure 2. ATR acoustic baseline signature highlights two events. Event 1 shows shift in the modulation frequency as a result to switching to back-up diesel. Event 2 is related to structural health monitoring objective and significant change in power as a result emergency coolant pump seal break leading to forced reactor shutdown.

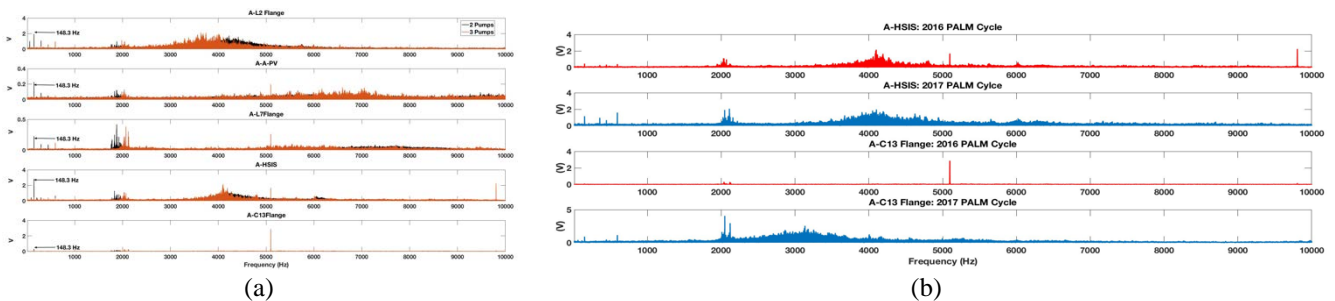


Figure 3. Fast Fourier transformation (FFT) of acoustic signal during (a) ATR normal operation and PALM cycle and (b) comparison of rabbit and C13 flange FFTs during 2016 and 2017 PALM cycles. Clearly high frequency component have disappeared in 2017 PALM cycle as a result of removal of rabbit tube.

## Benefits to DOE

This research is critical in advancing the Department of Energy’s nuclear energy mission by developing an advanced capability of in-pile temperature measurements for materials irradiation in research and test reactors. This aligns with the Nuclear Science User Facilities mission in the area of advance instrumentation for in-pile measurements. The research will enable direct technology- and capability-transfer opportunity to the nuclear industry to support current and next-generation reactor concepts. Successful completion of this research will significantly improve the quality and capability of the Laboratory to analyze in-pile data for materials and fuels and to carry out modeling and simulation

research and development. ATR has turned to the AMI to supply vibration data to help understand beryllium cracking near the hydraulic shuttle. The research augments the activities outlined within the Laboratory's Nuclear Science and Technology Directorate's Gateway to Accelerated Innovation in Nuclear Initiative.

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## Interns

Interns: Jasrah C. Stephenson, Alexandar Pharr, Joshua Hrisiko, and Dr. Andrei V. Gribok

## 15-060: Development of Efficient TREAT Modeling Capabilities with Graphite Data Improvement

Mark DeHart,<sup>1</sup> Ayman Hawari,<sup>3</sup> Todd Palmer,<sup>4</sup> Youho Lee,<sup>5</sup> Benoit Forget<sup>5,6</sup>

### General Project Description

This project comprises research projects from university researchers under the INL National University Consortium (NUC) to support modeling and experimentation in relation to the Transient Reactor Test Facility. Originally, this LDRD called for a collaborative effort between INL, Massachusetts Institute of Technology (MIT) and the University of New Mexico (UNM), and the project was eventually expanded to also include efforts at North Carolina State University (NCSU) and Oregon State University (OSU). Work includes Ayman Hawari's (NCSU) theoretical evaluation of graphite cross-sections compared to measured data; Wade Marcum's (OSU) supported research related to phonon transport in graphite using the INL Rattlesnake application in the first year, and Todd Palmer's research to develop a benchmark of the TREAT minimum core configuration. These were followed by work in advanced reduced-order modeling techniques. Edward Blandford and, later, Youho Lee (UNM) performed measurements and modeling to characterize the thermal-hydraulic performance of materials proposed for accident-tolerant fuels that will be evaluated in the first TREAT experiments. Last, Ben Forget at MIT led two research projects, both in the development of advanced methods based on the Monte Carlo approach for improving TREAT modeling capabilities.

### Summary

**NCSU:** Research has focused on two tasks: (1) establish a neutronic model using the Serpent Monte Carlo code of the TREAT M2 calibration experiment according to the information given in [1] and (2) establish a baseline graphite model that would enable the calculation of the reference phonon spectrum for graphite. Task 1 is showing reasonable agreement between calculated and measured flux distributions in test fuel pins, but with a bias that is being investigated. Models were improved as the result of a summer internship by an NCSU student. The Task 2 model has been completed and tested using the density functional theory code VASP (Vienna Ab initio Simulation Package). The model showed good agreement with measurements of phonon dispersion relations. Completion of both of these tasks supports improved modeling and validation for TREAT.

**OSU:** During the first year, the collaborators demonstrated that Rattlesnake, the neutron transport solver in MOOSE, could be used to compute the phonon distribution in heterogeneous materials, and that moments of this distribution could be used to predict thermal conductivity. Results for several test problems were generated and the Rattlesnake calculations were compared with values from the literature. In the second year, the reactor analysis package MAMMOTH was used to complete steady state calculations for the TREAT minimum critical core configuration. The fundamental neutronic properties were investigated as well as the effects of spatial homogenization and angular discretization on power distribution, eigenvalue, and integral reaction rates. Preliminary diffusion constant treatments in highly

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<sup>3</sup> North Carolina State University

<sup>4</sup> Oregon State University

<sup>5</sup> University of New Mexico

<sup>6</sup> Massachusetts Institute of Technology



anisotropic regions were developed. Current work involves the investigation of self-optimizing reduced-order systems of the neutron transport equation.

**MIT:** The two areas of research support TREAT modeling: (1) integration of the thermal neutron scattering of graphite in Monte Carlo simulations to facilitate sensitivity studies and uncertainty analyses, and (2) coupling of Monte Carlo methods with the MOOSE framework for coupled simulations. The methodology relies on two components: (a) functional expansion tallies (FETs) for representing power distribution in continuous space, and (b) continuous material tracking for sampling neutron travel in a continuously changing medium. Under the first, work has been completed integrating pre-processing capabilities directly in the Monte Carlo simulations to facilitate the generation of tables at all needed conditions. To improve versatility, MIT pursued the capability of sampling from the thermal neutron scattering on-the-fly. FETs were implemented and tested using Legendre polynomials whose coefficients are used to pass information to the finite element mesh of MOOSE, which greatly simplifies mapping of power and temperature distributions between the transport solution to a BISON solution. The first will improve understanding of uncertainties in TREAT graphite simulations; the latter has already been integrated into INL work to allow coupling of the Serpent Monte Carlo code with MOOSE-based tools to allow Monte Carlo-based simulations of TREAT. A student internship in 2017 was used to improve a model of TREAT within OpenMC for generation of weighted cross sections for MAMMOTH.

**UNM:** Activities at UNM included advance and receding contact angle measurements for different 310SS, Zirc-4, and FeCrAl samples oxidized in an autoclave under different simulated Light Water Reactors (LWRs) conditions for one year. The measured advance and receding angles are used to predict pool boiling Critical Heat Flux (CHF) using models reported in the literature. A second activity was to measure the pool boiling heat transfer and CHF of deionized water on these oxidized ATF samples and compare the experimentally measured CHF to those values predicted previously. Finally, UNM conducted water flow boiling CHF measurements under atmospheric pressure. The obtained results on the three activities listed above supported not only experiment design for early TREAT experiment with ATF sample, but also provides critical material and flow data needed for RELAP-7 simulation of those experiments.

### Benefits to DOE

All of the research in this LDRD advance the state of the art for modeling and simulation of TREAT and its experiments. Much of the work extends to a broader scope of reactor modeling. Hence, this work supports the DOE Nuclear Energy Modeling and Simulation (NEAMS) Program, specifically the current TREAT modeling and simulation work package within NEAMS. The various tasks are highly innovative and relevant to the DOE missions of transient testing and sustainability of the current commercial light-water reactor fleet. Measurements performed at UNM help simulate advanced cladding materials and assess them for failure prior to their being placed in a reactor, reducing testing time for fuels within a reactor and, potentially, the number of concepts that need to be studied. Activities at OSU and NCSU facilitate improved theoretical material behavior simulations, which will allow better simulation of TREAT, which, in turn, will reduce experimental error. Overall, the work at OSU has value for any graphite reactor, e.g., HTGRs, which are of interest to DOE. It allows better prediction of the behavior of reactor-grade graphite and helps to elucidate the complex physics of these materials. Finally, research activities at MIT will become important in high-performance computing and multi-physics by minimizing memory-intensive storage of cross-section data, eventually allowing modern methods, which tend to be data-bound, to be extended to full-core analysis and reduce uncertainty in core physics analysis for existing and proposed reactor designs.

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### Interns, Postdocs, and Staff

Interns: Jonathan Wormald, Nina Colby Sorrell, Anant Singhal, Anthony Alberti, Jackson Harter, Matthew Ryals, Carl Haugen, and Matt Ellis

Postdocs: Daniel LaBrier and Maolong Liu

Staff, Research Assistant Professor: Amir Ali

### **Collaborations**

Universities: North Carolina State University, Oregon State University, University of New Mexico, and Massachusetts Institute of Technology.

## 15-141: Interfacing MOOSE Components to Enhance Capability

Hongbin Zhang,<sup>1</sup> Carol Smidts,<sup>1</sup> Xiaodong Sun,<sup>1</sup> and Jinsuo Zhang<sup>1</sup>

### General Project Description

This project encompasses three research areas: the first is the development of a non-equilibrium chemical model for the assessment of chemical and corrosion reactions among coolant, cladding, and fuel resulted from fission-products release. The second is thermal hydraulics to support two-phase flow modeling and validation activities by investigating the thermal non-equilibrium five-equation drift-flux model (DFM) using the computational framework MOOSE. The third is the connection between RAVEN/RELAP-7 and the distributed test facility (DTF) for instrumentation and control (I&C) systems. A reduced-scale, hardware-in-a-loop (HIL) system to control steam-generator water-levels and a full-scale nuclear-power-plant simulator will be used to interact with RAVEN. This allows capabilities to be extended into the areas of digital I&C reliability and reliability testing.

### Summary of Scientific, Technical, and Programmatic Progress

#### *Release of Fission Products and Materials Corrosion*

The diffusion coefficient of Cs in simulated water was measured and the BISON model for Cs release from a defected fuel was developed. The diffusion coefficient of cesium iodide in boric acid water is measured using Nuclear Magnetic Resonance (NMR) technique at temperatures below boiling point of the coolant. The NMR DOSY measurement of Cs<sup>+</sup> in simulated LWR coolant chemistry shows the self-diffusion coefficient of Cs<sup>+</sup> is about  $3.04 \times 10^{-11}$  m<sup>2</sup>/s, and shows little dependence on Cs<sup>+</sup> concentration in the solution temperature in the testing range. The measured data is about 100 times smaller than Cs<sup>+</sup> in pure water, different solution composition, temperature difference, pH difference and also the measurement method difference will cause the difference. The cesium transport and diffusion through the fuel matrix and gap is modeled based on a fuel oxidation model. The BISON code is used to develop the cesium release model. The model developed can also be used to study the oxidation process of the fuel when contacting with water coolant. The oxidation model results from BIOSN agree with the results in reference very well which proves the model development using BISON. The cesium release model shows the time dependent cesium release after fuel defects reside on the fuel cladding, the radioactivity release to the coolant will be significant in the long term operation. The releasing of Cs into the coolant is significant when the fuel-water contact area is about 5%. And the releasing of Cs into the coolant will be significant when the diffusion coefficient of Cs in the fuel matrix increases 10 times.

#### *Thermal Hydraulics*

The five-equation drift-flux model (DFM) has been developed to address thermal non-equilibrium conditions and phenomena in LWRs. To relax the thermal equilibrium assumption in a mixture model, the energy conservation equation for the dispersed phase (gas phase) was derived from the Two-Fluid Model (TFM) as the fifth conservation field equation for the five-equation DFM. A mathematical study on system partial differential equations (PDEs) was also performed to examine its hyperbolic character, and therefore the “well-posedness” of the five-equation DFM. Due to its intrinsic hyperbolicity of system PDEs, this five-equation DFM can take advantage of the MOOSE framework using a finite element solver. For the closure of the five-equation DFM field equations, we revisited the existing constitutive equations or relations on the dispersed phase mass generation rate, interfacial energy transfer, distribution parameter, and drift velocity, specifically for important thermal non-equilibrium phenomena, such as subcooled boiling, choking flow during loss of coolant accidents, and flow instabilities in natural

circulation flow driven systems. Compared to other two-phase flow models, this five-equation DFM features relative simple governing equations with necessary physics included.

### ***Distributed Test Facility***

An external model was added to RAVEN to facilitate its connection to a hardware-in-the-loop test setup. This is a Python code module that takes values generated by RAVEN (e.g. a sampled variable), transmits it to the HIL system, and receives whatever outputs the HIL system generates and feeds them back into RAVEN. In this case, the value generated by RAVEN is to be used as the failure time of a component in the HIL, the main feed valve. The HIL setup receives this failure mode initialization from the external model, and begins running. When the HIL setup meets some terminating condition, either as a result of the induced component failure or not, it ceases operation and sends the test run time back to the external model which relays it further to RAVEN. In an effort to mitigate the undesirable transients and instability of the system under test in the DTF due to the overhead caused by significant time delays in a geo-distributed network, an improved algorithm for Task Allocation has been developed. This algorithm uses network graphs to compute the feasible configurations for the given computational nodes and software components. Furthermore, it uses stochastic dynamic programming to determine the most probable optimal dynamic allocation of software components at multiple computational locations by anticipating the changes in the network latency using time series models. When implementing an HIL system, the software must be synchronized to the hardware. This means that the software waits for input from the hardware before it can continue the next part of its calculation. Every computation step of the software must be faster than real time; no time margin or buffer can be built. Our devised method instead immediately provides several predicted values of the hardware response and the software continues running. Each of these predicted values is provided to a clone of the original software process, running in parallel. When the hardware does return its (real) value, the closest predicted value is found and the others can be discarded. To fully use RAVEN's capabilities, the failure modes of valves, pipes, and the intermediate heat exchanger in the turbine bypass system were considered in the test setup for method validation. The failure-modes-and-effects-analysis method was used to analyze the faults and effects propagation through the turbine bypass system. Equivalent behavior rules of the valves are being used to study the effect of the real failure modes and their influence on the system's performance.

### **Benefits to DOE**

This project benefits DOE by uncovering new thermodynamic data for fission products and extending the capabilities of the MOOSE/BISON. This work obtains additional thermodynamic data for fission products that are released in light water reactor (LWR) coolant and study the mechanisms of fission products release. The implementation of the MOOSE framework to solve the five-equation DFM offers a practical, yet accurate tool to model transient two-phase flow phenomena in LWRs. This work extends the application of the MOOSE framework in solving the thermal non-equilibrium two-phase flow model. The DTF provides the capability to test the reliability and performance of digital instrumentation and control systems; hence, it has high importance for the cybersecurity of nuclear power plants.

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### **Presentations**

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### **Interns and Postdocs**

Interns: Mike Pietrykowski, Rachit Aggarwal, Huijuan Li, Bobak Rashidnia, Sha Xue,

Postdocs: Shanbin Shi, Xiaoxu Diao,

## 15-142: New In-Core Neutron Diagnostics

Sebastien Teysseyre,<sup>1</sup> Adam Hecht,<sup>5</sup> and Jean-Claude Diels<sup>5</sup>

### General Project Description

Gamma radiation may displace electrons, which can have the effect of changing electron arrangement in the material and changing optical absorption, forming what is known as color centers. Neutron radiation may cause atomic recoils, which can also ionize the material, affecting color centers. Very distinct from gamma radiation, atomic recoils from neutron radiation change the structure of the material and can cause swelling or compactions. For transparent materials, this swelling or compaction can be seen in the change of the optical index of refraction. These changes can be exploited to measure a radiation field. That is, change in refractive index can be used to study bulk displacements and damage within a material nondestructively and to provide a gamma-blind mode of neutron dosimetry with a new range of materials that can be chosen for harsh environments.

This project focuses on examining the change in the index of refraction of  $\text{CaF}_2$  crystals as a function of fast-neutron radiation dose using irradiations in the Oregon State University reactor. The goals are to understand the correlation between dose and refractive index, to use this to develop crystals as a neutron dosimeter, and to set the groundwork to apply this understanding to standoff live-time readings, e.g., through optical coupling to the crystals through fiber optics. This would allow for live-time readouts of the neutron field in harsh environments, as within the TREAT reactor. Because color centers are produced in the crystals in these irradiations, they are also studied as a secondary and corroborating dosimetric method.

### Summary of Scientific, Technical, and Programmatic Progress

High precision refractive index measurements were performed on  $\text{CaF}_2$  crystals irradiated at the Oregon State University (OSU) TRIGA reactor. Three samples were examined following irradiation of  $10^{16}$ ,  $10^{17}$ , and  $10^{18}$  fast neutrons/cm<sup>2</sup>. The crystal swelled under irradiation, leading to a decrease in the index of refraction. The index change, from zero exposure, is presented in Figure 1 (left). This shows a clear decreasing trend. The refractive index of  $\text{CaF}_2$  is about 1.4 and the refractive index change values have estimated uncertainties of about  $2 \times 10^{-5}$ . Work is being performed to characterize and reduce uncertainty.

LAMMPS simulations were developed, including describing the interatomic interactions, for  $\text{CaF}_2$  crystals. Using these the displacements vs. energy deposited were simulated for low energies and a linear relation was found. Higher energies and higher doses would involve coalescing of vacancies into voids, which was beyond the scope of J. Morris' dissertation.

Color center formation was examined in the OSU irradiated crystals, shown in Figure 1 (right). Clear absorption peaks were identified and electronic structure was examined in the context of previous work on  $\text{CaF}_2$ . The absorption peaks reduce transmission at the particular wavelengths. These have different strength of response to irradiation but all track with irradiation. UV bleaching was also carried out to understand mobility of the color centers, and the faster populating color centers are also faster bleaching, relating to mobility of both populating and depopulating particular electron/hole locations.

Irradiations were performed at OSU to fill in the gaps in data below the highest irradiation for refractive index measurements, and below all three previous OSU irradiations for color center measurements. For coupling to fiber optics, literature reviews show some Si based fibers irradiated in the OSIRIS reactor to have an attenuation minimum near 790 nm, where we are performing this work [2].

Joe Morris completed his PhD dissertation, titled *High Precision Refractive Index Measurement Techniques Applied to the Analysis of Neutron Damage and Effects in CaF<sub>2</sub> Crystals*, in May 2017. Sara Pelka completed her MS thesis, titled *Examination of Color Center Formation in CaF<sub>2</sub> Crystals when Exposed to Gamma and Mixed Neutron/Gamma Fields*, in May 2017.

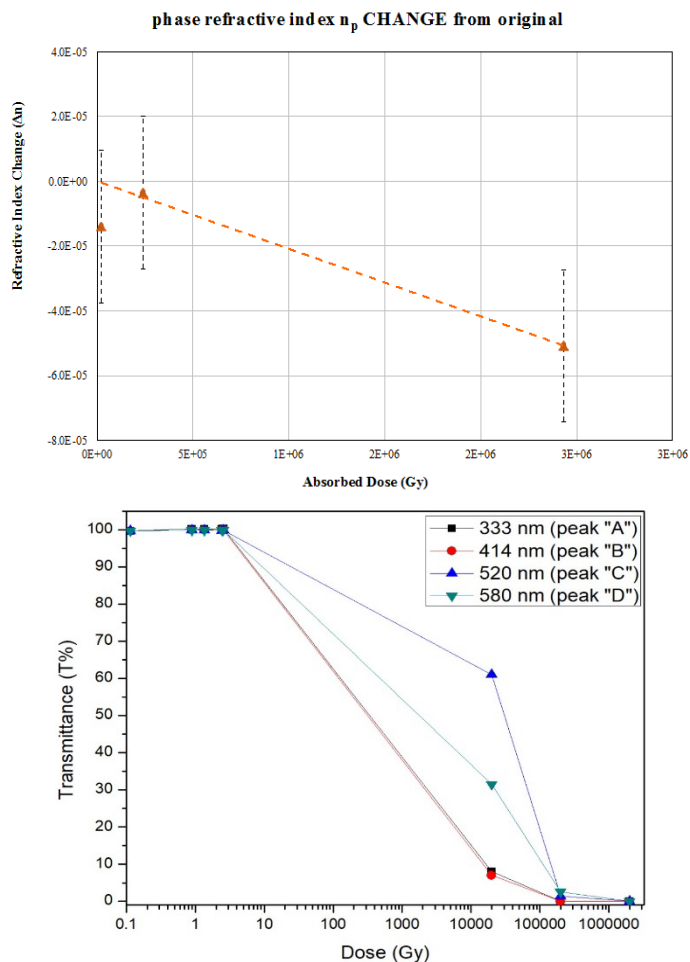


Figure 1. (Left). Refractive index change in CaF<sub>2</sub> crystals as a function of fast neutron dose from the Oregon State University TRIGA reactor. (Right) Color center formation for different color centers as a function of dose in CaF<sub>2</sub> crystals. The three doses to the right correspond to the OSU irradiations.

## Benefits to DOE

The project goal is to enable new types of neutron dosimetry measurements by nondestructive measurement of internal damage to crystals through fast and high precision index of refraction measurement. This opens a new range of materials for use in neutron dosimetry, including materials appropriate for harsh environments like those typical of pyroprocessing. This new dosimetric technique can be used for long-time, unpowered, integrating measurements or for live-time measurements. With microsecond-scale readout, differential measurements may be made that can enable live-time neutron characterization of neutron fields in the TREAT reactor.

## References

- [1] W. Primak, “Fast-Neutron-Induced Changes in Quartz and Vitreous Silica”, *Phys. Rev.* 110 (1958), p. 1240.
- [2] G. Cheymol, H. V. J.-F. Long and B. Brichard, *IEEE TNS* 55.4 (2008), pp. 2252–2258.

## Publications

- Morris, J.P., 2017, *High Precision Refractive Index Measurement Techniques Applied to the Analysis of Neutron Damage and Effects in CaF<sub>2</sub> Crystals*, PhD Dissertation, Nuclear Engineering, University of New Mexico, 2017.
- Pelka, S., 2017, *Examination of Color Center Formation in CaF<sub>2</sub> Crystals when Exposed to Gamma and Mixed Neutron/Gamma Fields*, Thesis, Nuclear Engineering, University of New Mexico, Sara Pelka, 2017.
- Masuda, K., E.I. Vaughan, L. Arissian, J.P. Hendrie, J. Cole, J.-C. Diels, A.A. Hecht, 2015, Novel techniques for high precision refractive index measurements, and application to assessing neutron damage and dose in crystals”, *Nuclear Instruments and Methods A* 784, 198 (2015)  
<http://dx.doi.org/10.1016/j.nima.2014.11.031>

## Publications in Preparation

- Morris, J., J. Hendrie, S. Pelka, S. Teysseyre, J.-C. Diels, and A.A. Hecht “High precision measurements of refractive index change in CaF<sub>2</sub> crystals as a function of reactor dose.”
- Morris, J., J. Hendrie, S. Pelka, S. Teysseyre, J.-C. Diels, and A.A. Hecht, “ Fabry Perot crystal rotation effects on nested cavity modes within a mode locked laser cavity.”
- Morris, J., J. Hendrie, S. Teysseyre, J.-C. Diels, and A.A. Hecht, “LAMMPS simulations and displacement energies on the CaF<sub>2</sub> crystal lattice.”
- Pelka, S., J. Morris, S. Teysseyre, J.-C. Diels, and A.A. Hecht,” Color center formation vs. dose in CaF<sub>2</sub> crystals from reactor irradiation.”

## Presentations

- Hendrie, J., A. Ladan, K. Masuda, A. Hecht, and J. C. Diels, 2015,” Nested Fabry-Perot in mode-locked lasers to monitor minute changes of index”, *CLEO: Science and Innovations 2015*, San Jose, California United States, 10–15 May 2015.

## Interns and Postdocs

Interns: Sara Pelka, Joe Morris, and Adam Hecht.

## 15-144: Investigation of Sonication Assisted Electrolytic Reduction of Used Oxide Fuel in Molten Salt

Shelly Li<sup>1</sup> and Haiyan Zhao<sup>7</sup>

### General Project Description

Electrolytic reduction is an integral step in pyroprocessing to treat used fuel from light water reactors (LWR) and other metal oxides. In the electrolytic metal oxide reduction, slow oxygen ion diffusion through the used fuel particulates inside the cathode basket to the anode is the process limiting step, which leads to low current efficiency, long operating hours, and re-oxidation of reduced metal fuels. Extensive R&D activities have been conducted in the past decade to improve the oxygen diffusion process associated with the electrolytic reduction of used LWR fuel in high temperature molten salts. However, sonication technology has not been explored for the purpose. Sonication is a mature technology to improve a variety of chemical/physical processes including chemical reactions and mass transports. This LDRD project provides a great opportunity to explore the possibility of improving electrolytic reduction of used oxide fuel in molten salts with ultrasound technique.

### Summary

All the experimental works have been conducted by graduate students under the supervision of Dr. Haiyan Zhao at CAES, the U of I. The collaboration with the university, especially the contributions made by graduate students, was essential for the accomplishments in FY-17.

In FY-17, we have focused on optimizing the setup for molten salt electrochemistry at lab scale and electrolytic metal oxide reduction in molten salts and finding a proper surrogate for UO<sub>2</sub>. The significant accomplishments include:

- Optimized electrode assembly for fundamental molten salt electrochemistry; improved fuel basket configuration with thicker center piece for metal oxide reduction purpose with improved results
- Established methods to identify the compositions of reduced samples using XRD and the Li<sub>2</sub>O compositions in salt using PH.
- Finished the sonication setup and tested with molten salts in fume hood and ready to test it in glovebox.

This LDRD project is under the initiative of Fuel Cycle Separations and Waste Forms. The PI at the INL and co-PI at the CAES have closely worked with the National Technical Director of Material Recovery and Waste Forms Development under the DOE NTRD programs. Further funding opportunities under the DOE NTRD and NEUP programs have been pursued.

Program development activities include:

1. Four full NEUP proposals were invited and submitted to NEUP-FY-17 CINR FOA based on the outcome of this project.
2. Apply for nuclear education grant program-curricula development sponsored by United States Nuclear Regulatory Commission for pyroprocessing technology at the University of Idaho;

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<sup>7</sup> Department of Chemical and Materials Engineering, University of Idaho at Idaho Falls (UI/CAES)

3. Apply NEUP-FY-18 CINR FOA;
4. Apply future DOE-BES EFRC calls.

### **Benefits to DOE**

The agitation through sonication will be expected to accelerate oxygen ion diffusion, improve the contact between the fuel particulate with the cathode and also drive the trapped O<sub>2</sub> molecules diffusing out of the packed fuel bed in the adhesive molten salt. Should the proposed research proceed as expected, it will successfully resolve one of key needs associated with scale-up pyroprocessing. The proposed research will expand expertise in the electrolytic reduction of used LWR fuels for pyroprocessing and further establish the INL as a world leader in innovative fuel cycle technology. The proposed research is also directly applicable to the projects for recycling rare earth elements under the Critical Material Institute (CMI). Should this proposal yield technical advances, funding would be sought through the DOE Nuclear Technology Research and Development (NTRD) Program as well as the CMI. The research team is seeking to protect intellectual property and publish information in the interest of the laboratory.

### **Publications**

*Journal of Electrochemistry Society*; in preparation, plan to submit by the end of 2017.

### **Presentation**

“Effect of Electrolyte Purity on Electrolytic Reduction of TiO<sub>2</sub>”, ANS, Las Vegas, November, 2016.

### **Invention Disclosures**

IDR#4430, Ultrasound Assisted Electrolytic Reduction of Used Oxide Fuel in Molten Salt.

### **Interns and Postdocs**

Interns: Meng Shi, Eugene Engmann, William Chan, and Amey Shiregkar.

### **Collaborations**

University: University of Idaho.



## 15-145: Advanced Neutron and X-Ray Imaging at TREAT

James K. Jewell<sup>1</sup> and Tony Hill<sup>8</sup>

### General Project Description

This LDRD focuses on development of advanced imaging options for future TREAT experimental program with the aim to develop a suite of possible imaging capabilities that will extend the scientific and engineering reach of TREAT to include a lower-length scale scientific testing program.

### Summary

This project plan starts with a broad analysis to identify spatial and temporal requirements for achieving the overarching goals of the program and the specific requirements as determined by potential users. A workshop was held on September 2nd & 3rd in the CAES auditorium that brought local experimenters and modelers together in order to begin identifying high-priority validation needs. The discussion focused on the development of appropriate sensitivity studies under the MOOSE framework that can support future cost-benefit analyses. The discussions were not limited to central position experiments but included ideas to evolve the TREAT core to include a lower-length scale irradiation position near the periphery that can be used parasitically, particularly during the time between central position irradiations, which could extend and complement the traditional TREAT experimental program. Discussions also focused on development of closer collaboration between modelers and experimentalists to properly design and analyze experiments of high value, as no organizational system is in place to cultivate and manage this relationship. Sensitivity studies are needed that provide quantitative basis (benefit) for experiments (cost) and requires initial uncertainty evaluations in existing models and covariance development. Experimentalists need a high fidelity simulation tool for the experimental regions that supports instrument/experimental design. The need for experimental analysis and data mining in MOOSE was discussed for the use of large-field SEM-based “Big Data” development.

Spatial energy deposition measurements can be considered critical for advancing the scientific impact of nearly all TREAT experiments. A rather simple system has been studied that would provide a) the previous burn-up profile along the axis of the fuel rod as it is being inserted into the TREAT reactor, and b) the energy deposited by TREAT along the axis of the rod as it is being retrieved from the reactor, thus determining the power coupling of the rod as a function of its length. This can be accomplished with the addition of an experimental collar or extension to the fuel cask, which is used to transport the fuel to and from the reactor. The extension would be positioned between the bottom of the cask and the top of the reactor. The extension will provide the shielded experimental access needed to “view” the fuel as it is moved into and out of the reactor. A simple horizontal slit (or slits) in the collar that runs from the inner diameter to the outer diameter will allow gamma rays to escape the central position and be measured by an HPGe system located on the outer diameter. The fuel can be stepped down from the cask, through the collar, and into the reactor, allowing gamma spectra to be measured as a function of length along the fuel rod. Long-lived isotope ratios will be used to determine previous history; short-lived isotopes will be used for the measuring the TREAT coupling. These measurements could significantly reduce the uncertainties associated with the specific irradiation conditions as a function of position within the test vehicle. The fluctuations in the neutron flux cannot be specifically predicted for each experiment, therefore, measurements must be carried out that quantify these variations in order to maximize the scientific impact. Signal to noise calculations have been estimated based on drawings of the Multi-SERTA test

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<sup>8</sup> Idaho State University

vehicle, which not only shield and scatter gammas but increase backgrounds due to activation. However, the neutron flux shape for the TREAT experimental position has only recently been estimated (poorly) and was not been incorporated into this study. GEANT4-based simulations were partially developed to identify the benefits of specifically designed HPGe “clusters” that are spectrally more efficient with lower background levels in the Compton continuum. This simulation also provided first estimates of the intrinsic backgrounds from Compton scattering within the dense nuclear fuel, which represents an irreducible background in the system and directly impacts the signal to noise requirements for such a system.

An advanced single gamma emission computed tomography system could provide true 3D isotopic distributions in fuel rods or pellets for determining axial burn-up and power profile, percent fission gas release and isotopics of fission gases, as well as the isotopic distributions within the fuel. A dedicated system has been envisioned that could be located above the hot cell in the Loop Insertion Cell (LIC). There have been a number of technological advances in computing, electronics and gamma detector design since the era of computed tomography began. A new simulation tool was developed specifically for carrying out basic sensitivity studies on the tomographic reconstruction code and eventually on global design parameters. Existing 3D codes, such as MCNP and GEANT, are expensive calculations given the overall inefficiency for the gamma detection system, which reduces to a highly restricted two-dimensional problem. The new 2D simulation code performs analytic line integrals across the idealized object in the measurement direction with an adjustable step granularity in the perpendicular direction that are summed to represent the flux of gammas through an adjustable collimation system. The new simulation code was used to quickly and efficiently generate data that were processed by modern computed tomography codes. It turns out that the intrinsic 2D resolution is fixed by the gamma collimation slit width, which will be ~1mm in a realistic system. The potential for high resolution (~120 micron) remains a possibility with 1mm apertures but will require significant effort in developing a new Bayesian unfolding algorithm (for instance) that maximizes the presented data in a true 3D space that accounts for variations in fuel density, diameter and curvature of rods. This approach would certainly require modern computing infrastructure and approximately 4-8 FTE years to develop the code. A more efficient unfolding algorithm will be needed in order to carry out further design sensitivity studies.

Approaches for validating the thermodynamic behavior of the TREAT fuel have been investigated. Under the assumption that fuel remnants are available, we foresee a set of experiments using highly instrumented fuel shapes that will be used as targets to provide critical feedback to the MOOSE-based V&V effort. One candidate is the central irradiation of small, bare TREAT fuel specimens that are highly instrumented for temperature mapping over the entire surface. The primary instrumentation challenges of such an experiment are the time response of thermocouples, which must have a time constant much shorter than a fast transient time scale (100ms), and the coupling technique for a large number of measurement points, which could be of order a hundred or more. Research has demonstrated that thin film thermocouples (125um layers) are capable of response times below a microsecond, making them prime candidates for fast pulse studies. These thermocouple layers are usually deposited by evaporation or sputtering techniques directly onto the surface of a sample using photolithography masks. The two layers are offset so that each pad has primary contact with the surface, along with a small overlapping area that forms the Seebeck junction. Each pad is also used for contacting the system with wires for voltage measurements by a remote data acquisition system. Complications arise in this application due to the radioactive nature of the specimen and the conductivity of fuel surface. We studied different approaches for simplifying the attachment of thin- film thermocouples and ways to electrically isolate the junction pairs from the fuel specimen surface or include the graphite in the thermocouple circuit.

TREAT science can also be enhanced by the proliferation of sensitive instrumentation around the experimental region for time dependent measurements of the local environment. Increased sensitivity and channel count can be extended beyond current format restrictions by the inclusion of electronic signal processing circuits between the instruments and the DAQ. An MCNP TREAT deck that includes the biological shield and basement volume was located at ANL and used to calculate the flux through the central experimental region and along potential cable paths through the reactor. These calculations can also be used to identify appropriate regions where electronics can be tested for use in future experiment designs.

### **Benefits to DOE**

This work supports the DOE NE Roadmap directive for science-based, independent effects measurements. Advanced imaging and monitoring capabilities could extent the scientific reach of the TREAT experimental program to time- and power-based dynamics at the meso-scale and would be the first of their kinds. It represents a novel approach to the detailed study of fuel at multiple length scales.

### **Presentation**

Tony Hill, 2016, “Advanced Neutron and X-Ray Imaging at TREAT”, LDRD Mid-Year Review, EROB Room 304b, June 28, 2016.

### **Interns**

Interns: Cody Milne and Bilguun Byambadorj

### **Collaborations**

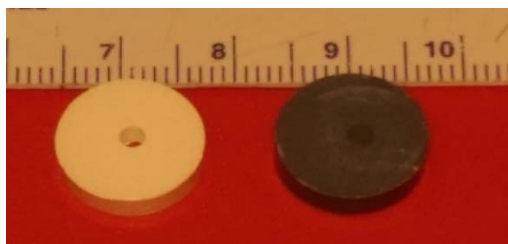
Universities: Idaho State University

## 16-003: Recycling of Tantalum-Containing Waste Materials to Recover Tantalum Metal

Prabhat K. Tripathy,<sup>1</sup> Michael R. Shaltry,<sup>1</sup> and Jerome P. Downey<sup>9</sup>

### General Project Description

In continuation of broader objectives, experimental research was extended to carry out the electrochemical reduction of mixed oxides, prepared both in a reducing as well as oxidizing atmosphere (Fig.1). Four mixed (sintered) oxide pellets (in the molar ratio 1:1) were chosen to study their electrochemical reduction patterns. The goal is to prepare the respective alloy powders (Ta-Ti, Ta-Hf, Ta-Nb and Ta-W) in just one unit operation from their respective mixed oxide compositions ( $Ta_2O_5+TiO_2$ ,  $Ta_2O_5+HfO_2$ ,  $Ta_2O_5+Nb_2O_5$  and  $Ta_2O_5+WO_3$ ). These alloy powders possess requisite high temperature properties (oxidation and corrosion resistance, high temperature strength, ductility etc.) and have been projected as future materials (mostly in structural components) in advanced nuclear reactor, space, defense, and automotive technologies. The conventional fabrication method of these alloy powders has been the co-melting of the alloy constituents, into the ingot, by a highly energy intensive melting process. Such a melting operation is usually repeated several times to render the alloy ingot homogeneous. The goal of the present project is to examine whether it is possible to prepare these high-melting alloy powders by a non-melting process directly from their oxide intermediates.



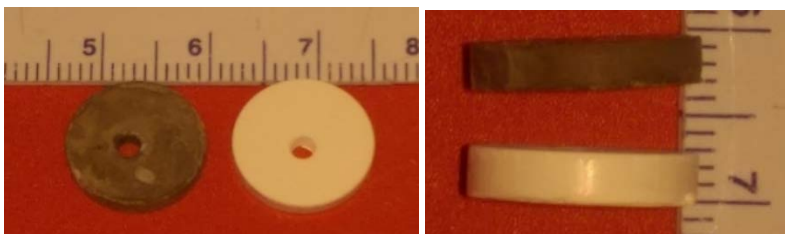
*Figure 1.  $Ta_2O_5+TiO_2$  pellet (left: air-sintered and right: sintered under pure hydrogen flow)*

### Summary

The specific goals of the project have been to (i) develop a generic molten salt electrometallurgical process for producing various engineering metals/alloys from their oxide intermediates (ii) develop recycling schemes for waste/discarded and recyclable engineering materials (iii) develop new process flowsheets to manufacture engineering metals and alloys with minimum environmental foot print and (iv) study the potential applications of new, hitherto untested, inert anode materials. Experimental research has indicated that better reduction efficiency as well as metal/alloy quality could be produced when the engineered oxide precursors were subjected to the electrochemical reduction in the calcium chloride-(1-5 wt.%) calcium oxide electrolyte at a temperature range of 800–950°C. These engineered oxide precursors were prepared by heating the green (compacted) pellets under a pure hydrogen flow at temperatures up to 1000°C. The reduction time in the case of the engineered pellets was observed to decrease by ~ 40% as compared to their counterparts (i.e. reduction of air-sintered oxide pellets). Also, the residual oxygen

<sup>9</sup> Montana Tech of the University of Montana

contents in the reduced metal/alloy, in the former group of pellets, were determined to be comparatively low. Such an observation was observed for the first time during the course of the present investigation and has not been reported in the scientific publications. Another important research finding is the possibility of producing a near-net-shaped product/component (Figure 2). Usually the oxide pellets (both single and mixed), upon reduction in a molten salt bath, get converted to powders/chunks. Because of their relatively fine size and larger surface areas, the reduced metals/alloys have been reported to pick up oxygen during subsequent washing (with water) to remove the entrapped electrolyte. It seems that careful manipulation of the reduction experiment can, in principle, result in the formation of a near-net shaped metal/alloy, something which is absent in the published literature.



*Figure 2. Electroreduced tantalum pellet could retain its shape: white – unreduced and grey – reduced pellets respectively. Slight reduction in the diameter (left) and thickness (right) of the reduced pellet were observed.*

The process flow sheets pertaining to the preparation of tantalum and alloys of tantalum (tantalum-niobium as well as tantalum-tungsten) have been developed. Process flowsheets pertaining to other two alloy systems (tantalum-titanium and tantalum-hafnium) are being developed. Superior performance characteristics of three platinum group metals (ruthenium, Ru, rhodium, Rh, and iridium, Ir), as inert anode materials, indicates that their compounds ( $M_xM_yO_z$ ,  $M_x = \text{Li/Ca}$ ,  $M_y = \text{Ru, Ir, Rh, Os}$  = oxygen) could possibly be developed as potentially low-cost oxygen evolving electrodes.

## Benefits to DOE

Refractory metals and their alloys, in general, and tantalum and its alloys, in particular, play crucial roles in nuclear, defense, aerospace, biomedical, and other industrial units. Tantalum-, niobium-, hafnium-, and tungsten-based alloys have been projected as structural materials for advanced nuclear reactors and space technologies. Ta-Hf alloys can be used as the precursor materials to fabricate super-hard materials (TaHfC) that can withstand ultrahigh temperature ( $\sim 4000^\circ\text{C}$ ) and may enable spacecraft to withstand very high temperatures while leaving and re-entering the earth atmosphere. The project has also shown feasibility of transforming the oxidized materials to their metallic stage, which can be directly put to use. Such a possibility opens up new opportunities for the recycling industries. The innovative approach, employed in the present project, offers an opportunity to develop new and energy-efficient manufacturing processes for the fabrication of a variety of engineering metals and alloys currently being used in advanced technologies. It is hoped that besides providing an edge to the INL's capabilities this project shall help foster innovation with technology solutions.

## Publication

Chorney, M.P., B.P. Hurley, P. K. Tripathy, and J. P. Downey, 2017, "Effects of Oxide Precursor Preparation Parameters on the Electrochemical Reduction of Tantalum Pentoxide in Calcium

Chloride Melt”, *The Minerals, Metals and Materials Society, TMS 2017, 146<sup>th</sup> Annual Meeting & Exhibition Supplemental Proceedings*, Springer, DOI:10.1007/978-3-319-51493-2\_62, pp. 651-5.

### **Presentation**

Chorney, M.P., B.P. Hurley, P. K. Tripathy, and J. P. Downey, 2017 “Recycling of Tantalum-containing Waste Materials”, *Annual Meeting and Exhibition, TMS*, Feb. 28–March 02, 2017, San Diego, CA

### **Invention Disclosure**

BA971-On the Use of Monolithic Metals as Potential Gas Evolving Electrodes in a Molten Alkaline Earth Metal Halide Electrolyte.

### **Interns and Postdocs**

Interns: Maureen P. Chorney and Bridger P. Hurley,

### **Collaborations**

University: Montana Technical University-Butte.



## 16-010: Development of a Fully Coupled Radiation Damage Production and Evolution Simulation Capability

Daniel Schwen,<sup>1</sup> Sebastian Schunert,<sup>1</sup> Javier Ortensi,<sup>1</sup> Xianming Bai,<sup>10</sup> and Yongfeng Zhang<sup>1</sup>

### General Project Description

Nuclear reactor components experience radiation damage due to energetic-particle radiation. This creates defects—such as vacancies and interstitials—in the regular atomic lattices, causes disorder in ordered compounds, and redistributes material, impacting the microstructure evolution, which ultimately determines macroscopic material properties. In this project, we aim to couple the simulation of radiation damage (MyTRIM), microstructure evolution (MARMOT), nuclide transmutation, and neutronics (MAMMOTH). The final deliverable will be a spatially resolved damage-calculation capability with ballistic mixing informed by MyTRIM, transmutation in MARMOT informed by MAMMOTH, and residual defect densities implemented using the phase field formalism.

### Summary

We completed coupling of the microstructure code MARMOT and MyTRIM in a flexible and highly efficient manner using a rasterization approach yielding maximum parallel scalability. MARMOT's FEM mesh is overlaid on the MyTRIM geometry, material properties are computed on each finite element and broadcast to each compute node for the MyTRIM simulation as collisions can span the whole domain. MyTRIM cascades parallelize over multiple MPI processes and threads. We demonstrated that the rasterization approach for coupling microstructure evolution and binary collision Monte-Carlo (BCMC) is feasible on ballistic mixing simulations where the BCMC introduces a new driving force that has previously not been accounted for in irradiation driven microstructure evolution simulations.

The neutron flux field is the driving force of the radiation damage and hence vital for an accurate simulation of radiation damage cascades. We implemented the capability of computing the (angular) nuclide recoil and nuclide fission rates that are used to construct PKA probability density functions. For sampling PKAs from fission reactions, ENDF data has been imported incorporating the distribution of mass and charge number of the fission products. ENDF data accurately represents the fission product distributions of more than 20 different fissionable targets for neutrons ranging from thermal energies (<1eV) up to fast neutrons (20 MeV).

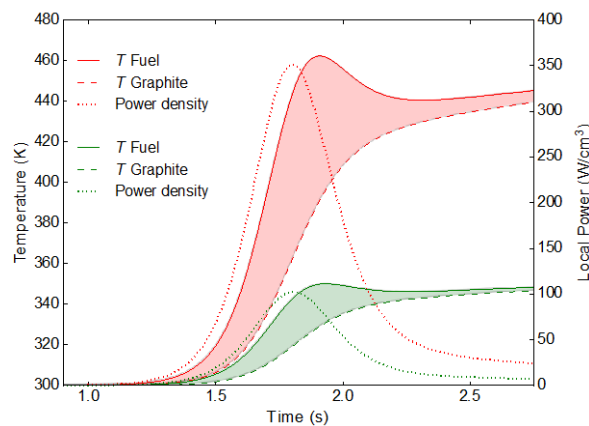
The utility of the coupled neutronics-BCMC simulation is demonstrated on a Transient Reactor Test Facility (TREAT) fuel particle, which has a size of the same order as the range of fission fragments and hence the fission energy deposition around it is neither uniform nor confined to the fuel. The BCMC algorithm has been accelerated to perform faster if lower spatial resolution for the energy deposition is acceptable.

We demonstrate that the sensitivity of the averaged temperatures in the fuel and graphite are noticeably different [but not overly sensitive] to the grain shape: differences of 5-10 K were observed. However, when comparing the peak fuel and graphite temperatures, we find large differences of up to 80 K even for the considered low power transient 15 (Figure 1). For a potential low-enrichment conversion of TREAT, this effect has strong implications for the reactivity of the core.

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<sup>10</sup> Virginia Polytechnic Institute and State University

We have started demonstrating the effect of micro-structure evolution driven by radiation damage using a coupled MAMMOTH-Magpie-MyTRIM model. A single fuel pellet is depleted over one full power year and the fuel isotopic composition MAMMOTH tracked via the depletion capability. The fission rate PDFs evaluated at multiple representative points in the pin are used to drive a BCMC simulation that provides fission gas source terms to a grand potential phase field model that tracks fission gas accumulation within grains and at grain boundaries. Fission gas bubble information are then used to modify the density at the MAMMOTH fuel pellet level. The university collaborator Co-PI Bai worked on parameterizing radiation damage in structural materials for mesoscale radiation damage models. Virginia Tech has used molecular dynamics simulations to calculate the cascade-induced defect numbers and defect diffusion coefficients in FeCr alloys with Cr concentration ranges from 0 to 20% at 300 K and 800 K. It is found that the total number of Frenkel pairs is not sensitive to Cr concentration. However, the fraction of Cr interstitials with respect to the total number of interstitials significantly exceeds (typically about twice to three times of) the Cr concentration in alloys. This work will be used to parameterize cluster dynamics simulations that extend the defect simulation past the ballistic phase.



*Figure 1. Temperature difference between fuel particles and graphite matrix during a simulated transient 15 at two locations in the core.*

## Benefits to DOE

Understanding radiation damage is essential for advancing fuel performance. However, understanding radiation damage requires such damage to be viewed in a coupled, multiphysics setting. The benefit of this LDRD is the development of the first tool for comprehensive studies of radiation damage and its evolution in a multiphysics environment. It will advance our understanding of the microscopic mechanisms governing the macroscopic behavior of fuels and structural materials, thus impacting both the ATF and LWRS Programs. It has already found application for the TREAT reactor directly impacting INL's mission. The tools developed in this LDRD enable researchers to better account for irradiation effects when predicting material performance of existing and newly designed reactor fuels, clads, and structural materials.

## Publications

Schunert, S., D. Schwen, P. Ghassemi, et al., 2017, “Heat Source Characterization In A TREAT Fuel Particle Using Coupled Neutronics Binary Collision Monte-Carlo Calculation,” *M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering*, Jeju, Korea, April 16-20, 2017 (published – conference proceedings).

Schwen, D. and S. Schunert, “Coupling binary collision Monte Carlo to finite element based microstructure evolution,” *Computational Materials Science*, in preparation.

Zabriskie, A., S. Schunert, D. Schwen, and R. Martineau, “Coupled multiscale neutronics binary collision Monte Carlo model of an LEU TREAT core,” *Annals of Nuclear Energy*, in preparation

## Presentations

Schwen, D. and S. Schunert, 2016, “Coupling Radiation Damage from Binary Collision Monte Carlo to Phase Field Microstructure Evolution”, *TMS 2016*, Nashville, TN. Conference presentation.

Schwen, D. and S. Schunert, 2016, “Coupling Radiation Damage from Binary Collision Monte Carlo to Phase Field Microstructure Evolution”, *MMM 2016*, Dijon, France (10/12/2016).

Schunert, S. and D. Schwen, 2016 “Heat Source Characterization in a TREAT Fuel Particle Using Coupled Neutronics-BCMC Calculations”, *International Conference on Mathematics & Computational Methods Applied to Nuclear Science and Engineering*, Jeju, Korea

Schwen, D. and S. Schunert, 2017, “Coupling radiation damage to phase field microstructure evolution and thermal transport”, *TMS 2017* San Diego

## Interns

Interns: Pedram Ghassemi and Marina Ferreira Fonseca Sessim

## Collaborations

Universities: North Carolina State University and Pennsylvania State University

## 16-013: Micromechanistic Approach and Critical Experiments for Quantitative Predictions of Delayed Hydride Cracking in Zirconium Alloys

S.B. Biner,<sup>1</sup> K.E. Ahmed,<sup>1</sup> P. Chakraborty,<sup>1</sup> D. Schwen,<sup>1</sup> and S. Teysseyre<sup>1</sup>

### General Project Description

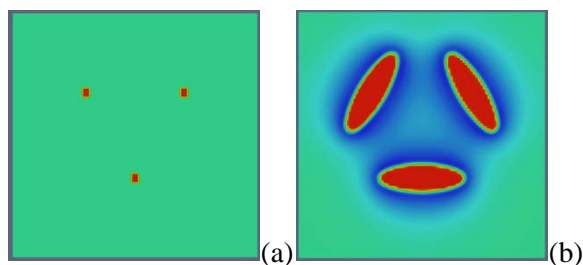
This proposal aims at the development of a micromechanistic phase-field model, validated with critical experiments, for quantitative predictions of delayed hydride cracking (DHC) in zirconium alloys.

### Summary

Our current progress is summarized in two sections below.

#### **Modeling and Simulation Studies**

A phase-field model for  $\delta$ -hydride evolution in Zr-alloys has been developed. The model correctly incorporates the misfit strains between the hydrides and the matrix phases on the evolution of the interfacial energy, leading to formation of the needle shape hydride phases for three different hydride invariants, as shown in Fig.1



*Figure 1. Evolution of three different hydride invariants from circular seeds. The hydrogen concentration is 0.1 in the matrix and 0.5 in the precipitate, with (a) the initial seed and (b) the final configuration of the precipitates.*

In addition, the incorporation of the thermodynamic database, based on the phase-equilibrium diagram, is currently being pursued for the quantitative analysis. This approach enables to model the dissolution/precipitation under thermal cycling as shown below in Fig.2.

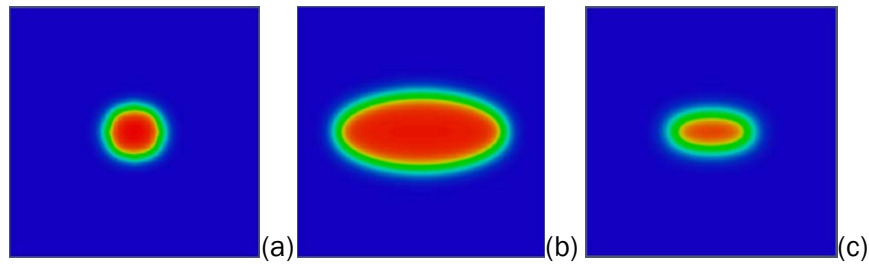


Figure 2. Modeling of hydride dissolution, with (a) initial seed at 500 K, (b) growth, and (c) dissolution of the grown precipitate when temperature is ramped to 800 K.

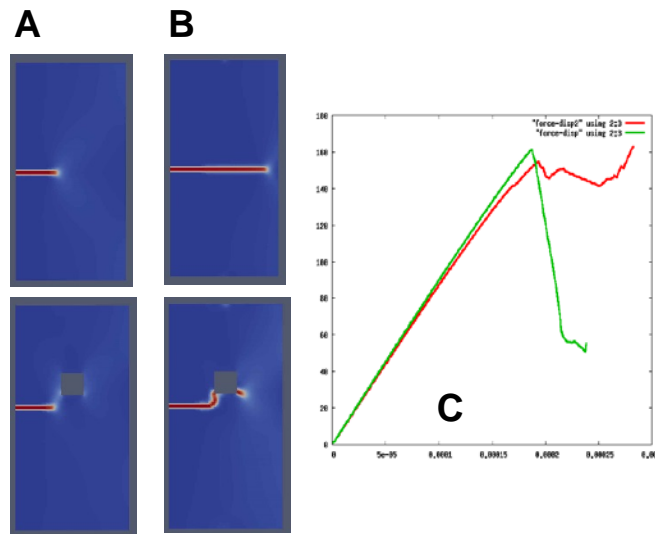


Figure 3. Simulation of fracture in SEN specimen (top a, b) and SEN specimen with a hole (bottom a, b). Column A is at the initial stages of the loading and column B is the final stages of the fracture. The red lines in the column A and B represents the crack. Fig.C is the resulting load-displacement curves.

For the evolution of the fracture behavior in delayed hydride cracking, a phase-field model based on the finite-element-method formulism has been developed. The simulation of cracking behavior in a single edge notch specimen and the simulation of crack and hole interactions are summarized in Fig.3, which agree very well with the available literature. One of the main objective of this effort is to elucidate two competing and conflicting theories/models that have been developed for delayed hydride cracking.

### Experimental Studies

We are able to produce hydride formation in a controlled manner in Zr-alloys. The delayed hydride cracking experiments on fatigue pre-cracked ¼ inch thick CT specimens are currently being performed at testing temperature of 525 °K.

## Benefits to DOE

The developments resulting from this proposal are also applicable to other hydriding alloy systems such as titanium, lithium etc.; therefore, it will clearly provide a fundamental understanding of DHC.

## Presentations

Ahmed, K.E., P. Chakraborty, D. Schwen, S. Tysseyre, and S. B. Biner, 2016, “The effects of crack-tip stress fields on the delayed hydride cracking”, *MST Annual Meeting* to be held in Salt Lake City during Oct 2016.

Ahmed, K.E., S.B. Biner, and D. Schwen, 2017, “Effect of crack-tip stress-field on the behavior of phase transition in two phase systems”, *MRS Winter Annual Meeting*, Nov-2017,

Ahmed, K.E., S.B. Biner, and D. Schwen, 2018, “Effects of stress on hydride precipitation and re-orientation: A phase-field model study”, *TMS Annual Meeting*, Phoenix March-2018.



## 16-026: Computationally Efficient Prediction of Containment Thermal Hydraulics Using Multi-Scale Simulation: Feasibility Study

Robert Youngblood,<sup>1</sup> Nam Dinh,<sup>3</sup> and Igor Bolotnov<sup>3</sup>

### General Project Description

The research is motivated by recognition that conventional high-resolution computational fluid dynamics (CFD) approaches are computationally overwhelming for simulation of the phenomenology of accident scenarios in reactor containment because these scenarios evolve over long time scales and extend over large length scales. The difficulties are even more pronounced when a sensitivity or uncertainty analysis is required to support risk-informed design and safety analysis of nuclear power plants; this entails simulation of many time histories in order to develop an understanding of the implications of the variabilities and uncertainties that affect the evolution of the scenarios. It is currently not feasible to analyze many scenarios using a high-fidelity code. The project's objective is to learn how to correct the results obtained from lower-fidelity simulations to agree with results obtained from a training set of high-fidelity simulations. Based on comparing low-fidelity results with high-fidelity results, we learn what is being lost in the low-fidelity simulations, and train a model such as a neural network to correct low-fidelity results to correspond to those obtained by higher-fidelity models. Once this is achieved, much more comprehensive analysis is possible using the low-fidelity simulations than would be practical using only high-fidelity simulations. If necessary, the overall results can be subsequently reconfirmed with a small number of high-fidelity simulations. In short, the project investigates a data-driven, multi-scale analysis framework that has the potential to enable computationally efficient simulation of thermal-hydraulic processes, initially in reactor containments and later potentially in other application areas.

### Summary

The work is being carried out in two parallel threads by two doctoral candidates, Han Bao and Botros Hanna.

Botros Hanna's work focuses on coarse-grained CFD, and has a multi-physics aspect. His work began with analysis of the turbulent natural convection case with volumetric heating in a horizontal fluid layer. Analysis of that problem was performed with a high-fidelity simulation (with fine mesh) and lower-fidelity, three-dimensional simulation (coarse mesh); based on the results, a method was developed for correcting the coarse mesh simulation by modifying the diffusion term in the energy equation to compensate for meshing effects. This global correction was presented as a function of mesh size. More recently, Hanna's work has examined turbulence in a lid-driven cavity, learning the correction from a much richer local data set (function values, first derivatives, second derivatives) in a more truly data-driven way. This work is the basis for Hanna's recent successful Preliminary exam; the current expectation is that he will defend his PhD thesis early in the next calendar year.

Han Bao's study focused on development and demonstration of the optimized mesh/model information system, "OMIS," which aims to advise on how to obtain the greatest accuracy possible from a coarse-mesh code by optimizing mesh and model, in order to enable mutual compensation of numerical error, model error and model uncertainty. The methodology assumes that the error in simulation of Figures of Merit (FOMs) using coarse-mesh thermal-hydraulic codes can be represented as a function of key Physical Features (PFs), model information (including model form and model parameter), and coarse mesh size. This error function for a specific physical condition can be obtained by training an appropriate Machine Learning (ML) algorithm, such as a neural network, based on results of training runs of the code.

Based on the assumptions and the demonstration of two single-FOM-PF case studies (1D conduction and 2D natural convection) in 2016, the framework for steady-state simulation has been revised and improved. In FY 2017, the system studied was a 2D mixed convection case with a cold-wall boundary condition at the top of the volume. Hot air was injected at the bottom of one sidewall and vented at the top of another sidewall. Natural convection and forced convection heat transfer occurred simultaneously in the volume. Four groups of convection models were defined in GOTHIC (a well-known tool for simulating thermal hydraulics) and used for coarse-mesh simulation with four different mesh sizes. Two PFs were identified and defined to represent this physical condition: the Reynolds number of inlet flow and the Rayleigh number with the temperature difference of top cold wall and inlet hot fluid. The FOM is the temperature distribution in the central line. Sixteen cases with different inlet air temperatures and velocities have been simulated using GOTHIC to obtain LF and HF data. A neural network with one hidden layer and twenty neurons was used for data training. The obtained OMIS regression model was then applied to predict the simulation error and optimized mesh/model information for three new conditions with different inlet air temperatures and velocities. Results showed that the prediction of error was very close to the real simulation error, and the respective Predicted Optimized Mesh/Model Information (POMI) was the same as the Real Optimized Mesh/Model Information (ROMI).

## Benefits to DOE

A specific benefit is improved capability to analyze containment phenomena; a more general benefit is the development of generally-applicable data-driven techniques for learning how to correct lower-fidelity simulations to approximate the results of higher-fidelity simulations, enabling the use of lower-fidelity models for very comprehensive analyses of complex situations. One specific benefit will be the ability to analyze scenarios evolving over long times and long length scales. State-of-practice capabilities for doing this involve lumped-parameter system codes. These system codes have improved over time, but there remains a need to do significantly better, in ways that this work is enabling. Of more general benefit, the data-driven multiscale simulation methodology that is being developed is applicable to other complex thermal-hydraulic processes that need to be analyzed in safety analysis of advanced energy systems.

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- Bao, H., N. Dinh, H. Zhao, H. Zhang, L. Zou, and R. Szilard, 2016, "A Study of BWR Mark I Station Blackout Accident: GOTHIC Modeling and Sensitivity Analysis," *International Congress of Advanced Nuclear Power Plants*, San Francisco, California, April 2016.
- Hanna, B., N. Dinh, and I. Bolotnov, 2016, "A Framework for Data-Driven Model Development for Coarse-Grained Computational Fluid Dynamics," *International Topical Meeting on Advances in Thermal Hydraulics 2016 (ATH 16)*, New Orleans, Louisiana, June 12 through 16, 2016.
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- Lin, L., 2016, "Assessment of the Smoothed Particle Hydrodynamics Method for Nuclear Thermal-Hydraulic Applications," Master of Science Thesis in Nuclear Engineering, North Carolina State University, 75 p, April 2016.

Botros N. Hanna, e. a., 2016, “High-fidelity simulation-driven model development for coarse-grained computational fluid dynamics”. *International Topical Meeting on Advances in Thermal Hydraulic*, New Orleans, LA.

### **Interns and Postdocs**

Interns: Han Bao, Yangmo Zhu, and Linyu Lin

### **Collaborations**

University: North Carolina State University

## 16-036: Neutron Microscope to Enable High-Resolution Neutron Tomography at INL

Kevin Tolman,<sup>1</sup> Boris Khaykovich,<sup>1</sup> Muhammad Abir<sup>1</sup>

### General Project Description

Neutron radiography is an important tool of post-irradiation examination of materials. At INL, the Neutron Radiography Facility (NRAD) is used for examining irradiated fuel elements. Usually, neutron-radiography instruments are designed as pinhole cameras, where a neutron beam from a small aperture with a diameter  $D$  illuminates a sample at a large distance  $L$ , where  $L/D$  is normally between 50 and 500. The spatial resolution of such a system improves with increasing  $L/D$  ratio and with decreasing the sample-to-detector distance. The high  $L/D$  ratio restricts the neutron flux on the sample, sometimes severely, as  $(D/L)^2$ . Powerful optical tools, such as focusing mirrors, if available for neutron radiography, might bring transformative improvements by increasing the spatial and temporal resolution and available neutron flux. The spatial resolution of such system does not depend on  $L/D$  ratio, allowing for significant increases in signal rates. Most importantly for INL, the large separation between the radioactive fuel samples and a detector would shield electronic detectors from damaging gamma rays. Therefore, existing indirect foil-film transfer detection, which requires manual handling of films, could be replaced by modern solid-state detectors, leading, in turn, to a fully automatic tomographic facility. The purpose of this project is to design such focusing mirrors, sometimes called Wolter mirrors, for the neutron-radiography application at NRAD at INL. The resulting facility is a magnification-one neutron microscope, where Wolter mirrors are placed between the sample and the detector and work as image-forming optics. In addition to imaging, instrumentation for neutron diffraction for studies of irradiated fuel at NRAD will be developed.

### Summary

In this project, we developed a solution, which would enable digital radiography and tomography of highly radioactive samples. The solution is based on the observation that in microscopes, in contrast to pinhole cameras, samples are separated from detectors by image-forming optics. We designed a neutron microscope, which employs axisymmetric neutron-focusing mirrors known as Wolter mirrors. Figure 1 shows the configuration of a thermal-neutron microscope. The mirrors utilize glancing-incidence reflection. Below a certain wavelength- and material-dependent angle, mirrors reflect neutrons with almost 100% efficiency. But above the critical angle, typically a few milli-radian (mrad), the reflectivity quickly diminishes. In such geometry, in order to produce an image, the beam must reflect from the mirrors an even number of times. For thermal neutrons, we designed the mirrors consisting of two identical pairs of confocal hyperboloid and paraboloid sections (Hyperboloid-Paraboloid-Paraboloid-Hyperboloid, or HPPH). The need for four reflections is dictated by the small critical reflection angle of thermal neutrons from surfaces. The performance of the proposed instrument is illustrated in Figure 2, which shows a simulated microscope image of hollow metal cylinders separated by 100-micron-wide openings, representing cracks in fuel elements. In addition to providing separation between the sample and the detector, Wolter mirrors lead to a signal rate increase **by a factor of up to 100**, an important improvement for relatively weak sources, such as the 250 kW NRAD reactor and other similar facilities.

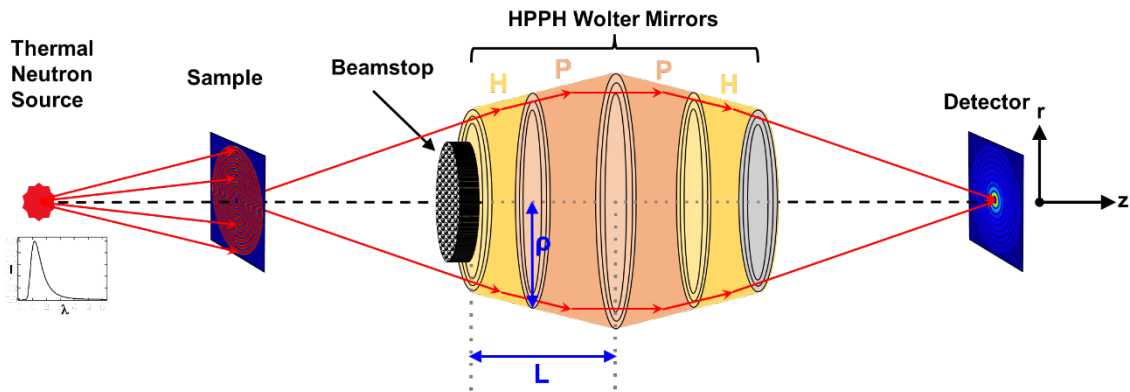


Figure 1. Schematics of the proposed neutron microscope optimized for thermal neutrons. The optics consists of nested sets of identical pairs of confocal coaxial Hyperboloid and Paraboloid sections (HPPH). The symmetric arrangement produces the optics of magnification  $M=1$ . Thermal neutrons are incident onto the sample at the upstream focal plane of the mirrors, and the image is formed at the detector at the downstream focal plane.

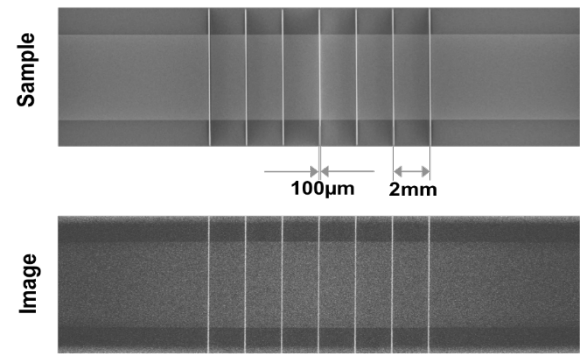


Figure 2: (a) Simulated neutron spectrum of NRAD in the thermal-neutron range. The source was simulated using both neutron transport (MCNP) code and a model Maxwellian Distribution in McStas, the ray-tracing software used to optimize the mirrors; (b) Simulated metal cylindrical sample (top) and its simulated image with a gap of  $100\mu\text{m}$  mimicking a typical crack/defect in the fuel sample, to be probed using the imaging optics.

## Benefits to DOE

The project benefits DOE by allowing a new post-irradiation examination (PIE) method to study irradiated nuclear fuel. Fully automatic neutron tomography would allow clear understanding of mechanical stability of irradiated fuel elements with high spatial resolution. The need for such investigations is clear because new fuel has been developed for existing and new nuclear reactors, driven by the national and international needs of developments in nuclear energy. The innovation of this project is in replacing a very old technology of pinhole imaging by modern focusing optics. By modernizing the existing neutron radiography and diffraction facilities at NRAD, INL would be positioned as an international leader in fuel development.

In addition, this project fosters close collaboration between Massachusetts Institute of Technology and INL, further improving scientific vitality of INL and helping training of students and postdocs.

## Publications

Rai, D.K., M. Abir, H. Wu, B. Khaykovich, and D.E. Moncton, 2018, “Focusing Mirrors for Enhanced Neutron Radiography with Thermal Neutrons and Application for Irradiated Nuclear Fuel”, *Nuclear Instruments and Methods in Physics*, A 879, 141 (2018);  
<https://doi.org/10.1016/j.nima.2017.10.013>

Morrell, J.T., 2017, “Experimental evaluation of polychromatic neutron diffraction”, Senior Thesis, Department of Nuclear Science and Engineering, Massachusetts Institute of Technology (2017).

## Presentations

Rai, D.K., H. Wu, M. Abir, B. Khaykovich, and D.E. Moncton, 2017, “Focusing Mirrors for Enhanced Neutron Radiography with Thermal Neutrons and Application for Irradiated Nuclear Fuel”, by, poster presentation at *NEUWAVE-9 Workshop*, Gaithersburg, MD, June 2017.

Rai, D.K., H. Wu, M. Abir, J. Giglio, and B. Khaykovich, 2017, “Neutron Focusing Mirrors for Neutron Radiography of Irradiated Nuclear Fuel at Idaho National Laboratory,”, presentation at the *American Physical Society* winter meeting, vol 62, number 4, 2017.

Abir, M. and B. Khaykovich, 2016, “Neutron focusing mirrors to enable high resolution neutron imaging at Idaho National Laboratory,” *International Topical Meeting of Neutron Radiography (ITMNR- 8)*, Beijing, China, 09/06/2016.

## Interns and Postdocs

Postdocs: Durgesh Rai and Muhammad Abir

## Collaborations

University: Massachusetts Institute of Technology



## 16-040: Integration of Prognostic Techniques and Probabilistic Safety Assessment for Online Risk Monitoring

Vivek Agarwal,<sup>1</sup> Andrei V. Gribok,<sup>1</sup> and Curtis L. Smith<sup>1</sup>

### General Project Description

Nuclear power plants use risk monitors to estimate system risk for ensuring safe and reliable operation of a plant. The existing risk monitors, based on probabilistic risk assessment (PRA), provide system risk based on the current plant configuration. Even though traditional PRA seeks realistic results, the assessment is based on Boolean logic (i.e., components have only two states: operational and failure), time-independent failure information (i.e., failure information is collected in time snapshots and not on a continuous basis), and assumptions that systems and components are non-repairable. As a result, traditional PRA in its present form, has limitations. These are (1) it is not capable of handling time-evolving scenarios; (2) it does not include system or component degradation or aging information; (3) it is a conservative risk estimate; and (4) it is unable to handle uncertainty due to changes in reliability of components and systems as a result of operational or external factors. This research is focused on an enabling approach to improve current risk monitors so as to consider time- and condition-dependent risk. The approach adapted in this research is integrating the traditional PRA models with condition monitoring and prognostic techniques. Mathematically, it can be interpreted as a transition from  $\{0,1\}$  to  $[0,1]$ . In  $\{0,1\}$  only Boolean states are considered whereas in  $[0,1]$  all the possible states between 0 and 1 (including 0 and 1) are considered.

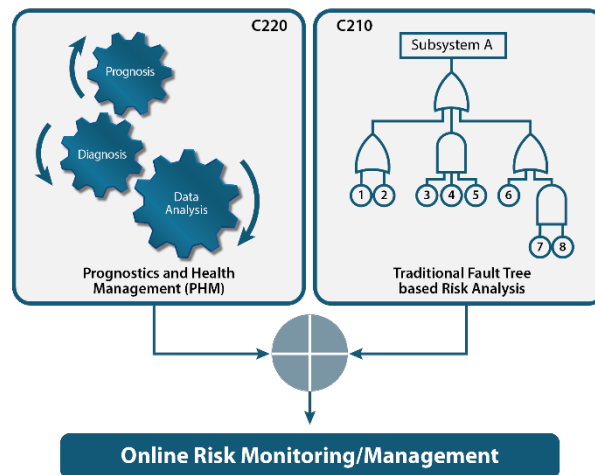


Figure 1. Enhancing traditional risk analysis with prognostics and health management.

### Summary

The first year of this three year project focused on understanding and identifying key assumptions that would be required to achieve online risk monitoring, followed by collecting measurement data including historical failure data across current fleet of light water reactors. The second year focused on analysis of data obtained from the US Nuclear Regulatory Commission (NRC) and INL’s Advanced Test Reactor (ATR) and implementing the findings in the traditional PRA models. The major highlights of the project to-date is summarized as follows:

- Component importance measures were identified that could be extended to repairable systems with non-binary states [1]. With too much emphasis on risk and safety significance importance measures, little attention is paid to the cost incurred to maintain systems and components. This led to the investigation in several cost-based importance measures [2] and preliminary result was published on cost importance measure.
- The risk monitor (RM) was developed as an add-on module within the INL's PRA software SAPHIRE and provided to us by the ATR staff (Figure 2). The RM is equipped with advanced capabilities of simulating scenarios, such as placing components out of service or in maintenance for a period of time. The RM helps better understand the effect of component failures on the top-event, and also foresees the effects of planned maintenance activities on the top-event probabilities.
- Analysis of NRC's database revealed that motor driven pump (MDP's) dominant failure mode Fail-to-Start is dictated by circuit breaker failures. Circuit breaker aging and repair were incorporated through Markov Chain model to compute accurate estimate of the MDP probability of failure over time. The results show that aging and repair have a significant impact on the evolution of MDP failure rates.
- A novel hazard-rate based model was developed to incorporate component degradation based on vibration measurements. Figure 3a shows four vibration measurements of MDP at ATR with bearing degradation along with the fitted exponential model. Figure 3b shows the evolution of probability of failure for the MDP using the instantaneous hazard-rate model. While the existing PRA overlooks degradation, the exponential hazard-rate based method can provide means to determine evolution of component probability of failure as a function of component performance measure, paving the way for incorporating online monitoring in PRA.
- Developed and validated a novel nonparametric empirical Bayes estimation technique which can be implemented in online monitoring systems. The new technique outperforms parametric Bayes estimates on the components' failure data collected from the NRC database.

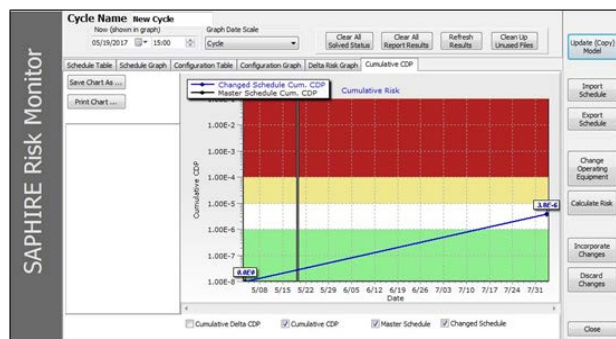


Figure 2. A snapshot of SAPHIRE risk monitor.

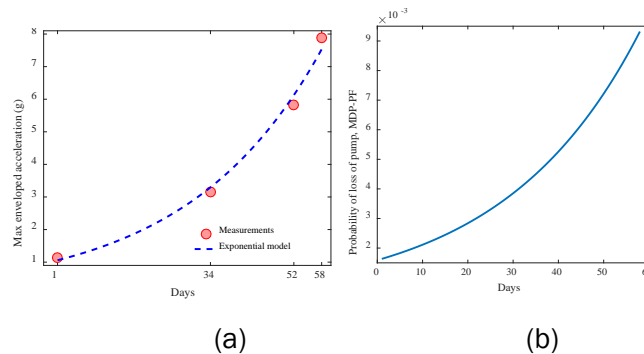


Figure 3. (a) Vibration data points indicating bearing degradation and exponential degradation model. (b) MDP probability of failure for 58 days period of bearing degradation.

## Benefits to DOE

The research will directly benefit the work being conducted under different DOE programs, including the Light Water Reactor Sustainability Program and Advanced Reactor Technologies, by enhancing the existing PRA capabilities to incorporate component aging and degradation. This research work facilitates and promotes inter-departmental collaboration at INL through an active partnership between the two departments of Human Factors, Controls, and Statistics (C220) and Risk Assessment and Management Services (C210) within the Nuclear Science and Technology Directorate (C200). Collaboration with ATR was established to support development of the technology using actual plant-equipment data. This research led to staff growth from 3 to 4 in the Controls group of C220 Department by hiring one postdoctoral researcher. Additionally, two interns were also hired as part of this project. As the technology developed under this project matures, the work will be pursued for application in nuclear, oil, and other critical-infrastructure industries.

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- [1] Van der Borst, M., and H. Schoonakker, 2001, "An overview of PSA importance measures." *Reliability Engineering & System Safety* 72.3 (2001): 241-245.
- [2] Wu, S. and F.P.A. Coolen, 2013, "A cost-based importance measure for system components: An extension of the Birnbaum importance." *European Journal of Operational Research* 225.1 (2013): 189-195.
- [3] Eide, S.A., T.E. Wierman, C.D. Gentillon, 2007, "Industry-average performance for components and initiating events at US commercial nuclear power plants." *NUREG/CR-6928*, (2007).

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- Yadav, V., V. Agarwal, A. V. Gribok, and C. L. Smith, 2017, "Dynamic PRA with Component Aging and Degradation Modeled Utilizing Plant Risk Monitoring Data," *International Topical Meeting on Probabilistic Safety Assessment and Analysis*, Pittsburg, Pennsylvania, September 24–28, 2017.
- Gribok, A. V., V. Agarwal and V. Yadav, 2017, "Specification of Prior in Empirical Bayes Estimation through Bayesian Deconvolution for Probabilistic Risk Assessment," *International Topical Meeting on Probabilistic Safety Assessment and Analysis*, Pittsburg, Pennsylvania, September 24–28, 2017.

Yadav, V., V. Agarwal A. V. Gribok and C. L. Smith, 2017, “Assessment of Dynamic PRA Techniques with Industry-Average Component Performance Data,” *10<sup>th</sup> ANS International Topical Meeting on Nuclear Plant Instrumentation, Control and Human Machine Interface Technologies*, San Francisco, California, June 11–15, 2017.

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Gribok, A. V., V. Agarwal and V. Yadav, “Performance of Empirical Bayes Estimation Techniques Used in Probabilistic Risk Assessment,” *Reliability Engineering & System Safety* (under review).

## Presentation

Agarwal, V., V. Yadav, A. V. Gribok and C. L. Smith, 2017, “Integration of Prognostic Techniques and Probabilistic Safety Assessment for Online Risk Monitoring,” National & Homeland Security Strategic Advisory Committee Meeting, Idaho Falls, Idaho, June 29, 2017.

## Interns and Postdocs

Interns: Payel Chatterjee and Brittany Layne Umbrage

Postdoc: Vaibhav Yadav

## 16-046: Development of a Synergistic Approach to Study Irradiated Materials Using Coupled Experiments and Simulation

Cynthia Adkins,<sup>1</sup> Dan Wachs,<sup>1</sup> Assel Aitkaliyeva,<sup>2</sup> and Michael Tonks<sup>1</sup>

### General Project Description

Understanding and predicting the effects of irradiation damage on material properties is possible only when state-of-the-art experimental characterization methods are used in conjunction with advanced mesoscale modeling and simulation. For this reason, DOE and INL have invested heavily in facilities and capabilities for microstructure characterization of irradiated materials, as well as the development of the MOOSE/BISON/MARMOT code system for predicting microstructure evolution and its impact on properties in fuel and cladding materials. This project shifts the focus from building capabilities to demonstrating the use and integration of these capabilities to shorten the nuclear fuel development cycle. To fully realize the benefits of tightly coupled experiments and simulation at the microstructural level, this project works in three areas: 1) developing experimental procedures to obtain the specific pre- and post-irradiation characterization data required for validation and uncertainty quantification of MARMOT models, 2) demonstrating the value of a coupled experimental and simulation approach on understanding critical thermal properties in a material of broad interest, and 3) understanding the evolution of microstructure under transient irradiation conditions and its impact on properties for use with TREAT.

### Summary

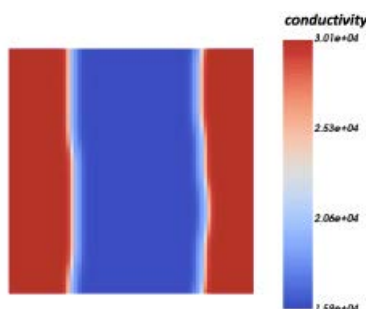
The project is conducting a systematic microstructural and thermal property characterization along with multi-scale modeling of nuclear fuels before and after irradiation. It will provide much needed linkage between thermal properties and microscopic scale observation. To achieve such characterization, a combination of complementary techniques, such as scanning/transmission electron microscopy (STEM, TEM) and others, was implemented. Microstructural characterization of the cast fuel, which includes analysis of the structure and chemistry of the primary, secondary, and impurity phases, and lattice defects, were conducted and the representative results were reported as input to the fuel microstructure model in MARMOT.

Microstructural characterization was linked to thermal properties analysis. Measurement of thermal properties, which are focused on thermal conductivity, phase transition temperatures, and enthalpy of the phase transitions, has been conducted on selected fuel alloys. Transition temperatures, enthalpies of transition, and heat capacities were determined employing a Differential Scanning Calorimeter/Thermogravimetric Analyzer (DSC/TGA). Thermal diffusivities and conductivities of the fuels were determined using laser flash analyzers (LFA). Phase transitions observed during DSC measurements were correlated with the phases observed in TEM.

As part of the coupled experimental and modeling approach, the experimentally determined phases and volume fractions of phases were used for direct reconstruction of the fuel microstructure in MARMOT. Phase diagrams suggest that U-Pu-Zr system consists of fourteen individual phases and a number of intermetallic phases. Each phase was evaluated for inclusion in the phase-field model based on the probability of the phase formation during the planned irradiation experiments. Isothermal decomposition simulations were performed by comparing the composition of equilibrium microstructures to equilibrium concentrations and overall phase fractions calculated from the mixture free energy expressions using the lever-rule. In addition to predicting microstructure evolution in binary systems, microstructure evolution of ternary U-Pu-Zr systems was simulated. The microstructure of the ternary system behaves similarly to

the binary systems and evolves to minimize surface area between the phases, as predicted. Comparison of modeling results to experimental data and phase diagrams show that the expected phases are present and that the components are partitioned to the appropriate phases.

The thermal conductivities of the alloys selected for the study were calculated and the representative result for U-Pu-Zr system is shown in Figure 1 in units of [nW/ $\mu\text{mK}$ ]. Calculated thermal conductivities throughout the microstructure agree with those calculated manually, which indicates correct implementation of the thermal conductivity model in MOOSE framework. The calculated effective thermal conductivities for the microstructure are  $1.74 \times 10^4$  nW/ $\mu\text{mK}$  in the horizontal direction and  $2.2 \times 10^4$  nW/ $\mu\text{mK}$  in the vertical direction. The effective thermal conductivity is lower in the horizontal direction because a low conductivity vertical strip impedes heat transfer, since it contains a lower concentration of the high conductivity uranium. These values are now being validated against experimental data that was collected in task 1. The results obtained as part of task 2 indicate that the phase-field model is capable of predicting equilibrium behaviors consistent with the free energy expressions, phase diagrams, and the experimental data. Combined with kinetics, mechanics, and conduction models, the phase-field model will aid in establishing a complete understanding of the link between microstructure evolution and bulk thermodynamic properties.



*Figure 1. Calculated local thermal conductivity for a U-Pu-Zr microstructure at  $T=773\text{K}$ , where  $x_U=0.45$ ,  $x_{Pu}=0.2$ , and  $x_{Zr}=0.35$ .*

To achieve the goal of developing thermal transport capabilities for metal fuel and predict the impact of rapid heat generation and its impact on the fuel behavior in MARMOT, PIs will create temperature-induced changes in the alloys using various furnaces. This will allow investigation of kinetic temperature effects without addition of the irradiation effects on microstructural evolution of the fuel alloys. The annealed alloys will be characterized in the same fashion as the as-fabricated alloys and the data will be used as an input to the developed phase-field model. Annealing data will be used as a benchmark to differentiate between temperature effects and irradiation-induced effects on microstructure. Furnace annealing temperature will match irradiation temperatures and annealing times will closely match the irradiation duration in TREAT to ensure consistency of the results. Steady-state irradiation at lower operating power lasting for hours (as opposed to minutes) will be used to produce desired microstructures. These data from the temperature induced microstructure will be provided to our student at UF to be incorporated into the phase-field modeling effort presented above and allow for completion of his PhD thesis.

## Benefits to DOE

This work will provide established procedures for coupling experiments with modeling and simulation to investigate critical material behavior in nuclear fuel. Such a coupled approach has the potential to provide detailed and quantitative understanding of atomic-scale in-reactor degradation behavior of nuclear fuels. This understanding is of critical importance to the development of next-generation reactor systems, as it is the evolution of the microstructure at the atomic scale that has the most profound impact on bulk properties and in-reactor performance. These procedures will include the application of various complementary techniques to provide a detailed characterization of the fuel before and after irradiation. As a result of this effort, DOE will have the kind of information needed to provide a more thorough understanding of radiation response of metallic fuels and shed light on their future as fuel for next-generation fast reactors.

## Publications

Aitkaliyeva A. and C. Papesch, 2016, “Identification of subsurface phases in ternary U-Pu-Zr fuel”, *Journal of Nuclear Materials*, Vol. 473, p. 75, 2016.

Aitkaliyeva, A., C. A. Papesch, and S. Middlemas, 2016, “Evaluation of Microstructure and Thermal Properties of U-24Pu-15Zr Alloy”, submitted to *Journal of Nuclear Materials*, November 2016, currently under revision.

## Presentations

Aitkaliyeva, A., 2017, “Coupled experimental and simulation approach to study transmutation fuels”, Invited Talk, to be presented at *2017 Materials Science & Technology (MS&T)* meeting, Pittsburgh, PA, October 8-12, 2017

Aitkaliyeva, A. and C. A. Papesch, 2017, “Microstructural characterization of Pu-Zr fuels”, to be presented at *Microscopy & Microanalysis (M&M 2017)* Conference, St. Louis, MO, August 6-10, 2017.

Papesch, C.A., A. Aitkaliyeva, and S. Middlemas, 2017, “Phase verification and thermophysical properties evaluation of Pu-Zr alloys”, to be presented at *American Nuclear Society (ANS) Annual Meeting*, San Francisco, CA, June 11-15, 2017.

Hirschhorn, J., A. Aitkaliyeva, C. A. Papesch, and M. Tonks, 2017, “A phase-field model for the U-Pu-Zr system”, to be presented at *American Nuclear Society (ANS) Annual Meeting*, San Francisco, CA, June 11-15, 2017.

Middlemas, S., A. Aitkaliyeva, and C. A. Papesch, 2017, “Evaluation of microstructural and thermal properties of U-Pu-Zr metallic fuels”, to be presented at *American Nuclear Society (ANS) Annual Meeting*, San Francisco, CA, June 11-15, 2017.

Aitkaliyeva, A., C. A. Papesch, and M. Tonks, 2017, “Coupling experiments and simulations to understand metallic fuel behavior”, to be presented at *American Nuclear Society (ANS) Annual Meeting*, San Francisco, CA, June 11-15, 2017.

Middlemas, S., C. A. Papesch, and A. Aitkaliyeva, 2017, “Evaluation of thermophysical properties and microstructure of U-Pu-Zr metallic fuels”, presented at the *33rd International Thermal Conductivity Conference (ITCC) and the 21st International Thermal Expansion Symposium (ITES)*, Logan, UT, May 15-18, 2017.



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- Aitkaliyeva, A. and C. A. Papesch, 2016, "Microstructural characterization of metallic transmutation fuels", Presented at *14th International Exchange Meeting on Actinide and Fission Product Partitioning and Transmutation (14IEMPT)*, San Diego, CA, October 17-20, 2016.
- Aitkaliyeva, A., 2016, "Microstructural evolution in metallic fuels", Invited Talk, Presented at *2016 ANS Winter Meeting and Nuclear Technology Expo*, Las Vegas, NV, November 6-10, 2016.
- Aitkaliyeva A. and C.A. Papesch, 2016, "TEM identification of phases in metallic Pu-based fuels" *2016 Microscopy and Microanalysis Conference*, Columbus, Ohio, July 2016.
- Aitkaliyeva, A., J. Madden, and C. Papesch, 2016, "TEM investigation of phases formed in ternary U-Pu-Zr systems" *2016 TMS Annual Meeting & Exhibit*, Nashville, TN, February 2016.

## 16-050: Stress Corrosion Cracking Testing in Supercritical Carbon Dioxide

Sebastien Teyssyre<sup>1</sup> and Julie Tucker<sup>4</sup>

### General Project Description

The supercritical carbon dioxide (sCO<sub>2</sub>) Brayton cycle is being considered for power conversion systems because of its high efficiency. However, implementation this technology in the field requires the selection of structural materials that will withstand exposure to high temperature sCO<sub>2</sub>. This project had two objectives: generating sCO<sub>2</sub> corrosion data and extending the capability of the existing Oregon State University (OSU) sCO<sub>2</sub> loop from a simple corrosion loop to a loop with stress corrosion cracking testing capability and in-situ crack growth-rate measurement.

The corrosion test matrix included Ni-based alloys (e.g., Inconel 625, Haynes 282) and their joints (diffusion bonding, laser welding, brazes) at temperatures ranging from 300 to 750°C, based on the alloy class, research-grade sCO<sub>2</sub> (99.999% purity). Post-test evaluation of samples was performed by mass change measurements and analysis of the surface corrosion product films with scanning electron microscopy-energy dispersive spectroscopy (SEM-EDS), x-ray diffraction (XRD) and transmission electron microscopy (TEM) to identify the corrosion-product structure and chemistry.

Stress corrosion cracking activity consisted primarily to adapt a testing rig developed at INL for in-pile testing to use in the OSU corrosion loop. The rig uses a pneumatic bellow to apply load to the specimen. The objectives were to develop the first sCO<sub>2</sub> testing capability, but also to gather additional information about a recently developed design.

### Summary

Corrosion experiments have been and continue to be carried out in the previously built sCO<sub>2</sub> autoclave at Oregon State University. Due to frequent issues with this system, the timetable was significantly pushed back. However, several exposure campaigns were initiated and characterization of exposed 800H samples at 650 and 750°C (exposure in sCO<sub>2</sub> performed at the University of Wisconsin- Madison, air and argon exposure performed at OSU) was performed. The characterization of alloy 800H showed that exposure at 750°C for 600h lead to significant void density underneath the oxide layer and internal oxidation (figure 1) so a rapid degradation of the material.

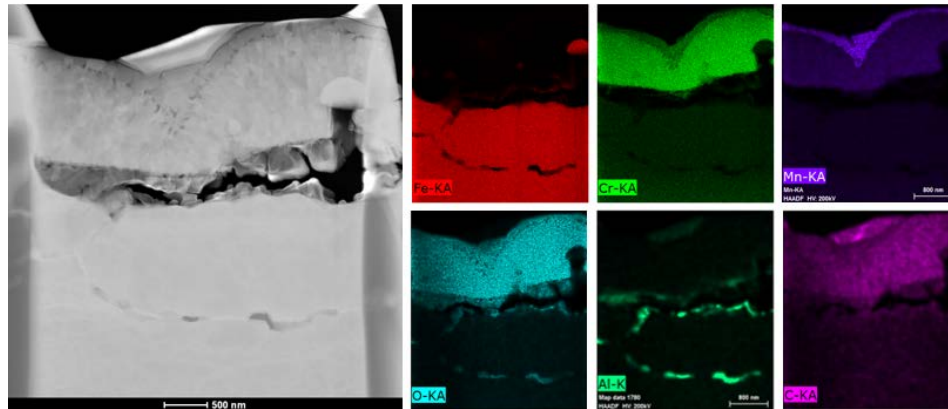


Figure 3. TEM of scale and matrix for 800H exposed for 600 hrs. at 750°C and corresponding EDX maps.

A set of stainless steels were exposed to conditions that most closely resemble the list of materials, temperature, and pressure of interest to the stress corrosion cracking exposures. The goal is to determine the material damages without application of any stress to assess the potential formation of initiation sites and the oxidation kinetics. In this study, we are examining alloys 316, 316L, 347H, C-20, and P91 at 500 °C and 20 MPa at 200 hr. intervals. The mass change plot can be seen in Figure 4.

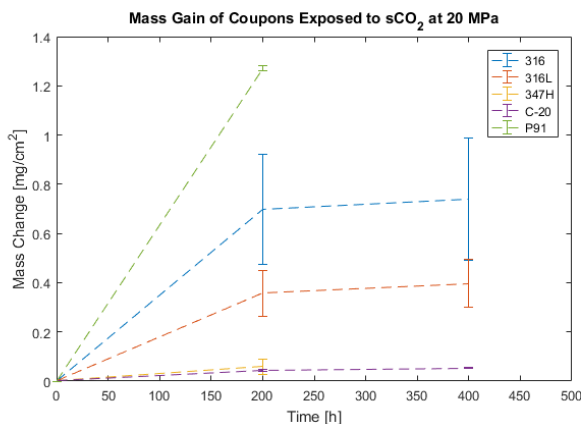


Figure 4: Weight change data for exposed SS at 500°C.

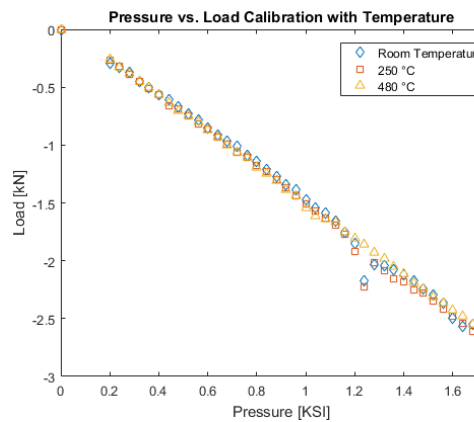


Figure 3: Calibration of SCC rig at temperature.

The stress corrosion cracking rig, its control mechanism and its crack length measurement capability have been installed. The rig was calibrated for applications in the range of load and temperature of interest. **Error! Reference source not found.** shows the evolution of the load applied by the rig as a function of internal bellow pressure at various temperatures. It is clear from this data that the in-situ devices can be calibrated at room temperature and the pressure/load relation does not change.

The device was used to propagate a fatigue crack at temperature in an air environment. The system showed its ability to load the sample, propagate a crack and follow the crack length. However this test also showed two limitations of this device. As room temperature air was used to activate the system, load cycling also led to temperature cycling of the bellow. Then, it was shown that there was a limit in the crack length at which the specimen can be efficiently loaded because when the crack is deep, the opening of the testing rig led to misalignment of the bellow with its support. The bellow failed in this condition.

## Benefits to DOE

The sCO<sub>2</sub> Brayton cycle is being considered for power conversion systems for a number of nuclear reactor concepts, including the sodium fast reactor, fluoride salt-cooled high-temperature reactor, high-temperature gas reactor, and several types of small modular reactors. Supercritical CO<sub>2</sub> Brayton conversion will benefit efforts in the offices of Nuclear Energy, Fossil Energy, Energy Efficiency, and Renewable Energy. To be able to deploy such technology, it is necessary to select suitable materials to be used for the components working in this environment. This work develops stress corrosion cracking testing capability to generate the first stress corrosion cracking data in supercritical sCO<sub>2</sub> and support corrosion experiments which are critical for material selection.

## Publication

Adam, B., L. Teeter, J. Mahaffey, M. Anderson, and J. Tucker, “Effects of Corrosion in Supercritical CO<sub>2</sub> on the Microstructural Evolution in an Fe-Ni Superalloy”, In progress.

## Presentations

Teeter, L., B. Adam, T. Wood, S. Teysseyre, J. Tucker, 2017, “Environmentally Induced Cracking of Energy System Materials in sCO<sub>2</sub>”, *Symposium of the Pacific Northwest Chapter of the AVS*, September 8 (2017), Corvallis OR.

Teeter, L., 2017, “Corrosion Research and Current Activities at Oregon State University”, *1<sup>st</sup> International Network Meeting of the European School of Materials*, March 31 (2017), Saarbrücken Germany [Invited].

Teeter, L., J. Mahaffey, M. Anderson, S. Teysseyre, and J. Tucker, 2017, “Corrosion of Fe-Ni-Cr Alloy 800H in Supercritical CO<sub>2</sub> and its Effects”, *TMS Annual Meeting and Exhibition*, Feb 27 (2017), San Diego CA [poster].

Teeter, L., B. Adam, R. Repukaiti, T. Wood, S. Teysseyre, and J. Tucker, 2017, “SCC in sCO<sub>2</sub> for Energy Systems Materials”, Oregon State University Graduate Research Expo, February 22 (2017), Corvallis OR [poster].

## Interns and Postdocs

Interns: Lucas Teeter and Thomas Wood

## 16-055: Capability Extension for Multiscale, Multi-Application development within the Multiphysics Object-Oriented Simulation Environment

Cody Permann,<sup>1</sup> David Andrš,<sup>1</sup> Derek Gaston,<sup>1</sup> John Peterson,<sup>1</sup> Andrew Slaughter,<sup>1</sup> Brian Alger,<sup>1</sup> Yidong Xia,<sup>1</sup> and Fande Kong<sup>1</sup>

### General Project Description

MOOSE is Idaho National Laboratory's premier modeling and simulation framework. It forms the basis for several mature INL nuclear science research and development applications, including both MARMOT and BISON, and is also used in private industry and by a number of different academic institutions in the US and abroad. The purpose of this project is to implement several high-impact, cross-cutting, multi-physics coupling capabilities within the MOOSE framework and its physics modules. As part of this work, a new continuous integration toolkit, CIVET, was developed in order to incorporate these new features into the framework while maintaining high software quality standards and compatibility with existing applications.

### Summary

The CIVET toolkit is now the single most important component of the continuous integration process used by MOOSE and its dependent applications. CIVET is based on a client-server event model, with the client handling dozens of requests for automated regression testing and verification of software quality metrics each day. Each CIVET event triggers one or more jobs to run on dedicated build servers, either inside the INL or at collaborator institutions. Each job is composed of user-customizable building blocks called "recipes." Since it was open sourced, CIVET has run approximately 3 million regression tests per week in support of approximately 25 public MOOSE Pull Requests (on GitHub), and around 1 million regression tests per week in support of INL MOOSE-based applications such as BISON, MARMOT, RattleSnake, RELAP-7, and others. CIVET also maintains log files for all the jobs it runs, ensuring traceability and creating a connection between the requirements, design, implementation, and verification of integration for each piece of code that is merged into MOOSE and its dependent applications.

Significant progress has also been made on the task of implementing the mortar finite element method based on Lagrange multipliers within the MOOSE framework. The mortar finite element method, and mixed finite element methods in general, have a rich mathematical underpinning and an important connection to problems of both practical engineering interest and computational methods development. This work focuses on two use cases which are critically important to MOOSE-based applications: the "gap heat transfer" capability, and the ability to enforce solution continuity across non-conformingly meshed 1D and 2D manifolds. Our approach follows that of Yang et al, (*Int. J. for Num. Meth. Engng.*, vol. 62(9), p. 1183-1225) for defining the slave surface smoothed outward nodal normals, nodal projection (and inverse projection) operators, and mortar segment definition, parameterization, and assembly operations. These capabilities have been implemented and verified to work for the relatively simple model problem of thermal contact in both the continuity and gap heat transfer applications. Ongoing work is focused on the thermomechanical contact problem, which has many of the same implementation characteristics as the thermal contact problem, but is formulated in terms of a variational inequality, more sophisticated governing equations, and deforming meshes.

## Benefits to DOE

As an open source toolkit, CIVET is a high-visibility symbol of DOE's interest in and dedication to continuous integration techniques for improving, tracking, and maintaining high performance computational science software. CIVET has already led to closer ties with external collaborators who are interested in the traceability, usability, and maintainability of their applications in relation to the underlying MOOSE framework. Furthermore, since CIVET is a general tool, and not tied explicitly to MOOSE, we also expect that it will also be adopted by other software development teams within the DOE complex, and be a key component of these teams NQA-1 certification planning processes.

The RDG method has significantly extended the capabilities of MOOSE with regard to nuclear reactor/facility design and safety analysis in extreme conditions, and has facilitated an INL LDRD project on the development of a multi-dimensional CFD code for analyzing the integrity of nuclear reactor containment vessels subjected to extreme thermal and overpressure-loading conditions. Future applications will include a fluid-solid interaction (FSI) model involving coupled reactive fluid flow, and solid structural mechanics in reactors. To be developed in a unified framework, the MOOSE FSI model is expected to provide additional robustness and other advantages over traditional FSI coupling strategies.

## Publications

- Alger, B., et al, 2016, "CIVET: Continuous Integration, Verification, Enhancement, and Testing," Technical Report, INL/MIS-16-40463, Idaho National Laboratory.
- Schwen, D., L. Aagesen, J. Peterson, and M. Tonks, 2017, "Rapid multiphase-field model development using a modular free energy based approach with automatic differentiation in MOOSE/MARMOT," INL/JOU-17-41181, *Computational Materials Science*, vol. 132, pg. 36-45, May 2017.
- Kong, F., et al., 2017, "A fully coupled two-level Schwarz preconditioner based on smoothed aggregation for the transient multigroup neutron diffusion equations," INL/CON-17-40867, *Linear Algebra and Its Applications*, under review
- Peterson, J., et al, "An implementation of the mortar finite element method in MOOSE," Tech. Report, Idaho National Laboratory, in preparation.

## Presentations

- Slaughter, A., et al, 2017, "Continuous integration for large-scale scientific software development," *U.S. National Congress on Computational Mechanics (USNCCM 14)*, Montréal, Québec, Canada, Jul. 17-20, 2017.
- Slaughter, A., et al, 2016, "Lessons from Nuclear Energy: Building Snow and Avalanche Simulation Tools using a Common Open-Source Framework," INL/CON-16-38566, *International Snow Science Workshop (ISSW)*, Breckenridge, CO, Oct. 3-7, 2016
- Permann, C., et al, 2017, "Continuous integration for large-scale scientific software development," *SIAM Conference on Computational Science and Engineering*, Atlanta, GA, Feb. 27-Mar. 3, 2017.
- Peterson, J., et al, 2017, "An overview of the MOOSE framework and its modules," *SIAM Conference on Computational Science and Engineering*, Atlanta, GA, Feb. 27-Mar. 3, 2017.
- Kong, F., et al, 2017, "A class of parallel hybrid algorithms based on field-splitting, AMG and ASM in MOOSE," INL/CON-17-40867, *18th Copper Mountain Conference on Multigrid Methods*, Copper Mountain, CO, Mar. 26-31, 2017.

## **Invention Disclosures, Patents, Copyrights**

CIVET (<https://github.com/idaholab/civet>) was released as open source software on November 29, 2016 under the Apache 2.0 license.

## **Interns and Postdocs**

Intern: Sonia Pozzi.

Postdoc: Robert W. Carlsen.

## **Collaborations**

Universities: University of Wisconsin and Università della Svizzera Italiana, Lugano, Switzerland.



## 16-058: Predicting Radiation-Induced Microstructural Change via Implementation and Validation of Multiscale Cluster Dynamics in MOOSE

Cody Permann,<sup>1</sup> Michael Short,<sup>6</sup> and Miaomiao Jin<sup>1</sup>

### General Project Description

The long-time evolution of radiation-induced defects is a crucial issue for accurate prediction of material properties under irradiation. Studying the radiation-defect cluster distribution can contribute to the successful design of various radiation-resistant materials, not limited to nuclear applications, and predict their stability under irradiation. The most common tool for long-term evolution of radiation-induced microstructural change is cluster dynamics (CD), which tracks the flow of defects in and out of various defect clusters in size space. Calculations are carried out using a rate-theory construction, with both classical normal rate theory (NRT) and production bias model (PBM) taken into account for realism. Relevant parameters, including defect motilities and cluster-absorption/emission rates, are derived mostly from atomic-level simulations. For quantities such as the binding energy of a vacancy to a void, for example, empirical thermodynamics-based correlations are used. However, most CD codes are neither extendable to other situations, nor formulated in a way that allows for the coupling of intermediate variables and final outputs to other multiphysics simulations. For example, if one were to be able to evolve accurately the radiation-induced microstructure of silicon carbide using CD, it could be easily coupled to solid mechanics and thermal models of its degradation under irradiation. Finally, correct outputs of CD simulations are directly verifiable using standard analytical techniques such as transmission electron microscopy (TEM), differential scanning calorimetry (DSC), and transient grating spectroscopy (TGS).

The governing equation for cluster dynamics is given below. This equation is adapted from rate theory describing the production, growth, and elimination of defect cluster of several sizes with spatial resolution.

$C_j$  is the concentration of defect size  $j$ . On the right hand side, first term  $G_j$  is the direct point defect or small cluster generation rate, the second to fourth terms represent absorption and emission, and the last term quantifies the elimination rate of defects at other microstructural sinks such as dislocations, grain boundaries, or free surfaces. Notice that  $G_j$  considers the clusters remaining after annealing radiation damage cascades. Defect clusters larger than 2 nm are visible under TEM for relatively easy verification. As a rough estimation, a 5 nm spherical cluster has a size  $\sim 4.4 \times 10^4$ . It implies that to describe a general system of defect cluster distributions, at least tens of thousands of simultaneous, low-order size-space equations need to be solved at each spatial node.

### Summary

At this point, several parts of this project have been implemented in a prototype MOOSE-based application, some ahead of proposed three-year schedule:

1. The generation of defect clusters has been calculated based on the binary collision approximation (BCA), and annealing of damage cascades with molecular dynamics code (LAMMPS). The production rates of various cluster types and sizes has been pre-computed with spatial dependence.

2. A family of custom actions has been built in the MOOSE-based application to automatically generate constituent kernels for each variable. These constituent kernels each account for a single term from the Master equation above for each type and size of cluster on each spatial node. Flexible treatment of mobile and immobile defect clusters, the production of defect clusters, and interaction coefficients has been completed. New parameters or radiation damage scenarios can be easily constructed, by utilizing the include/source files and the corresponding input file. Absorption and emission rates for all defects can be flexibly pre-compiled into a user object.
3. Due to computational cost, there is an upper limit to the largest cluster in the system, which can be tailored directly in input file according to experimental observations. Nevertheless, the more defect species involved, the more difficult it becomes to solve the full set of equations numerically. To relieve the computational burden of solving one equation for each defect species, one may group all sizes into a number of bins and then solve one equation for each bin. This method has been implemented based on the publications of Golubov et al.<sup>i</sup>The results have been tested to agree well with the discretely solving of each species.
4. Extensive verification and validation has been performed this fiscal year using the MOOSE-based CD implementation. Several simulations have been performed and the results have been compared to several experimental datasets available in the published literature. Specifically, we focused on self-ion irradiation in tungsten at 30K <sup>ii</sup>to explain the deviation from power law in experimentally measured defect size distribution. We varied typical parameters in self-ion irradiation to explore the mobility of self-interstitial atom (SIA) clusters, dose rate, incoming particle energy, and total dose. A number of expected results have been observed and are in agreement with other studies: The SIA cluster mobility is very important in determining the final defect size distribution. An upper limit to the mobility of SIA clusters of size six yields results very close to experimental measurements. Also as expected, a higher dose rate limits the defects' ability to cluster into larger groups, since more annihilation of SIAs and vacancies is anticipated with less relaxation time between damage cascades.

## Benefits to DOE

A full cluster-dynamics capability benefits DOE by providing higher-fidelity scale bridging between traditional molecular-dynamics simulations and mesoscale simulations. When complete, this bridging will enable a new class of simulations capable of furthering our understanding of various materials under irradiation, which directly benefits nuclear energy research. These capabilities will also further INL's lead nuclear lab leadership position in terms of modeling and simulations capabilities. When the final product is implemented in the MOOSE framework, it will be immediately available to other MOOSE-based applications further increasing our simulation capabilities portfolio. The cluster dynamics implementation also challenges the upper limits of our computational capabilities.

## 16-070: Characterization of Neutron Beamlines at the Neutron Radiography Reactor

Aaron E. Craft,<sup>1</sup> Sam H. Giegel,<sup>1</sup> Glen C. Papaioannou,<sup>1</sup> Chad L. Pope,<sup>1</sup> and George R. Imel<sup>8</sup>

### General Project Description

The Neutron Radiography Reactor (NRAD) sits beneath a large hot cell at the Hot Fuels Examination Facility and is designed specifically for neutron radiography of both highly radioactive and non-radioactive materials using two different neutron beams. The unique capabilities offered by NRAD and its neutron beams are well-suited for various research and development activities. However, information about these neutron beams is very limited. This project seeks to characterize the two neutron beams at the Hot Fuels Examination Facility's East and North Radiography Stations to provide users with detailed information about these beams, including beam flux, spatial distribution, energy spectrum, divergence/collimation, and gamma content. This project will measure these characteristics for both the radiography stations' neutron beams. The same beam characterization techniques will be extended to the neutron beam at the Transient Reactor Test Facility once operational. Characterization of these facilities will provide information that is essential for developing advanced digital neutron imaging capabilities, planning experiments and beamline upgrades, and providing data for validation of neutronics models.

### Summary

Characterization of neutron beams includes a suite of experimental measurements. The methods for performing these measurements are well-documented but can be technically challenging and quite involved. Users may require that the beam satisfy quality standards as a high-quality neutron imaging facility. This analysis per American Society for Testing and Materials standards is relatively simple and is included in this project. Additionally, users may desire more detailed measures of beam quality such as beam uniformity, divergence, length-to-diameter ratio (L/D), neutron energy spectrum, and gamma content of the beam. This information is essential for extracting quantitative data derived from neutron radiographs generated at the NRAD facility. Some of these measurements require special devices and meticulous data processing and analysis. This project is well-suited as a Masters of Science thesis topic, where it will receive the meticulous efforts of a full-time graduate student. Sam H. Giegel, a graduate student from Idaho State University in the Nuclear Engineering Department, is the primary researcher of this project. Sam will be advised by professors at Idaho State University (Chad Pope and George Imel) and INL staff (Aaron Craft and Glen Papaioannou) who are experts in the facilities being characterized and the methods used. A literature review has been compiled of characterization techniques for neutron beams and previous characterization efforts. Materials required for the measurements have been acquired, and a major portion of the data needed for this effort have been collected. One of the valuable outcomes of this work is to inform validation of radiation transport models of the reactor and neutron beams. Models are being developed using Monte-Carlo n-Particle (MCNP) for the North and East Radiography Station beamlines, and validation is occurring concurrently with characterization measurements. Neutron beam flux and beam profile measurements have been performed on both beamlines. The beam profiles reveal a relatively uniform beam over the field of view. The average neutron beam flux in the North Radiography Station is  $\sim 4.5 \times 10^6$  n/cm<sup>2</sup>s at L/D=185 and East Radiography Station is  $\sim 9.5 \times 10^6$  n/cm<sup>2</sup>s at L/D=125, both with  $2\sigma$  standard deviation of 3%. Multi-foil activations are complete, and the data will be used to calculate the neutron energy spectrum. The activation results will provide inputs for energy-spectrum unfolding software and for validating MCNP models. The resulting energy spectrum from the unfolding software will be compared to that of the

MCNP model. The neutron energy spectrum will be a major focus of the Thesis document and a journal publication. Two novel devices for characterizing neutron beams and imaging systems have been identified and are under development as part of this project. The first is a new device used to measure the effective L/D of neutron beams and the second is a device to measure the basic spatial resolution of neutron imaging systems. Each of these two efforts represents a new contribution to the neutron imaging scientific community. The L/D measurements will be included in the thesis and could be the topic of a publication depending on the device's performance. Dr. Craft is developing the line-pair gauge as a new standard through the American Society for Testing & Materials. . This project includes measurement of the gamma energy spectrum directly in the neutron beams using a high-purity germanium detector. These measurements will be included in the thesis and a journal publication.

### **Benefits to DOE**

Projects developing advanced nuclear fuels require neutron imaging capabilities to evaluate the condition of irradiated fuels and inform subsequent examinations. The neutron imaging capabilities provided by the neutron beams at NRAD directly support the primary mission of INL to advance nuclear energy in the United States. Characterization of these facilities will provide information that is essential for developing advanced digital neutron imaging capabilities, planning experiments and beamline upgrades, and providing data for validation of radiation transport models. This project supports a graduate student, Sam Giegel, from Idaho State University.

### **Interns and Postdocs**

Intern: Sam H. Giegel

### **Collaboration**

University: Idaho State University

## 16-071: Evaluation of Advanced Digital Neutron Imaging Systems for PIE of Nuclear Fuel

Aaron E. Craft<sup>1</sup>, Anton S. Tremsin<sup>11</sup>, and Glen C. Papaioannou<sup>1</sup>

### General Project Description

The current state-of-the-art for neutron imaging of irradiated fuel is the transfer method using converter foils with computed radiography plates or film, which is time-consuming and expensive. The gamma sensitivity of digital neutron imaging systems has been the precluding factor for their use for this application. This project seeks to test and develop advanced digital neutron imaging detectors for their applicability to evaluate irradiated nuclear fuel.

### Summary

A major component of this project relies on a collaboration with Dr. Anton Tremsin at University of California–Berkeley (UC-Berkeley), who develops state-of-the-art micro-channel plate (MCP) neutron imaging detectors for real-time neutron imaging. These imaging systems are less sensitive to gamma radiation than other digital neutron imaging systems, and this project seeks to test their feasibility for imaging highly-radioactive fuel in neutron beams with high gamma radiation content, such as those at NRAD. In FY-16, this project produced the first digital neutron radiographs ever acquired at INL in the North Radiography Station neutron beam despite its high gamma content (Figure 1). The MCP system was able to produce neutron radiographs in this gamma field without significant degradation of image quality, lending optimism to the prospect of using the MCP system to image irradiated fuel. Activities scheduled for the end of September 2017 will attempt to acquire neutron radiographs of an irradiated fuel pin. The information gained from these efforts will inform development of a theoretical background for production of novel MCP plates more suitable for imaging in high-radiation environments. A Monte Carlo n-Particle (MCNP) model of the North Radiography Station is being developed to inform development of digital imaging systems and potential modifications to the beamline to make it more suitable for digital neutron imaging.

The transfer method currently used to produce neutron radiographs introduces a compounded point spread function that decreases the effective spatial resolution by approximately 60%. Image processing techniques may be able to deconvolve this point spread function to sharpen digitized radiographs and gain back some of the 60% lost spatial resolution. A collaboration with Dr. Elise Barney-Smith, a Professor of Image Science at Boise State University, is evaluating image processing techniques using digitized neutron radiographs in an effort to improve image quality. The initial results from this image processing tool are promising, and further evaluations are underway.

This project is also supporting a graduate student at Colorado School of Mines to develop neutron contrast agents doped in liquid penetrants to enhance visualization of internal features of nuclear fuel elements. Initial results of multi-angle neutron radiography of samples treated with these techniques revealed internal cracking in internal coolant channels that were not detectable using other techniques. This work emphasized the value of neutron tomography and digital neutron imaging, demonstrating significant relevance to this project.

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<sup>11</sup> University of California-Berkeley

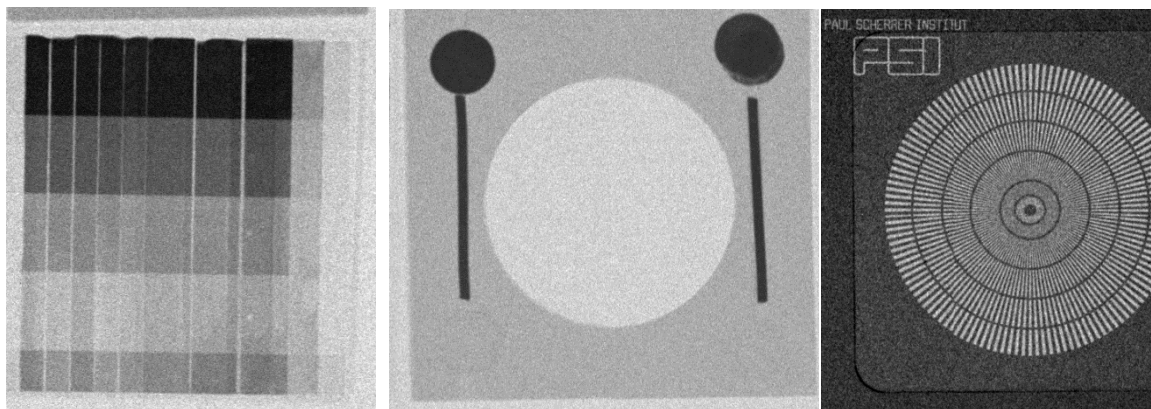


Figure 1. Radiographs of a sensitivity indicator (left) and beam purity indicator (right).

## Benefits to DOE

This project seeks to evaluate the applicability of advanced digital neutron imaging systems for post-irradiation examination of nuclear fuel and to further develop INL's neutron imaging capabilities to be more suitable for digital imaging systems. If successful, this project would lead to a system that could provide routine use of neutron computed tomography for post-irradiation examination of nuclear fuels and significantly improve the quality of data compared to current capabilities. This new capability would clearly demonstrate INL's leadership in nuclear fuels testing and promote the technical superiority of nuclear energy research and development in the United States.

## Publications

Digital neutron and gamma-ray radiography in high radiation environments with an MCP/Timepix detector, *Journal of Nuclear Materials*. (submitted for publication).

Image processing techniques to improve image quality of digitized neutron radiographs produced using the transfer method. *Journal of Imaging Science and Technology*.

Neutron contrast agents to enhance internal features in neutron imaging. *Physics Procedia*.

## Interns and Postdocs

Interns: Nicholas M. Boulton and Russell Jarmer.

## Collaborations

Universities: Oregon State University and Colorado School of Mines.



## 16-096: Supporting Operator Performance and Situation Awareness in Highly Automated Nuclear Power Plants

Katya Le Blanc<sup>1</sup> and Johanna Oxstrand<sup>1</sup>

### General Project Description

The objective of this project is to investigate the impact of high levels of automation in complex, safety-critical systems and to demonstrate ways to enable optimal situation awareness for human operators in those systems. Specifically, this research will demonstrate how to design human-automation interaction to support optimal situation awareness, workload, and plant performance in a multi-unit small modular reactor.

### Summary

INL researchers worked with NuScale personnel to design realistic scenarios for investigating operator performance under a variety of levels of automation. NuScale power has defined a preliminary human automation interaction design, where many of the plant's functions are fully automated, but some functions have an intermediate level of automation. INL researchers developed three interfaces for a boron dilution task with varying levels of automated support for the operator. The research worked with operations, engineering, and human factors staff at NuScale to design an experimental test for evaluating the effect of each of the three interfaces on human performance and situational awareness. One of the interfaces developed by the INL team has been adopted by NuScale as a template for all automation processes in the control room. This interface will be updated based on the results of this and future studies, resulting in a design that optimally supports operators in automated tasks.

INL researchers supported methodology development for the workload analysis NuScale conducted as part of their request for exemption to the Nuclear Regulatory Commission (NRC) staffing rule. We advised NuScale on how to perform and analyze several common workload measurement tools and provided several suggestions on how to develop criteria for characterization of acceptable workload. NuScale adopted several of our suggestions, including using workload at an existing operating plant as baseline criteria for workload comparison. NuScale noted that the discussions we had on workload methodology helped them develop their own expertise and enhanced their ability to successfully present their approach to NRC. The workload analysis is an important part of NuScale's request for exemption to the NRC staffing rule, which is one of the greatest challenges to licensing the NuScale design. Supporting the workload analysis directly supports NuScale's licensing efforts.

The researchers designed an experiment to test the dilution display's effect on performance, situational awareness, and workload. The researchers worked closely with NuScale operations engineers, human factors engineers, and simulator engineers to design scenarios and performance measures for the experiment. Testing of the experimental protocol and initial data collection began the week of June 13, 2016, and continued through September 20, 2016. Experimental data collection was slightly delayed due to challenges with the NuScale simulator and delays in their workload analysis for NRC that took priority over this work. Data collection was complete in February 2017 and researcher have analyzed a large amount of simulator log and observational data and are preparing a paper to submit to *Safety Science*. Based on the methodological expertise demonstrated in this LDRD project, NuScale Power has asked the INL team to participate in Integrated System Validation testing of the control room design in FY 18. This work will be funded by NuScale.



## Benefits to DOE

This work supports design of human automation interaction in the nuclear industry and will also inform use of advanced technologies that may be installed in existing light water reactors as part of control-room upgrades and design of systems installed to support grid modernization and hybrid energy systems. This work comprises scientifically rigorous research in close collaboration with industry. We meet several key challenges in conducting scientific research in full-scale simulator studies, thus advancing the science of human performance measurement in the nuclear context. This work supports licensing of a small modular reactor and demonstrates an effective collaboration between INL and NuScale that benefits the entire nuclear industry and any industry that has human-automation interaction challenges:

- NuScale provides the platform, facilities, operational expertise, and operators for conducting high-quality research to understand human/automation interaction
- Interfaces developed and tested in this work will be implemented in the NuScale control room, and the concepts can be applied to related work in other Office of Nuclear Energy programs
- Support of NuScale's licensing directly supports the DOE mission of deploying a small modular reactor.

## Publications

Le Blanc, K.L. Z. Spielman, R. Hill, R. Snuggerud, B. Pearse, J. McLerran, J., and R. Flamand, 2017, "A Human Automation Interaction Concept for a Small Modular Reactor Control Room", INL/CON-17-41509 in proceeding of *10th International Topical Meeting on Nuclear Plant Instrumentation, Control and Human Machine Interface Technologies*, San Francisco, CA, 2017.

## Presentations

Presented project to 2016 Nuclear Science and Technology Advisory committee on May 17, 2016, INL/MIS-17-42380. Presented a poster at NH&S Strategic Advisory Committee Meeting on June, 29, 2017

## Interns and Postdocs

Intern: Rachael Hill

Postdoc: Wei Zhang

## Collaborations

Universities: Brigham Young University-Idaho and Michigan Technological University

## 16-149: In-core Qualification of Developmental Instrumentation

Joshua Daw<sup>1</sup> and Joe Palmer<sup>1</sup>

### General Project Description

The purpose of this project is to perform out-of-core characterization of several sensors under development for in-core use. This testing is necessary preparation for potential in-core tests, as a basis for comparison with in-core results. The sensors tested are primarily ultrasonic and fiber-optic temperature sensors. The physical principles these sensors are based upon can be used for sensors capable of measuring many parameters in addition to temperature (i.e., strain, pressure, displacement, etc.). Thus, successful demonstration of these sensors will lead to further sensor development for an extended range of parameters.

### Summary

Ultrasonic thermometers (Figure 1) using various materials and numbers of sensor segments were fabricated, calibrated, and evaluated for accuracy and stability (examples shown in Figure 2). UTs show good stability over long duration tests, but the accuracy is currently limited by jitter in the measurement of delay time with standard ultrasonic testing equipment, as temperature is correlated to the travel time of acoustic pulses (Figure 3). This effect reduces with increasing temperature and sensor length, but accuracy is currently limited to an estimated 40°C. Improvements to the stability of time measurement could theoretically improve the accuracy of temperature measurements to levels similar to thermocouples but with comparatively reduced drift. Short of this, much effort was spent in improving the mechanical design of the UT and the fabrication process. This has resulted in marked improvements to the sensor-to-sensor consistency, robustness, and speed of manufacturing.

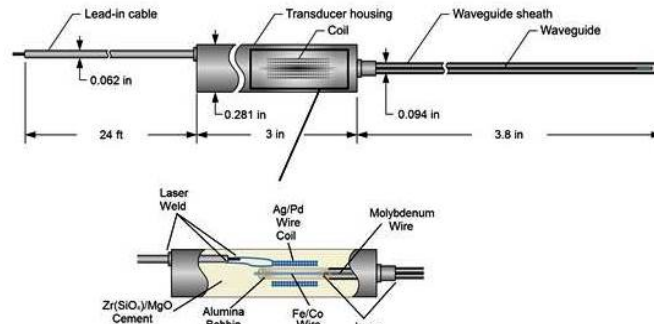


Figure 1. Diagram of basic UT construction

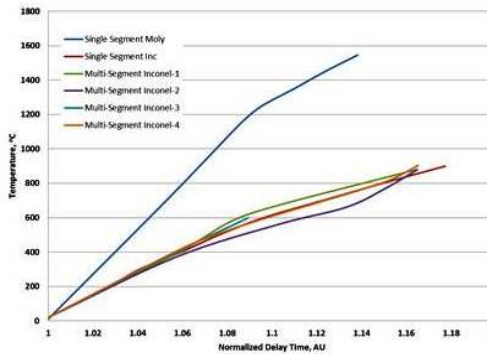


Figure 2. Calibration curves for UT materials and configurations of interest

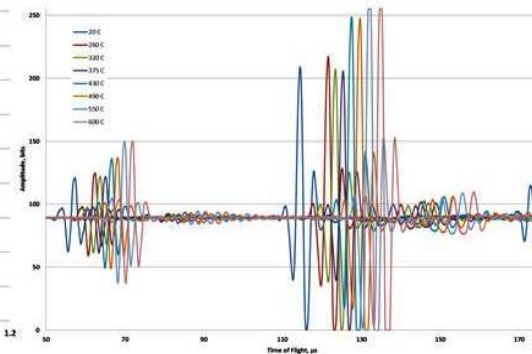
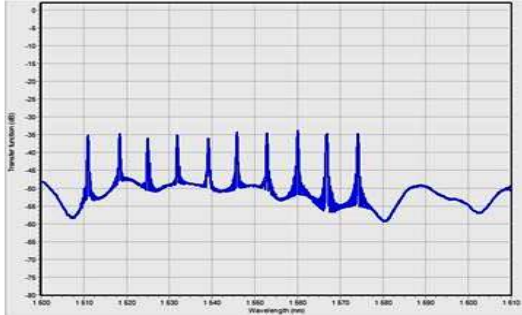


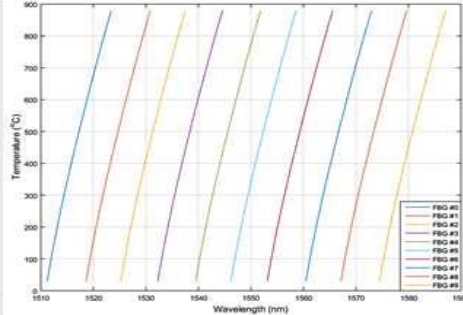
Figure 3. Signal characteristics of a single segment UT with changing temperatures

Fiber-Bragg gratings (FBG) sensors measure the shift in the Bragg wavelength of the grating as temperature changes. The shift is measured at each grating allowing for multiple measurements along the length of the fiber. Long-term use of standard Bragg gratings at temperatures beyond 400–500°C leads to drift and reduced reflectivity resulting in failure of the gratings. Type-I UV laser written FBGs are multiplexed into a standard single mode silica optical fiber and regenerated through a high-temperature annealing process. Regenerated type-I FBGs have been shown to withstand temperatures up to 900°C and potentially up to 1295°C. Figure 4 shows a scan of the fiber Bragg sensor provided by the French Atomic and Alternative Energy Commission (CEA) that was evaluated at HTTL, each of the 10 FBGs reflects a different wavelength and is calibrated separately to a polynomial fit that was provided with the sensor. The calibration curves for all 10 FBGs are shown in Figure 5. The FBG sensors were observed to have an initial accuracy of approximately 1°C, but experienced an average temperature drift of more than 10°C between the first and second heating cycles. The cause of this drift is unknown as the maximum test temperature was well below the maximum recommended use temperature provided by CEA.

**Multi-Point Fiber-Bragg Grating Optical Fiber Temperature Sensor**

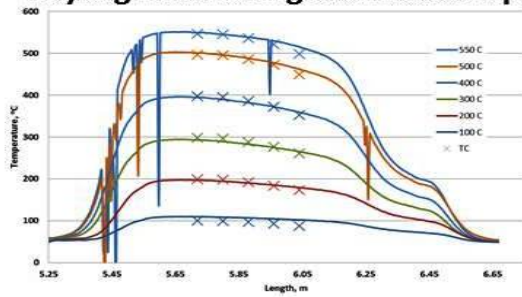


**Figure 4. Reflection spectrum for FBG optical sensor at room temperature**

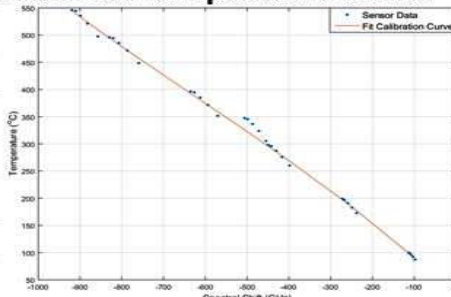


**Figure 5. Calibration curves for 10 FBGs in CEA probe**

**Rayleigh Scattering Distributed Optical Fiber Temperature Sensor**



**Figure 6. Measured temperatures along full length of optical fiber (resolution ~1mm)**



**Figure 7. Calibration curve for a single point along fiber**

The distributed optical fiber sensor is an unaltered single mode silica fiber that uses the natural defects and density fluctuations in the amorphous glass. Swept wavelength interferometry (SWI) is used to measure the Rayleigh backscatter as a function of the length of the optical fiber. The Rayleigh backscatter is caused by the random defects and density fluctuations in the fiber. For any given fiber the Rayleigh backscatter signal is random but constant, up to certain temperatures, and the thermal expansion in the fiber causes a shift in the reflected spectrum of the fiber. This shift can be calibrated to an initial reference scan of that fiber creating a distributed temperature sensor. The distributed sensor was tested up to 550°C and did not show any evidence of drift. Figure 6 shows the temperature profile in the furnace measured by the distributed sensor for temperature steps up to 550°C, with pointwise thermocouple measurements shown by “X” markers. Although no drift was observed, for temperatures above 500°C temperature errors began to manifest at points along the fiber. This is likely caused by defect annealing. These temperature errors persisted during cooling and represent a permanent change to the calibration of the fiber. This can be corrected between heating cycles by obtaining a new baseline scan. Figure 7 shows a temperature calibration curve for a single point on the fiber.

**Benefits to DOE**

Development of advanced in-core instrumentation is critical to DOE’s energy-security mission to provide world-class facilities for advancing nuclear science and technology. Successful completion of this effort has resulted in sufficient out-of-core characterization of new ultrasonic and fiber optic temperature sensors to allow for characterization during in-core testing necessary to qualify the sensors for regular use in irradiation tests. Based, in part, on the results of this LDRD, ultrasonic thermometers and fiber-optic

temperature sensors are scheduled for inclusion in two irradiation tests. These include AGR 5/6/7 in the ATR, which will include one ultrasonic thermometer and two FBG sensors, and an already-started, year-long irradiation at the Massachusetts Institute of Technology Research Reactor (MITR). The MITR irradiation includes three UTs, both single and multi-segment, and multiple fiber optic sensors of both FBG and Rayleigh types.

### **Interns and Postdocs**

Intern: Kelly McCary.

### **Collaboration**

University: Ohio State University.

## **16P6-003FP: Phenomena Identification and Ranking Table Technique Applied to the MEGA-POWER Heat Pipe Reactor Concept**

James W. Sterbentz,<sup>1</sup> James E. Werner,<sup>1</sup> Michael G. McKellar,<sup>1</sup> Andrew J. Hummel,<sup>1</sup> John C. Kennedy,<sup>1</sup> Richard N. Wright,<sup>1</sup> and John M. Biersdorf<sup>1</sup>

### **General Project Description**

This LDRD project completed its main goal of performing and completing a multi-disciplinary technical review of the Los Alamos National Laboratory (LANL) Mega-Power heat pipe-cooled fast reactor concept. The Phenomena Identification and Ranking Table (PIRT) technique was applied to the Mega-Power concept to identify those phenomena that dominate specific safety-related issues. The PIRT review was subdivided into four assessment areas: (1) Reactor Normal and Accident Conditions, (2) Heat Pipes, (3) Reactor Materials, and (4) Power Conversion. The INL PIRT assessment was documented and published in an INL external report (limited distribution) entitled, “Special Purpose Nuclear Reactor (5 MW) for Reliable Power at Remote Sites Assessment Report--Using Phenomena Identification and Ranking Tables (PIRTs)”, INL/LTD-16-40741, Revision 0, January 2016.

This LDRD project has been a unique opportunity for INL. INL gained an intimate understanding of the LANL Mega-Power reactor concept and, through the PIRT, became aware of the key design issues that may prevent the LANL concept from achieving deployment. INL evaluated and discussed these design issues over the course of the PIRT assessment process with LANL. To circumvent the LANL concept issues, INL invented two alternative core design concepts that are significantly more robust in terms of safety and ability to be fabricated than the LANL concept. These two INL alternative design concepts (Design A and Design B) have been protected by patent applications filed. The second major goal of the LDRD was dedicated to evaluating the two INL alternative micro-reactor core designs in terms of neutronics, thermal-hydraulics, materials, heat-pipe design, and manufacturability.

### **Summary**

The preliminary analyses for the first INL alternative core design (Design A) looks extremely promising. The thermo-mechanical stresses around the SS316 heat pipes and fuel are substantially lower (factor of 10) than those calculated for the LANL concept. This implies the reactor core can operate safely under normal operating conditions, but can also operate with one or more failed heat pipes. In addition, Design A fuel elements are relatively easy to fabricate with existing commercial techniques and will not require extensive research and development programs like the LANL concept. Design B exhibits comparable reactor performance to Design A, but with even less stress issues. Although Design B is not yet as mature as Design A, like Design A its core components are also readily fabricable with existing commercial techniques.

### **Benefits to DOE**

Both the Department of Energy and the Department of Defense have expressed keen interest in micro-reactors recently. Both are currently looking at the use of small nuclear reactors (micro-reactors) to supply electrical power to off-grid and remote installations. The LANL concept has been highlighted by DoD as a potentially viable reactor concept. INL's two new core-design concepts are improvements over the LANL concept. It is hoped that recent discussions between INL (Dr. K.P. Ananth and Dr. Kemal Passamehmetoglu) and DOE NE-1 will lay the ground work for future programmatic funding (in FY-18)

for both the INL and LANL concepts. INL has established a close working relationship with LANL and hopes to continue this collaboration in the future.

## Publications

Sterbentz, J.W., J.E. Werner, M.G. McKellar, A.J. Hummel, J.C. Kennedy, R.N. Wright, and J.M. Biersdorf, 2017, “Special Purpose Nuclear Reactor (5 MW) for Reliable Power at Remote Sites Assessment Report--Using Phenomena Identification and Ranking Tables (PIRTs)”, INL/LTD-16-40741, Revision 1, April 2017.

Sterbentz, J.W., J.E. Werner, A.J. Hummel, J.C. Kennedy, R. O’Brien, A.M. Dion, and R. N. Wright, 2017, “*Preliminary Assessment of Two Alternative Core Design Concepts for the Special Purpose Reactor,*” INL/EXT-17-43212, Revision 0, October 2017.

## Presentations

Phenomena Identification and Ranking Table assessments of the Special Purpose Reactor (LANL concept). INL-LANL technical meeting at the Idaho National Laboratory on February 7-8, 2017.

“Technical presentations on heat pipes and the Hot Isostatic Press technique applicable to the fabrication of their steel monolith”, Los Alamos.

Dr. K.P. Ananth , 2017, “Portable Special Purpose Nuclear Reactor (2MW) for Remote Operating Bases and Microgrids”, to the *2017 Joint Service Power Exposition*, May 1-4, 2017, Virginia Beach, VA.

Dr. J.W. Sterbentz, 2017, “Special Purpose Reactor”, INL NS&T Program Advisory Review, June 7, 2017 at the Idaho National Laboratory.

## Invention Disclosures, Patents, Copyrights

Attorney Docket No. 2939-P13471US (BA-952). “*Modular Nuclear Reactors, Fuel Structures, and Related Methods.*”

## Interns, Postdocs, and Staff Support for Graduate Studies

Intern: Axel M. Dion.

## Collaboration

University: Ecole Polytechnique University in Paris, France.



## 17A1-024FP: Design to Enable Narrow Pulse Width in Transient Tests

Nick Woolstenhulme,<sup>1</sup> John Bess,<sup>1</sup> Jim Parry,<sup>1</sup> Joe Palmer<sup>1</sup>

### General Project Description

The Transient Reactor Test Facility (TREAT), constructed in the late 1950s, provided thousands of transient irradiations before being placed in standby in 1994. It will soon resume its crucial role in nuclear-heated safety research. While the facility's flexible design and multi-mission nature saw historic experiments for numerous reactor fuels and transient types, TREAT was never specifically adapted to address very brief pulse transients akin to postulated light water reactor (LWR) reactivity initiated accidents (RIAs). Since the behaviors of fuel under these conditions depends strongly on energy input duration and resulting cladding time/temperature response under pellet cladding mechanical interactions, this LDRD project was conceived to develop pulse-narrowing capabilities for the future of TREAT.

### Summary

TREAT is currently capable of performing transients to achieve pulse's whose Full-Width at Half Maximum (FWHM) duration is <100ms, and perhaps as narrow as 72 ms, but not squarely in the desired range of 25-65 and 45-75 ms FWHM required for simulating hot zero power RIAs for Pressurized and Boiling Water Reactors (PWR and BWR), respectively. Kinetic models of TREAT were exercised to determine which nuclear parameters most affected pulse duration. These investigations showed incremental improvements for minor facility enhancements including increased reactivity step insertions (to initiate the power pulse) and slightly-increased transient rod drive speed for pulse termination ("clipping") via uprated rod drive system pressure. This transient rod speed improvement opportunity was communicated to TREAT personnel and is currently under consideration for inclusion in regularly scheduled revisions to the facility's capability basis.

Modern nuclear models demonstrated three-dimensional computational tools can be used to optimize the core power peaking profile to permit increased reactivity step insertions. By replacing peak fuel assemblies with graphite dummies, fixing TREAT's various non-transient control rods at deliberate positions to hold down the "hot side" of the core, and balancing against the required excess reactivity needed in the transient rods, the limiting fuel assembly power can be reduced on the order of ~20%. This is a remarkable discovery of latent capability in the TREAT facility, not only in enabling the subject capabilities for reduced pulse widths, but also for "uprating" the core's transient energy capacity by a significant amount. Investment in computational developments which automate the experiment-specific optimization process will be needed to streamline this strategy into a useful design tool.

Although it is believed that these two minor improvements can enable TREAT to access the relevant pulse width range for BWRs, there is some uncertainty in the achievable pulse width based on general lack of "prompt pulse fast clip" transients in the historic database. For this reason, a series of similar transients have been planned to be performed in TREAT following its imminent restart. These tests will address the relevant physics for prompt pulse fast clip transients to aid in model benchmarking. This work will likely result in the first formal publication achieved under this LDRD.

While incremental improvements can likely enhance TREAT's capability into BWR-relevant missions, the aforementioned kinetic models also demonstrated that the briefer PWR pulse shapes can only be achieved with a to-be-designed advanced clipping system. Literature review and three-dimensional fuel performance modeling were performed to ensure that such a capability was relevant. The results of these

studies, combined with the prevalence of PWR-type plants in today's current fleet, demonstrated that an enhanced clipping capability will be essential for TREAT to access this important mission area.

Several enhanced clipping concepts were explored including pneumatically-driven light weight clipping rods and neutron poison gas injection into in-core chambers. For a number of engineering reasons, the gas injection concepts were prioritized for further development. Several viable poison gases were evaluated for nuclear affects and design considerations. Most neutron poison gases were determined to be infeasible for this application, but enriched  $^{10}\text{BF}_3$  remained a viable candidate despite complications with containing this chemically-reactive gas. A rare isotope of helium ( $^3\text{He}$ ), however, was found to offer the greatest benefits for clipping design and overall performance. Owing to the cost of  $^3\text{He}$ , innovative mechanical concepts were explored which minimized the total amount of gas needed in the system. A unique concept, inspired by TREAT's experiment design paradigm of self-contained, compact, package-type assemblies, showed great promise for enabling a  $^3\text{He}$ -based system with a reasonable cost. Pending future evaluations of crucial design components, such as fast-acting valves, this design concept will likely become the focal point of future work under this LDRD to lay the foundation for its ultimate deployment at TREAT.

## Benefits to DOE

This project will develop the information needed to deploy a set of capabilities which are crucial in enabling TREAT to adequately address a major component of nuclear safety research in direct support of the most prevalent reactor types in the industry. The pulse-narrowing strategy is not yet sufficiently mature to perform detailed resource-level and deployment-timing evaluations, but it is reasonable to expect that this capability will be impactful for DOE Office of Nuclear Energy programs, such as accident-tolerant fuel research. This capability will also be crucial for industrial partners to resolve data gaps in performance of state-of-the-art fuels. Last, innovative LWR nuclear companies who will likely access TREAT's capabilities through the Gateway for Accelerated Innovation in Nuclear Program will benefit greatly from accident-testing capabilities which faithfully represent the postulated conditions to establish license-supporting safety tests.

## References

- [1] Crawford, D. C., A. E. Wright, R. W. Swanson, and R. E. Holtz, "RIA Testing Capability of the Transient Reactor Test Facility," *Proceedings of the IAEA Technical Committee Meeting on Fuel Cycle Options for LWRs and HWRs, Victoria, Canada, May 1998*, IAEA-TECDOC-1122, pp. 99-109.
- [2] "Nuclear Fuel Behaviour Under Reactivity-imitated Accident (RIA) Conditions, State-of-the-art Report", *OECD-NEA Report NEA/CSNI/R (2010)1*, 2010.

## Publications

External publications will be forthcoming in years 2 and 3. An INL internal report was prepared during year 1 to facilitate future publication as referenced below:

Woolstenhulme, N. E., J. Bess, C. Davis, L. Dusanter, C. Folsom, J. Parry, T. Shorthill, and H. Zhao, "Conceptual Report on Narrowing TREAT's Pulse Width for Enhanced LWR RIA Simulation", INL Internal Report INL/INT-17-43163, September 2017.

## **Presentations**

Woolstenhulme, N.E., 2017, “TREAT Transient Shaping,” Poster Presentation at GAIN Fuel Safety Research Workshop, Energy Innovation Laboratory, Idaho Falls, Idaho, May 2-4, 2017.

Woolstenhulme, N. E., 2017, “Update on Experiment Design Preparations for TREAT,” Presentation at *OSU IRP Meeting*, Argonne National Laboratory, Illinois, May 23-24, 2017.

“TREAT Transient Shaping,” webpage for forthcoming TREAT website, scheduled for publication October 2017.

## **Interns and Postdocs**

Interns: L. Dusanter, C. Folsom, and T. Shorthill.

## **Collaboration**

University: Utah State University.

## 17A1-070FP: Multi-Purpose Non-Destructive Examination Station in the ATR Canal

Nick Woolstenhulme,<sup>1</sup> Tom Eiden,<sup>1</sup> and Adam Robinson<sup>1</sup>

### General Project Description

The Advanced Test Reactor (ATR) is one of the most capable test reactors ever constructed for obtaining fuel- and material-performance data from in-core instrumentation during irradiation, but these instruments are often limited by geometric or environmental constraints. Typical hot-cell-based post-irradiation examinations (PIE) also serve to provide crucial performance data, but typically only long after irradiation is complete for logistical reasons (e.g., cooling and shipping). Another currently-undervalued data opportunity is poolside nondestructive examination (NDE) in the ATR canal, performed during routine outages (i.e., mid-irradiation exams) or post-irradiation cooling. Most ATR experiments, driver fuel, and dosimetry are routinely discharged to ATR's relatively large canal during outages; making it an ideal venue for poolside NDE. While isolated projects have deployed limited in-canal NDE capabilities at various points in ATR's history, no integrated efforts have yet enabled the full scientific opportunity of a multi-purpose NDE station. This LDRD project addresses this prospect by investigating user needs to downselect the most impactful NDE technologies, developing an ATR NDE System (hereafter referred to as ANDES), and laying the groundwork for its future deployment.

### Summary

A survey of past, present, and future ATR specimens of interest determined that ANDES should address various specimens including cylindrical capsule experiments, plate type specimens, exposed-cladding fuel rodlets, slender flux wires, and ATR driver fuel assemblies. A structured trade study was used to perform "market research" based on the value proposition of enabling increased scientific opportunities for these specimen types through in-canal NDE. Approximately 40 experts participated including technical leads representing the user community, personnel experienced with in-canal work, and NDE/instrumentation experts. This phase of the project was performed earnestly to prioritize NDE capabilities that are viable to implement and faithfully represent the user community's needs. The collation of NDE needs, downselection of candidate techniques, and first-order evaluations for facility implementations yielded outcomes appropriate to provide the basis for follow-on work focused toward conceptualization and design innovation during this LDRD's remaining two years.

One of the most resounding and cross cutting needs identified for ANDES was spatial measurement of specimen and dosimeter radioisotopic distribution. This capability's will enable comparison to as-run neutronic models for data-informed experiment adjustments in subsequent cycles (e.g. lobe power, irradiation duration) as well as burnup benchmarking data for more efficient driver fuel management. A collimated gamma beam and detector system will be included in ANDES to serve this vital data need. Owing to the multitude of ATR experiments which are entirely encapsulated, this system will also enable gamma computed tomography (CT) through exchangeable collimator slits, controlled specimen rotation, and the option for placement of a gamma source opposing the collimator for gamma transmission CT techniques. Similar approaches have been demonstrated to some level of dimensional resolution at other test reactor projects and synergetic but not duplicative research will be performed in the near future under a recently-awarded Nuclear Energy University Partnerships project.

It was also determined that ANDES should have a non-contact metrology system based on underwater laser-based 3D surface scanning to provide highly-resolved dimensional data on exposed specimen surfaces,

noting that similar systems have been at commercial nuclear plants 0. This metrology system, as well as the gamma characterization system, will be able to operate in two different “urgency modes” so that outage measurements can be performed more quickly with reduced resolution and vice versa for end-of-irradiation specimens during longer cooling periods. Similarly, the need for an enhanced visual-based imaging system was prioritized based on the successful use of underwater videography currently at ATR, except that ANDES will pair such a system with a more precise mechanically-stabilized arrangement and acuity/dimensional standards to enable semi-quantitative videography.

Last, the mechanical fixtures, electromechanical systems, and data acquisition equipment needed to enable the ANDES capability package were recognized as non-trivial fields expected to require innovation and ingenuity to ultimately forge the path to ANDES implementation. These considerations and other were evaluated against facility considerations and resulted in selection of a preferred canal location for ANDES on the east wall of the “working canal” area.

### Benefits to DOE

ANDES will create an opportunity for gathering mid-irradiation data that can be used develop continuous performance correlations, rather than just end-state data, to greatly aid in understanding and modeling of advanced nuclear fuels and materials. ANDES can also be used to examine whether specimens are performing acceptably, bolstering confidence in continued irradiation, or to gage progress on parameters such as burnup, reducing uncertainties in core models, and enabling adjustments to achieve specific irradiation targets. Additionally, most fueled experiments spend several months, and sometimes even years, waiting in the canal during decay-heat cooling periods prior to shipment for PIE. These cooling periods could be used productively for non-destructive PIE. ANDES will help reduce the cost of irradiation and PIE campaigns and accelerate the fuel-development cycle to break down some of the main barriers to deploying advanced nuclear technology.

### References

- [1] Andersson, P., S. Holcombe, and T. Tverberg, 2016, "Inspection of a LOCA Test Rod at the Halden Reactor Project using Gamma Emission Tomography," *Proceedings of the Top Fuel 2016 Conference*, September 11-16, 2016, Boise, Idaho.
- [2] Newton labs website, “[http://www.newtonlabs.com/Specialty\\_Scanners.htm](http://www.newtonlabs.com/Specialty_Scanners.htm)” and [http://www.newtonlabs.com/nuke\\_nm200uw\\_hardware.html](http://www.newtonlabs.com/nuke_nm200uw_hardware.html)

### Publications

External publications will be forthcoming in years 2 and 3. An INL internal report was prepared during year 1 to facilitate future publication as referenced below:

Woolstenhulme, N.E., D. Choe, T. Eiden, D. Imholte, J. Jennings, E. Nef, A. Robinson, and S. Swanson, 2017, "Needs, Concepts, and Rationale for In-Canal Examination at the Advanced Test Reactor", INL Internal Report INL/INT-17-43244, September 2017.

## 17A1-086FP: Development of a Complete Kinetic Model for Free-Radical-Induced Degradation of Formic and Oxalic Acids

Peter Zalupski,<sup>1</sup> Bruce Mincher,<sup>1</sup> Dean Peterman,<sup>1</sup> Gregory Horne,<sup>1</sup> Christopher Zarzana,<sup>1</sup> Cathy Rae,<sup>1</sup> Dayna Daubaras,<sup>1</sup> and Stephen Mezyk<sup>12</sup>

### General Project Description

This research project targets a quantitative understanding of chemical processes that could lead to the complete mineralization of organic species exposed to ionizing radiation. When ionizing radiation interacts with matter, strongly oxidizing and reducing ionic and radical species are produced. These radicals attack any molecular species in their path, initiating arrays of chemical reactions. Depending on the application, the free-radical-induced degradation of molecules may be beneficial (for example, by inflicting damage on organic pollutants for wastewater-treatment purposes) or detrimental (by impairing working chemical reagents in separations processes). The incurred damage typically transforms the target molecules to simpler chemical species until only water and carbon dioxide remain (i.e., complete mineralization). Formic and oxalic acids are the last stable organic species produced immediately prior to mineralization, as they exist in a metastable equilibrium that delays the mineralization outcome. The goal of this work is to quantify the full free radical chemistry of formic and oxalic acids to afford a predictive modeling tool of interest to scientists studying radiation chemistry in a variety of research fields, such as advanced oxidation for environmental remediation, nuclear fuel cycles, nuclear medicine, atmospheric chemistry, and space exploration. The project combines a variety of experimental tools (particle accelerators, gamma irradiation, mass spectrometry, laser flash photolysis) to study mechanisms of degradation pathways and kinetic rate constants for reactions with radical species. The experimental data generated by this research project aids in the construction of a kinetic model for the quantitative prediction of the free-radical-induced degradation of formic and oxalic acids.

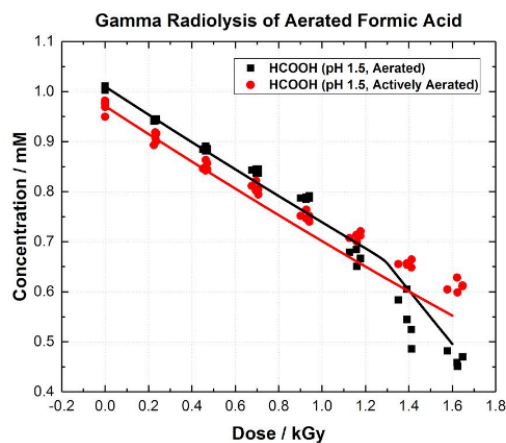


Figure 1. Degradation trend of formic acid, measured in (●) sealed system (full  $O_2$  consumption at 1 kGy), and (■) aerated system

<sup>12</sup> California State University at Long Beach

*(constant O<sub>2</sub> delivery). Solid lines represent initial multi-scale model predictions.*

## Summary

Degradation trends for formic and formate have been established by combining  $\gamma$ -irradiation, high performance liquid chromatography (analysis of degradation products in liquid state) and gas chromatography (analysis of CO<sub>2</sub> and H<sub>2</sub> production due to radiolytic damage). Formic acid (pH 1.5) and separately formate (pH 9.0) solutions were irradiated in the Nordion Gammacell 220E <sup>60</sup>Co irradiator in sealed vials (O<sub>2</sub> is consumed after delivery of ~1 kGy dose), as well as in aerated configuration (O<sub>2</sub> is present throughout). Figure 1 shows the developed degradation trends for formic acid after both irradiation scenarios (O<sub>2</sub> consumed and present) were analyzed using HPLC. Two distinct trends have been consistently acquired during numerous studies, showing that presence of oxygen slows the degradation rates of formic acid and formate. For sealed experiments the rates of production of carbon dioxide and hydrogen gas (resulting from the degradation of formic acid) track well with the observed accelerated rate of analyte degradation resulting from total consumption of oxygen.

The multi-scale model[1] was developed for the formic acid / formate chemistry to predict degradation mechanisms on the basis of reported kinetic data for chemical reactions expected from radiolysis of water. The model allows for comprehensive representation of reaction kinetics as a set of coupled ordinary differential equations, which are simultaneously solved by the FACSIMILE Kinetic Modelling Software package. The model predicts the degradation track of formic acid (Figure 1, solid lines) very well, suggesting that the sudden acceleration ~1 kGy is due to the enhanced formation of OH<sup>•</sup> radical via scavenging of H<sup>•</sup> by the produced H<sub>2</sub>O<sub>2</sub>. When oxygen presence is maintained throughout the OH<sup>•</sup> production is controlled by O<sub>2</sub>, yielding a relatively linear decay of formic acid. The degradation of formate is faster, relative to formic acid, due to its faster reactivity with OH<sup>•</sup> radical.

Additional notable scientific accomplishments include (1) measured rate constants for reactions between formic and formate species and •OH free radical using LINAC pulse radiolysis method at Notre Dame Radiation Laboratory, (2) established the laser flash photolysis methodology to study free radical reactivity. Some programmatic progress worth mentioning includes (1) the establishment of a collaborative relationship with Idaho State University via Adjunct Research Faculty hiring in the area of Degradation Chemistry/Mass Spectrometry, (2) acquired status of guest research assistant professor at the Notre Dame Radiation Laboratory (Zalupski).

## Benefits to DOE

This LDRD builds the tools and expertise to continue the expansion of a very highly regarded radiation-chemistry research in support of NE programs, it provides for transition of skills from a retiring Laboratory Fellow with expertise in this area, and it opens new potential customers and markets for radiation chemistry research.

## References

[1 ]Horne, G.P.; Donoclift, T.A.; Sims, H.E.; Orr, R.M.; Pimblott, S.M. *J. Phys. Chem. B*, 2016, 120, 11781-11789.

## Interns and Postdocs

Postdoc: Gregory Horne



## Collaboration

University: University of Manchester, UK

## 17A1-093FP: Digital Neutron Imaging of Irradiated Nuclear Fuel Using a Gamma-Discriminating Scintillation System

Aaron E. Craft,<sup>1</sup> Glen C. Papaioannou,<sup>1</sup> Christian Grünzweig<sup>13</sup>

### General Project Description

This project seeks to design, develop, and demonstrate a novel digital neutron imaging system for examination of irradiated nuclear fuel. The gamma-sensitivity of digital neutron imaging systems has been the precluding factor for their application to radioactive objects. The proposed imaging system uses a dysprosium-doped scintillator screen, which produces a latent image in the form of neutron activation of the dysprosium. The activated screen can then be positioned away from the neutron beam and radioactive object into a light-tight enclosure where the image can be read by a digital camera. The approach investigated by this project should enable imaging highly radioactive objects. The imaging system would be capable of producing digital neutron radiographs in a matter of minutes, allowing acquisition of over one hundred images in a single day, which is far more than the current production capacity of only fourteen radiographs per day using the current capabilities. The project includes development of a novel neutron scintillator screen and readout process that allows for complete discrimination of gamma radiation emitted from the irradiated nuclear fuel. This innovative neutron imaging system would enable routine use of neutron tomography for post-irradiated examination of nuclear fuels, which would significantly improve the quality of data produced compared to current capabilities.

### Summary

This project has completed the first of its planned three year term. Efforts in the first year focused on proof of principle of a dysprosium-doped delayed neutron scintillator screen and development of a camera-based imaging system that would use the new screens once developed. The project moved further than originally proposed in development of a camera-based neutron imaging system for testing the dysprosium-doped screens once available. A prototype camera-based neutron imaging system was constructed and tested in the East Radiography Station. The prototype system was able to acquire 32 neutron radiographs in less than 12 minutes, which is impressive compared to the current throughput limit of 14 radiographs per day. Dr. Burkhard Schillinger, a professor and colleague from Technical University Munich and expert of neutron beamline and imaging system design, visited INL to collaborate on these activities. Drs. Schillinger and Craft collaborated on a simple and inexpensive system architecture for a neutron computed tomography that could be inexpensively implemented by facilities developing initial neutron imaging systems to demonstrate their utility and gain experience.

The lessons learned from testing a simple prototype camera-based system will be incorporated into design of this second camera-based neutron imaging system in the summer of 2017. Significant radiation shielding and informed system geometry would largely determine the success of a camera-based neutron imaging system in the high gamma content of the neutron beams at the Neutron Radiography Reactor (NRAD). The beam characterization efforts of another project will inform radiation transport models of the imaging system shielding. In support of these efforts, this project supported a summer intern, Miranda Wachs, and subcontractor, Nick Boulton, to help develop an updated prototype imaging system. The camera enclosure has been designed and fabricated. The system will be ready for testing once shielding has been assembled and the electronics installed.

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<sup>13</sup> Paul Scherrer Institute

As proof of principle of the novel scintillator screens, cesium iodide scintillator material was deposited onto the surface of dysprosium foils. These screens were then tested in a neutron beam with a cadmium edge specimen as the object. The activated scintillator screen was read out by digital camera, which successfully produced a digital image from the light emitted from the screen. This test demonstrated the feasibility of such a screen for digital neutron radiography, establishing proof of principle for use of such screens for examination of irradiated nuclear fuel. These screens are completely insensitive to the gamma radiation emitted from the fuel because of the transfer away from the irradiated fuel for readout. Further tests are still planned to measure the light output as a function of time and neutron exposure, but it is expected to follow the well-known activation and decay behavior of dysprosium.

### **Benefits to DOE**

Projects developing advanced nuclear fuels require neutron imaging capabilities to evaluate the condition of irradiated fuels and inform subsequent examinations. The neutron imaging capabilities provided by the neutron beams at NRAD directly support the primary mission of DOE to advance nuclear energy in the United States. If successful, this project would provide an innovative new neutron tomography capability for post-irradiated examination (PIE) of nuclear fuels that would significantly improve the quality of data produced compared to current capabilities and represent a new state-of-the-art for neutron imaging of highly-radioactive objects and would clearly demonstrate DOE's leadership in nuclear fuels testing and evaluation.

### **Interns and Postdocs**

Interns: Nicholas M. Boulton and Miranda Wachs.

### **Collaboration**

Universities: Oregon State University and Idaho State University.

## 17A1-105FP: Safety Margin Evaluation for Experiment Irradiation in ATR

J. W. Nielsen,<sup>1</sup> P. E. Murray,<sup>1</sup> Lin-Wen Hu,<sup>1</sup> Kaichao Sun,<sup>1</sup> A. Dave,<sup>1</sup> and R. L. Marlow<sup>1</sup>

### General Project Description

The current safety basis for the Advanced Test Reactor (ATR) ensures that plant protection criteria are maintained for all Condition 2 events by verifying that, for a Condition 2 flow coastdown transient and condition 2 reactivity insertion accident, the departure from nucleate boiling ratio (DNBR) is greater than two [1]. This limitation may not be applicable to reactor experiments because the quantity of fissionable material and fission-product inventory in experiments is much less than that of the reactor core and may prevent or limit future experimental testing in the ATR. In particular, fueled experiments may be excluded from irradiation in ATR if the desired fission power cannot be achieved due to these safety criteria. This LDRD evaluates the DNBR limit using various subcooled critical heat flux (CHF) correlations and considers the impacts of changing the limit to the onset of nucleate boiling (ONB). The project will provide recommendations to support safety basis changes that can expand the experimental operating envelope of the ATR without a compromise in safety.

### Summary

The INL has worked in collaboration with the Massachusetts Institute of Technology (MIT) to evaluate the margin of safety with respect to experiments irradiated in ATR. As part of the research the INL has selected the Mini-Plate 1 High Power (MP-1 HP) experiment as a case study. The MP-1 HP experiment challenged the ATR safety limits for a loss of flow accident, which limits the  $DNBR > 2$ . INL in conjunction with MIT has successfully quantified the safety margin of the MP-1 experiment. Initially the project evaluated the various CHF correlations with respect to flow coast down transient. Using various correlations, the CHF ratio was determined for steady-state conditions and peak transient conditions. Additional investigation has been performed to evaluate the use of CHF correlations in a transient condition. The literature search has revealed the use of these correlations, which were obtained from steady-state experiments, may be conservative for use in evaluation of short period transients.

The MIT collaborators performed a statistical analysis evaluating the uncertainty in various parameters (i.e., mass flux, power, and pressure) using an MIT developed MATLAB model. The use of the MATLAB software allowed for evaluation of CHF correlations that are not embedded into the RELAP5 software. Concurrently, INL performed a statistical analysis using the RAVEN software developed at INL coupled with RELAP5, using the Groeneveld 2006 CHF correlations. A summary of the CHF ratios for several correlations is presented in Table 1. Several cases have been considered, varying in power multipliers considered. Case 1 represents a nominal operating condition. Case 3 represents the most conservative scenario where the power is 152% greater than nominal ( $P=2.52 P_n$ ).

Correlation	Outer Channel		Inner Channel		Correlation	Outer Channel		Inner Channel	
	Mean	3 $\sigma$	Mean	3 $\sigma$		Mean	3 $\sigma$	Mean	3 $\sigma$
<b>Steady-State Case 1: <math>P = 1.00P_n</math></b>									
LUT	8.960	0.460	8.678	0.446	LUT	6.441	0.329	6.193	0.319
SRL	10.170	0.769	10.860	0.824	SRL	7.020	0.531	7.548	0.573
HM OCC	11.120	0.581	10.760	0.557	HM OCC	7.921	0.425	7.598	0.407
<b>Steady-State Case 2: <math>P = 1.82P_n</math></b>									
LUT	4.601	0.237	4.403	0.227	LUT	3.144	0.162	2.981	0.154
SRL	5.394	0.409	5.765	0.436	SRL	3.580	0.271	3.865	0.291
HM OCC	5.680	0.304	5.422	0.292	HM OCC	3.803	0.213	3.578	0.202
<b>Steady-State Case 3: <math>P = 2.52P_n</math></b>									
LUT	3.114	0.161	2.952	0.153	LUT	2.041	0.108	1.899	0.102
SRL	3.799	0.288	4.047	0.305	SRL	2.486	0.189	2.634	0.200
HM OCC	3.816	0.208	3.600	0.200	HM OCC	2.413	0.140	2.216	0.131
<b>Peak Transient Case 1: <math>P = 1.00P_n</math></b>									
<b>Peak Transient Case 2: <math>P = 1.82P_n</math></b>									
<b>Peak Transient Case 3: <math>P = 2.52P_n</math></b>									

Table 1: CHF evaluation using the 2006 Groeneveld CHF Look-up table (LUT), Savannah River Laboratory correlation (SRL) and the Hall-Mudawar Outlet Condition correlation (HM OCC). Left table is evaluated at steady-state conditions, and the right table is evaluated at peak-transient conditions.

The above results demonstrate, that at nominal steady-state or peak transient conditions, a significant amount of margin in safety of experiments inserted into ATR. The limit of DNBR < 2.0 is only breached by the LUT during a peak transient with Case 3 power multipliers. In order to further address the limit, this project is evaluating the Onset of Nuclear Boiling, Onset of Significant Voiding, and Onset of Flow Instability, and will provide the appropriate recommendation for a revised safety limit.

## Benefits to DOE

The INL vision for the Advanced Test Reactor is to be the national and international materials and fuels irradiation testing facility of choice. The current safety basis limits the capabilities of irradiating fueled experiments in ATR. This research utilizes modern techniques for evaluation of safety margin (e.g., risk-informed safety-margin characterization) to adequately quantify the safety margin for ATR experiments. Evaluation of modeling parameters such as CHF correlations and consideration of the uncertainties in those correlations supports the methodology for safety margin characterization, expanding the ATR capabilities. The expansion of ATR capabilities has the ability to attract new experimental programs for fuels testing that would otherwise be performed elsewhere. As ATR is the only high performance research reactor (HPRR) in the DOE complex that routinely performs fuel irradiation tests, fuels testing that cannot be accomplished in the ATR would have to be tested in international reactors such as BR-2 in Belgium or the Halden reactor in Norway. Expanding the capabilities of ATR is critical in maintaining and furthering the INL mission as the lead laboratory for nuclear energy research.

## References

- [1] "Experiment and Irradiation Facilities - Upgraded Final Safety Analysis Report for the Advanced Test Reactor," SAR-153 Chapter 10, Rev. 23, April 2016.

[2] “Guidelines for Preparing and Reviewing Applications for the Licensing of Non-Power Reactors: Format and Content (NUREG 1537 Part I)”, NUREG-1537, February 1996.

## **Publications**

Dave, A., J. Morrell, and K. Sun, “Safety Margin Characterization for ATR Experiments,” Draft Report.

Dave, A., J. Morrell, K. Sun, L. Hu, J. Nielsen, P. Murray, and R. Marlow, 2017, “Safety Margin Evaluations for ATR In-core Experiments supporting LEU U-Mo Fuel Development,” Submitted abstract to 2017 TRTR conference.

## 17A1-111FP: Design of Low Activation Retrievable Sample Holder for TREAT Irradiation of Science-Based Specimens

Nick Woolstenhulme,<sup>1</sup> Assel Aitkaliyeva,<sup>1</sup> and Steven Hayes<sup>1</sup>

### General Project Description

The Transient Reactor Test Facility (TREAT), constructed in the late 1950s, provided thousands of transient irradiations before being placed in standby in 1994 and will soon resume its crucial role in nuclear-heated safety research. The latter half of TREAT's historic operation was best known for integral-scale testing of fuel specimens under postulated reactor-plant accident conditions, but TREAT's underappreciated earlier history included simpler phenomena identification tests that elucidated fundamental behaviors and paved the way for these integral-scale tests. Advances in modern computational capabilities and a resurgence of interest in novel reactor technologies create an opportunity for emphasizing modernized, science-based and separate-effects test capabilities once again at TREAT. An innovative approach to this testing was conceived to leverage minor radioactivity built in during brief TREAT irradiations by arranging small fresh-fuel specimens in low activation hardware so that they could be easily extracted and shipped for post-irradiation examination (PIE) within weeks. The concept was termed the minimal-activation retrievable capsule holder (MARCH) irradiation vehicle system, and development began under this LDRD project in FY-17.

### Summary

The genesis of the MARCH concept emerged in response to the irradiations proposed under another LDRD (16-046), which aimed to irradiate small metal fuel alloys in well-monitored environments and characterize the resulting microstructural changes. Three core components of the MARCH system were developed in order support this irradiation and others like it including: 1) A containment structure termed the Broad Use Specimen Transient Experiment Rig (BUSTER), 2) A high temperature heater module (capable of 700°C), and 3) An assembly which supports and encapsulates the specimens termed the Characterization-scale Instrument Neutron Dose Irradiation (CINDI) module. This LDRD is currently supporting final preparations to enable the initial CINDI irradiations in TREAT during FY-18. Similar irradiations pertaining to irradiation-impacted pseudo-equilibrium phases in metal fuel alloys have also been proposed as having potential for future DOE funding if the present LDRD were successful in developing the core capability.

Additionally, a period of initial brainstorming, idea-gathering, and informal market research led to the invention of other module capabilities. One of these modules, termed the Separate-Effect Test Holder (SETH), enables transient irradiations of various "centimeter-scale" fuel specimens for separate-effects tests such as melt progression studies, phenomena indentation, and in-situ properties measurements. The SETH module's larger capsule displaces the heater module and is filled with room temperature inert gas in order facilitate stable boundary conditions for separate-effects experiment with reduced engineering/fabrication burden for performing these tests. Since TREAT's safety containment requirements are ascribed primarily to the reusable BUSTER pipe, the SETH capsule is able to be arranged with low-activation materials and off-the-shelf consumables; combining to create a well-placed tool for timely and cost-effective science-based irradiations. The SETH module was conceptualized under this LDRD to become the base concept for a variety of other potential irradiation opportunities, some of which are already funded separately to branch off of the LDRD project and develop their specific test



adaptations. Like CINDI-based tests, irradiation performed using SETH are currently foreseen to be some of the first performed in the restarted TREAT. Figure 5 shows an overview of the MARCH system.

Another module similar to SETH, but which makes use of thicker capsule walls, built-in low-temperature electrical heaters, and capsule-to-specimen liquid metal bond, was created and termed the Temperature Heat-sink Overpower Response (THOR) module. THOR was invented to enable a relevant capability for simulating specimen temperature response and the early stages of fuel performance under transient overpower conditions. The THOR module was only peripherally and briefly approached under this LDRD as it was quickly adopted by other funding sources for its value in testing of sodium fast reactor fuels.

Lastly, a revolutionary module concept emerged with the objective to create a safety/engineering envelope that enables irradiation of simple specimens, such as instrumentation, to be performed as affordably as typical out-of-pile testing. While this module, termed the Transient Instrument and Materials Maximum Irradiation Envelope (TIMMIE) includes some basic hardware, its true innovation is a safety analysis philosophy based on pre-populated nuclear/thermal parameters in a straightforward calculation tool. The TIMMIE analysis tool permits safe irradiation of pre-analyzed materials based only on their constituent masses; bypassing the cost of geometric specific modeling/reporting. This transformative idea was initially conceptualized under this LDRD and later adopted for further maturation by funding sources aimed toward development of advanced in-pile instruments.

## **Benefits to DOE**

Development of the MARCH system will continue to attract experimenters from DOE, industry, and academia to branch off from the foundational work performed under this LDRD to develop their experiment-specific modules or adaptations. In a pattern similar to TREAT's early history, the MARCH system will support science-based irradiations to provide pioneering data sets for modern model validation, identify fundamental behavior to sharpen fuel-research focus, and advance the state of nuclear safety advancements by cultivating broad interest in transient science. Based on the current outlook, science-based MARCH irradiations will not only be eventual in TREAT, but will likely be the inaugural irradiations in the restarted TREAT. This will be a tremendous achievement in highlighting capability deployment and ensuring that TREAT's emerging staff and operational bases are solidified in a diverse way to support data needs from within the broader spectrum of nuclear-fuel technology developments.

***The MARCH System***

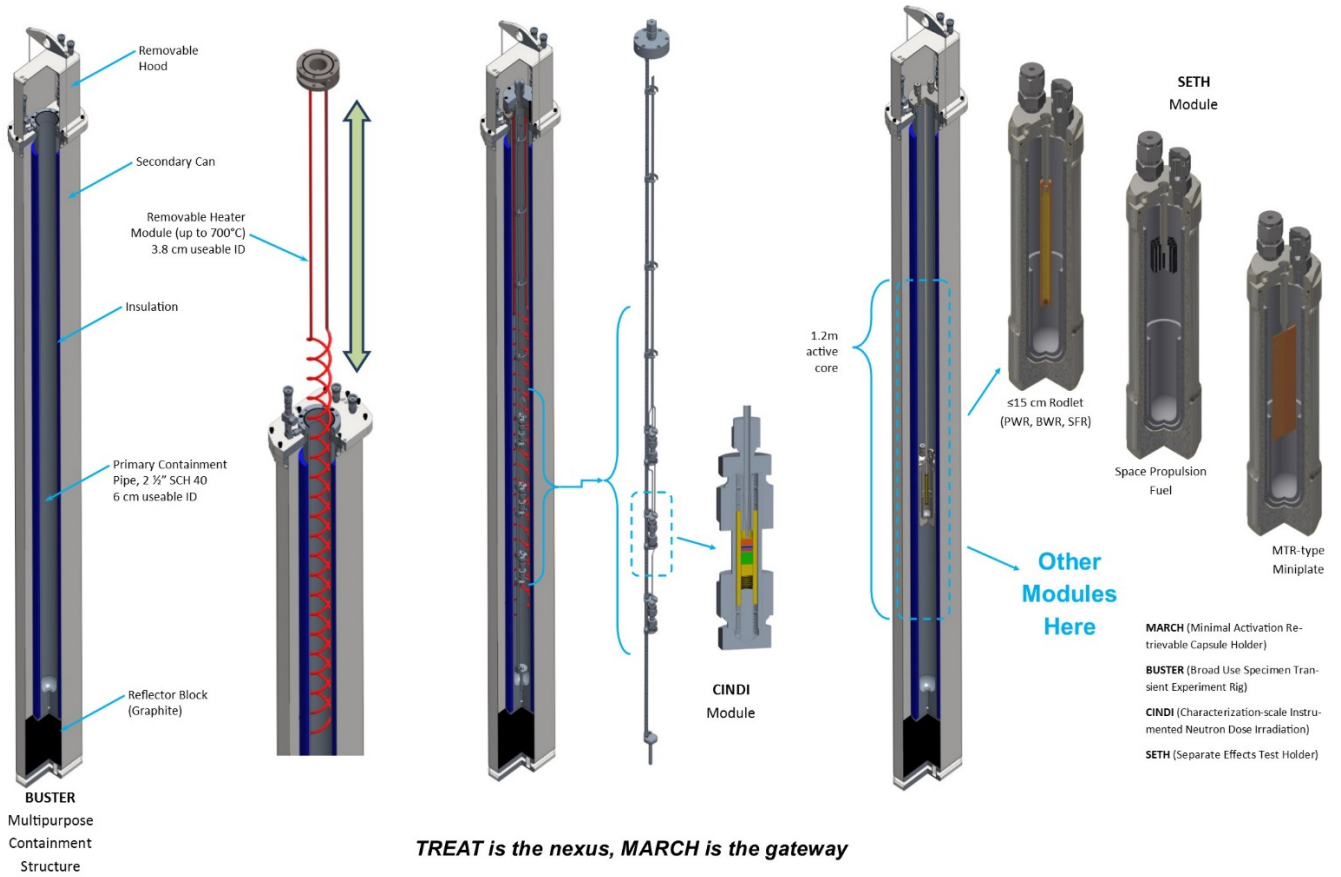


Figure 5: MARCH System Overview.

## Publications

External publications will be forthcoming in years 2 and 3. An INL internal report was prepared during year 1 to facilitate future publication as referenced below:

Woolstenhulme, N. E., C. Baker, D. Chapman, C. Hill, C. Papesch, E. Rosvall, and S. Snow, 2017, " Conceptual Report for the Minimal Activation Retrievable Capsule Holder Irradiation Vehicle System ", INL Internal Report INL/INT-17-43170, September 2017.

## Presentations

Woolstenhulme, N. E., 2017, "Static Capsules for TREAT Irradiations," Poster Presentation at GAIN Fuel Safety Research Workshop, Energy Innovation Laboratory, Idaho Falls, Idaho, May 2-4, 2017.

Woolstenhulme, N. E., 2017, "Update on Experiment Design Preparations for TREAT," Presentation at *OSU IRP Meeting*, Argonne National Laboratory, Illinois, May 23-24, 2017.

"The Minimal Activation Retrievable Capsule Holder (MARCH) System," webpage for forthcoming TREAT website, scheduled for publication October 2017.

## 17A1-124FP: Systematic Error Control in Cross Section Library Generation for Novel Reactors

Zain Karriem,<sup>1</sup> Abderrafi M. Ougouag,<sup>1</sup> Gerhard Strydom,<sup>1</sup> Jui-Yu Wang<sup>1</sup>

### General Project Description

Currently, efficient and accurate analysis and design of nuclear reactors can be performed using reactor physics methods and computer codes that represent the physical problem with low energy and spatial detail without significant loss of fidelity. Retention of the necessary fidelity hinges on the availability of suitably prepared ultra-fine-energy group (U-FEG) nuclear cross section libraries that incorporate an accurate representation of the physics. Such U-FEG libraries are further processed to generate energy condensed and spatially homogenized cross section data for use in the low-order neutronic models. Although the current state of the art of cross sections preparation incorporates all the relevant physical principles governing neutron-nuclei interactions, the actual methods as implemented are still often *ad-hoc* and marred by the use of many approximations. In particular, no prior existing method attempts to quantify or control the systematic process-inherent error in the resulting multigroup cross sections. None includes a rational algorithm-based determination of the sufficient extent of supercells, and only one addresses the Doppler Effect on resonant scattering kernels. In addition, all these methods have further inadequacies when dealing with multiple levels of heterogeneity and interpenetration of spectra. Therefore a comprehensive formal theory is needed for a mathematically rigorous approach to the front end of nuclear data processing. The goal of this project is to develop such a theory and associated computational methods. The goal is to remedy all the shortcomings just listed and give reactor physicists the ability to generate nuclear cross data using a collection of methods in which the systematic error of a given data set may be quantified and controlled.

### Summary

The first year of this project, FY 2017, focused on three main tasks: (i) establishing a baseline infrastructure for cross section data processing, (ii) developing theoretical methods and (iii) carrying out initial code implementation of the newly developed theory. Item (i) has been achieved through the acquisition, installation, and testing of a two-prong capability, the NJOY and PREPRO codes, for processing basic nuclear data from Evaluated Nuclear Data Files (ENDF/B). While each code can be used independently of the other, the possibility of interlacing modules from the two codes allows the incorporation of new modules and the exploration of novel data processing schemes. Item (ii), theoretical developments, included (a) a theory for error control in ultra-fine multigroup cross sections generation, (b) a method for the Doppler broadening of arbitrary-shape 0 K cross sections from ENDF/B files and (c) application of the theory from (a) to cross sections as retrieved from ENDF/B files and Doppler broadened using the methods from (b). All were completed, and the practical result is an energy group structure that allows quantification of the error in ultra-fine multigroup cross sections and the production of data suitable for subsequent processing and use downstream in neutronics computational suites. Item (iii), code implementation of the new theory has been successfully carried out. This required the creation of two auxiliary codes for retrieval of data from ENDF/B files and for Doppler broadening per the methods developed in this project.

The computer code starts with a conventional equal-lethargy-bins semi-fine group structure and allows the user to specify the relative error that is tolerated in the cross sections in going from a continuous energy cross section representation to a fine-group representation. The program then proceeds to refine the equal-lethargy-bins group structure into a fine-energy group structure that ensures the user-specified relative error is not exceeded. *Figure 6* shows preliminary results for the theoretical selection of the energy group structure for a uranium fueled reactor.

FY 18 will see the evaluation of the use of the theoretically selected energy group structure; the development, implementation and testing of theory to treat spatial homogenization. The planned goal for FY 19 is to develop a cross section processing code suite that implements the developments of FY 17 and FY 18 into a single automated data processing tool.

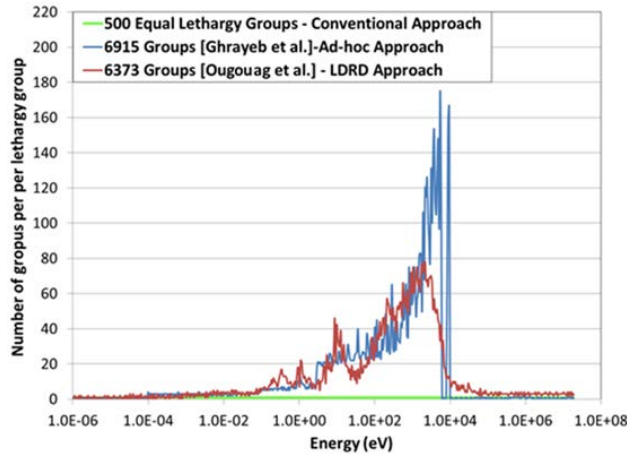


Figure 6: Preliminary results for theoretically based energy group selection compared to conventional and ad-hoc energy group selection results (Note that the LDRD structure does not yet include refinements from unresolved resonances).

## Benefits to DOE

This project will provide the means to generate data for new and novel reactors without the need to rely on operating reactor experience, which is the case for legacy methods. The success of this project will ultimately provide a better state-of-the-art cross section generation capability that will be useful to INL and beyond to other laboratories and the nuclear industry.

## Publications

Ougouag, A. M. and Z. Karriem, 2017, “Annual Progress Report for LDRD project 17A1-124FP: Systematic Error Control in Cross Section Library Generation for Novel Reactors”, 09/2017 (In preparation)

Karriem, Z., 2017, “Processing Cross Sections with NJOY and PREPRO”, 09/2017 (In preparation)

Ougouag, A. M., 2017, “Systematic method for quantifying and controlling relative error in ultra-fine group cross sections”, September 2017 (In preparation)

Wang, J.W., Z. Karriem and A. M. Ougouag “Fortran code implementation of a fine-energy group structure generation algorithm incorporating systematic error control”, 2017, 09/2017 (In preparation)

## Interns and Postdocs

Intern: Jui-Yu Wang.

## Collaboration

University: North Carolina State University.

## 17A1-150FP: Advanced Manufacturing of Metallic Fuels and Cladding by Equal-Channel Angular Pressing

Cheng Sun,<sup>1</sup> Randall S. Fielding,<sup>1</sup> Tomas M. Lillo,<sup>1</sup> James I. Cole,<sup>1</sup> and Caizhi Zhou<sup>14</sup>

### General Project Description

Advanced manufacturing of nuclear fuels and materials is a component of the INL's core missions of discovering innovative nuclear energy solutions. Improving the performance of currently used fuels and cladding via advanced manufacturing techniques is at relatively low cost compared to development of new materials. Nanostructured materials exhibit an enhanced irradiation tolerance due to the significant volume fraction of high-angle grain boundaries that serve as sinks or recombination centers for radiation-induced defects. The project aims to manufacture nanostructured metallic fuels and cladding materials through equal-channel angular pressing (ECAP) and examine the irradiation performance of the manufactured materials. ECAP is a low-cost advanced manufacturing technique that produces ultrafine ( $100 \text{ nm} < \text{grain size} < 1 \text{ }\mu\text{m}$ ) or nanocrystalline grain sizes ( $< 100 \text{ nm}$ ) in metals and alloys through application of severely plastic deformation to achieve exceptional grain refinement of coarse-grained (grain size  $> 1 \text{ }\mu\text{m}$ ) metals and alloys. Our research is anticipated to impact the research and development of nuclear fuels and cladding by establishing a low-cost and advanced manufacturing technique and developing nanostructured metallic fuels and cladding. This project is directed-basic research in nuclear engineering and materials science disciplines, and fits into INL's strategic area of advanced nuclear energy.

### Summary

In FY 17 (Year 1), our project was focused on the design and construction of ECAP setups and on the manufacturing of steel fuel cladding Grade 91. The ECAP setup is being built in Center of Advanced Energy Studies (CAES) for manufacturing non-radioactive steel fuel cladding and other metals. Figure 1 shows the schematic illustration of the ECAP setup. Figure 2 (left) shows the furnace, which will be installed around the die. Figure 2 (right) shows the die with backpressure slider bar. Figure 3 shows the hydraulic press that is being used for loading in the ECAP setup. Finite element modeling (FEM) was performed by Missouri University of Science & Technology to facilitate design of the ECAP dies and identification of optimum parameters during ECAP processing. This FEM analysis was used to test the die design and bolts to ensure the integrity of the system up to  $900^\circ \text{ C}$  during processing with different combinations of temperature and stress. In addition, FEM analysis was performed to determine optimum processing conditions (temperature, pressure/backpressure, and speed) in order to increase the uniformity of the shear and optimize the microstructural evolution of the samples during ECAP. The microstructure characterization of pre-ECAP Grade 91 stainless steel has been characterized using transmission electron microscopy and Automatic Crystal Orientation and Phase Mapping, as seen in Figure 4-5. In terms of university collaborations, two ISU graduate students have been working on designing and building the ECAP setup at CAES.

### Benefits to DOE

Research on developing a low-cost advanced manufacturing technique for nuclear fuels and cladding will benefit DOE-NE programs, including fuel-cycle-research and development (FCRD), and light water reactor sustainability (LWRS) programs. Follow-on proposals may also be solicited to design new ECAP dies and processes for manufacturing tube-shaped fuel cladding.

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<sup>14</sup> Missouri University of Science and Technology



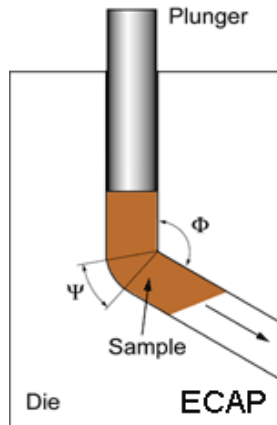


Figure 1. schematic of ECAP.

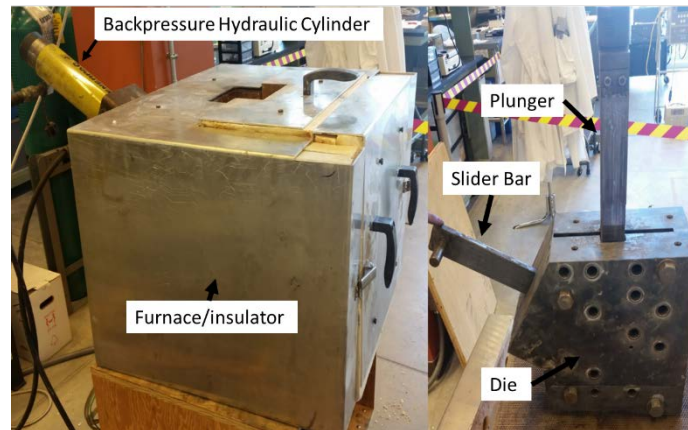


Figure 2. The outer insulation of the furnace around the die with the backpressure cylinder (left) and the die with the backpressure slider bar (right)



Figure 3. Hydraulic press that is used for loading in the ECAP experiment setup. The maximum load is 150 tons.

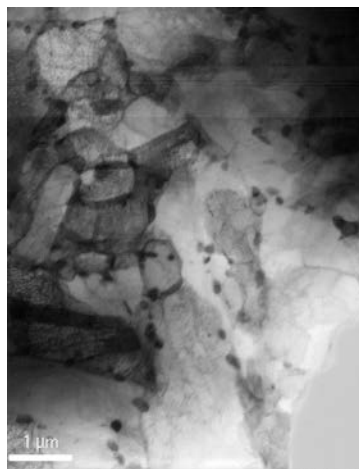


Figure 4. TEM image of pre-ECAP Grade 91 stainless steel. The average grain size is  $\sim 1 \mu\text{m}$ .

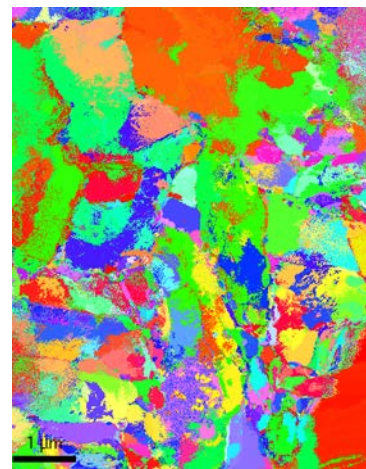


Figure 5. Orientation mapping of pre-ECAP Grade 91 stainless steel using EBSE-TEM procedure.

## Interns, Postdocs, and Staff support for Graduate Studies

Interns: Ryan Carnahan, Andrew Hoffman, and Tianju Chen.

Staff Support: Professor Caizhi Zhou.

## Collaborations

Universities: Idaho State University and Missouri University of Science and Technology.



## 17A1-164FP: Application of Traditional Risk Assessment Methods to Cyber Manipulation Scenarios

Katya Le Blanc,<sup>1</sup> Robert Youngblood,<sup>1</sup> and Vivek Agarwal<sup>1</sup>

### General Project Description

This project will (1) adapt an existing risk-analysis method for application to the problem of identifying vulnerabilities to cyber-manipulation in nuclear facilities, (2) demonstrate the modified method on a simple test facility (the Idaho State University flow loop), and (3) apply the refined method on a larger scale to a realistic facility, the Human Systems and Simulation Laboratory (HSSL). Existing risk-assessment tools have some strengths for the intended application; for example, they are adapted to generate, and work with, large scenario sets. But they also have certain weaknesses: many of them make implicit assumptions about the probabilities of combinations of events that are inapplicable to this application, and some existing methods are not well adapted to analyzing the kinds of failure modes that cyber-manipulation could inject. Accordingly, the project will begin by defining characteristics needed for an effective risk-assessment methodology for cyber-manipulation scenarios, followed by a review of existing scenario-based risk-assessment methods against these characteristics. We will then assess the efficacy of each method based on both system response and plant response to cyber manipulation.

### Summary

The team completed a literature review of existing cyber manipulation scenarios. The review looked at a total of 34 methods for cyber risk assessment, focusing on methods that could be used in control systems and NPPs. The review categorizes the methods based on the functionality it provides, the domain it is applied to/developed for, the stage of risk assessment methods it applies to, and whether the method has been validated or applied to real-world system. The review revealed that few if any of the methods have been validated and many of them have not been applied to real-world systems, and many will not likely scale well to large, complex systems. This literature review helped identify the gaps in existing risk analysis methods for cyber security in NPPs. The results of the literature review will be presented in a summary report on June 30<sup>th</sup>, 2017 and a journal article will be prepared and submitted by September, 2017.

The team worked with cyber security researchers to define the characteristics needed in a risk assessment method to address cyber manipulation scenarios and evaluated existing methods against the characteristics. This revealed that many cyber risk methods rely heavily on the concept of vulnerability to estimate the likelihood of attack. Vulnerability is a hard concept to capture and is not always directly related to the likelihood of an attack. Our work will investigate ways to better characterize likelihood in the cyber context. Another gap in many existing approaches is that many of them feature a top down approach to identifying scenarios and consequences. A journal article is in preparation and will be submitted by September 30, 2017.

The team developed cyber-attack scenarios for a simple control loop system using an approach based on logic modeling. The advantage of logic modeling is that it is straightforwardly verifiable, and it systematically produces a catalog of possible outcomes. However using logic modeling for control loops and modeling event timing is particularly challenging, so the approach may have to be modified to accommodate the more complex systems. The methodology allows the system to be modeled in a way that identifies unique consequences and interactions to the system due to cyber components.

To facilitate the first empirical test of the methodology, the team has established a subcontract with ISU. The team conducted an experimental evaluation of the scenarios on September 15, 2017 at the ISU Flow loop.

The team has also begun efforts to scale up to test a cyber manipulation scenario of auxiliary feedwater pump in the generic Pressurized Water Reactor model housed in the Human System simulation Laboratory. All of these

activities will be unique efforts to empirically validate scenarios generated as part of a risk methodology Both the flow loop test and the HSSL test will include a human –in the-loop component to investigate the effects of misleading system operators.

## Benefits to DOE

The potential consequences of cyberattack are significant, and existing methods for identifying and analyzing the possible scenarios are deficient. Therefore, the significance of making progress on this front is potentially great. Additionally, many nuclear utilities are considering employing technologies that may increase the cyberattack surface of nuclear power plants. As plants embark on modernization efforts to increase efficiency and develop cost savings, many digital technologies may be incorporated into the control room and beyond. While most utilities are likely to avoid modifying safety systems, the consequences of a cyber manipulation on the upgraded non-safety systems could have severe economic consequences. This work will help ensure the continued safety of operating plants by characterizing the cyber risk while still enabling modernization efforts that can enhance the economic competitiveness of nuclear power plants. This work will also build capabilities for DOE that will enable simulation of cyberattack scenarios and human-in-loop testing of cyberattack scenarios, as well as building staff competency in this important area.

## Publications

The following papers are in preparation: 1)A paper describing the results of the literature review , 2)A paper describing the crosswalk between the characteristics required for a method to address cyber manipulation and the review of methods 3) A paper describing the cyber manipulation scenarios developed for the flow loop and the result of the testing will be submitted to a risk journal 4) A paper describing the results of the human-in-the-loop testing of the scenarios in the ISU flow loop will be submitted to *Human Factors*.

## Presentations

“Application of Traditional Risk Assessment Methods to Cyber Manipulation Scenarios”, presented at NH&S Strategic Advisory Committee Meeting on June, 29, 2017.

Youngblood, B., 2017, presented at the Extended Probabilistic (ePRA) Risk Assessment Workshop.

## Invention Disclosure, Patents and Copyrights

None

## Interns, Postdocs, and Staff Support for Graduate Studies

Post Doc: Wei Zhang.

Staff Support: Ryan Pitcher.

## Collaborations

Universities: Michigan Technological University and Idaho State University.

## 17A1-201FP: Human Reliability Analysis for Advanced Reactor Technologies and Systems

Ronald Boring,<sup>1</sup> Shawn St. Germain,<sup>1</sup> and Harold Blackman<sup>15</sup>

### General Project Description

Human reliability analysis (HRA) is a framework to identify and quantify the human component of system risk. While originally developed primarily for nuclear energy applications, HRA has been adopted in other safety-critical areas, like oil and gas, aerospace, and defense. Originally designed to model human operators in analog control rooms, HRA has not kept pace with advances in digital human-machine interfaces (HMIs). Digital technologies are being incorporated into control rooms in the form of control-room modernization and new builds. These digital HMIs potentially change the types of tasks operators perform (e.g., more monitoring due to increased automation). As a result, human-error types and probabilities may be different from those found in analog control rooms. Still, HRAs for new reactors are being completed with methods that predate digital HMIs. This LDRD seeks to bring HRA methods up to date with contemporary and future digital HMI technologies. Specifically, the project is reviewing human failure events that are specific to digital HMIs, crosswalking existing HRA methods to these human failure events, adapting HRA methods where there are shortcomings, and developing new guidance for HRA methods to address digital HMIs.

### Summary

Efforts during the first year of the project have entailed a multi-pronged approach to gather information about experiences with digital HMIs and establish collaborators for out-year activities. INL staff are conducting an ongoing literature review and operating experience review of advanced HMIs, including surrogate industries to nuclear power like chemical process control, where digital HMIs have been in place for several decades. Additionally, INL initiated two research efforts to gain firsthand empirical insights:

1. One issue that has been identified in digital control rooms is the so-called keyhole effect, in which operators develop a sort of tunnel vision by focusing on their own consoles. This has in some cases resulted in a decrease in mutual awareness in the control room—the sense of awareness what others are doing. In extreme cases, this has resulted in a breakdown in required threeway communications in the control room between reactor operators and supervisors. INL has developed and completed a survey of subject matter experts and operators to determine contributing factors to mutual awareness and experiences in analog vs. digital control rooms. Additionally, INL developed a mutual awareness self-report scale to be used in control room settings. The goal is to identify the impact of mutual awareness on human reliability and model it in an HRA method.
2. There remains a shortage of empirical data to inform human error probability estimates. This fact holds true for HRA in analog environments, but there is an even greater paucity of data for digital interfaces. The prospect of large-scale operator studies is beyond the scope of this project, but there is opportunity to collect data using simplified environments to full-scale control rooms. Working with INL, University of Idaho (UI) has developed Rancor, a microworld simulator. Rancor represents a simplified nuclear power plant control interface, on which students can be trained to proficiency quickly. The environment allows collection of larger sample sizes of participants than would be possible for an actual plant simulator, with the caveat that the results of student operators using a simplified control interface may not always generalize to reactor operators at an actual plant. However, the approach allows large-scale data collection and precise experimental control. Rancor has been developed and piloted in 2017 and is planned for an extensive series of studies to inform HRA in 2018 and 2019. Professor Karin Laumann of the Norwegian University of Science

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<sup>15</sup> Boise State University

and Technology (NTNU) plans to use the microworld to gather HRA data through a university funded grant. Professor Carol Smidts of the Ohio State University likewise plans to work with the microworld through an in-kind collaboration.

A key element in the first year of the project has been enlisting collaborators who are actively engaged in human reliability for advanced HMIs. These collaborators, who have significantly represented international partners with experience using advanced HMIs, provide in-kind access to valuable insights on HRA and opportunities to work together in the remaining two years of the project. INL met with human factors and probabilistic risk staff at Nuscale Power, Korea Atomic Energy Research Institute, Korea Hydro and Nuclear Power, U.S. Nuclear Regulatory Commission, and Canadian Nuclear Safety Commission to gain insights into their HRA modeling of digital HMIs and multi-unit and highly automated plant designs. INL is using these insights to create a report on future directions for HRA.

### Benefit to DOE

Already early in the project, domestic and international companies, universities, and regulators have shown tremendous interest in working with INL. Particularly promising is the use of the microworld to collect HRA data specific to digital HMIs, with assistance by NTNU. NTNU has noted that oil and gas companies would be very interested in a version of the microworld customized to an oil or gas production process, and it is anticipated that this will lead to external funding opportunities related to training and risk assessment. Additionally, the chance to conduct an HRA trade study to assist a vendor in 2018 promises to establish a method to support human factors validation for developers of digital HMIs. Work proposed from a U.S. Department of Defense contract in 2018 has identified a task at INL to summarize insights into human error using digital interfaces—essentially a report summarizing findings from the first year of this LDRD. These efforts combine to demonstrate the wide-ranging value of the research approach and the opportunity for follow-on funding. Through continued work on the LDRD and emerging collaborations, the project promises to ensure more robust HRA for licensing of digital HMIs, ensure continued safe operator performance with new technologies, and establish the applicability of HRA outside the nuclear energy sector. Advancing the state of the art in HRA will help ensure continued safe operation of facilities within the DOE and across the energy sector.

### Publications

- Blackman, H., and R. Boring, 2017, “Assessing dependency in SPAR-H: Some practical considerations”, In R. Boring (ed.), *Advances in Human Error, Reliability, Resilience, and Performance (Advances in Intelligent Systems and Computing)*. Heidelberg: Springer Verlag, pp. 13-19.
- Boring, R., H. Blackman, and M. Rasmussen, 2017, “Preliminary considerations for human reliability analysis for verification and validation of new designs”, *Proceedings of the PSAM Topical Conference on Human Reliability, Quantitative Human Factors, and Risk Management*.
- Lew, R., R. Boring, and T. A. Ulrich, 2017, “Ensuring operator reliability in digital control rooms”, *Proceedings of the 2017 American Nuclear Society Nuclear Power Instrumentation & Controls and Human-Machine Interface Technology (NPIC HMIT) Conference*, pp 8-18.
- Lew, R., T. A. Ulrich, R. Boring, and S. Werner, 2017 (in press), “Applications of the Rancor microworld nuclear power plant simulator”, *IEEE Proceedings of Resilience Week 2017*, pp. 143-149.
- Savchenko, K., H. Medema, R. Boring, and T. Ulrich, 2017, “Comparison of mutual awareness in analog vs. digital control rooms”, In R. Boring (ed.), *Advances in Human Error, Reliability, Resilience, and Performance (Advances in Intelligent Systems and Computing)*. Heidelberg: Springer Verlag, pp. 192-199.

St. Germain, S., R. Boring, G. Banaseanu, Y. Akl, and H. Chatri, 2017 (in press), “Multi-unit considerations for human reliability analysis”, *Proceedings of the PSAM Topical Conference on Human Reliability, Quantitative Human Factors, and Risk Management*.

## **Presentations**

Boring, R., K. Savchenko, R. Lew, T. Ulrich, T, 2017, “The think-aloud protocol method to facilitate three-way communication in digital control rooms”, *2017 American Nuclear Society Nuclear Power Instrumentation & Controls and Human-Machine Interface Technology (NPIC HMIT) Conference*, San Francisco, June 11-15, 2017.

## **Invention Disclosures, Patents, and Copyrights**

None

## **Interns, Postdocs, and Staff Support for Graduate Studies**

Interns: Ms. Kateryna Savchenko and Thomas Ulrich.

Postdoc: Dr. Martin Rasmussen.

Staff Support: Dr. Harold Blackman, Dr. Karin Laumann, Dr. Roger Lew, and Dr. Carol Smidts.

## **Collaborations**

Universities: Boise State University, Norwegian University of Science and Technology, University of Idaho, and Ohio State University

## 17A1-223FP: New Approach for PIE Using Modular Transportable Instrumentation

Daniel Jadernas,<sup>1</sup> Aaron E. Craft,<sup>1</sup> Robert O'Brien,<sup>1</sup> and Scott Moore<sup>1</sup>

### General Project Description

Traditional post-irradiation examination (PIE) methodology requires the use of remote equipment in large hot cell facilities, creating expense and a long-duration research cycle. Additionally, the remote nature of instrumentation, imposes geometrical requirements, and harsh environments within hot cells limit applicable technologies and hardware, hinder maintenance, and complicate upgrades. The goal of this project is to develop a novel high-efficiency PIE apparatus capable of delivering a higher throughput, increased flexibility, and both new and higher-quality existing data streams that provide a significant positive impact on the nuclear-fuel research and development cycle. The system will be capable of performing multiple and correlative non-destructive examination (NDE) functions concurrent with increased efficiency and simplified maintenance and upgrades.

While this project will develop some instrumentation for proof-of-principle experiments, the focus of this project is to develop the platform for PIE using a novel approach. The proposed platform, called modular examination instrument for transportable nuclear energy research (MEITNER), is a mobile post-irradiation system composed of a stack of shielded modules capable of housing various non-destructive examination systems while providing access to the highly-radioactive objects contained therein. Non-contact measurements will be used, where possible, to provide flexibility in the geometries that can be examined to accelerate examination and to provide three-dimensional data. Potential PIE capabilities include visual examination, dimensional inspection and profilometry, surface-layer composition studies, gamma emission tomography, ultrasonic examination, eddy-current testing, radiographic examination, and others.

The modular approach of the platform also allows rapid and cost-effective development of novel PIE methods. The relatively transportable nature of this system allows it to be implemented anywhere with a crane, a cask, and an in-floor pit or similar facility, including the Advanced Test Reactor (ATR), the Transient Reactor Test Facility (TREAT), the Hot Fuel Examination Facility (HFEF), and the North Radiography Station (NRS) of the Neutron Radiography Reactor (NRAD) at HFEF.

Upon successful implementation of this project, MEITNER would:

1. Decrease fuel cycle R&D time consumption and cost by >50%
2. Increase the reliability and quality of the data output and enhance capabilities of existing techniques
3. Enable inexpensive and rapid development of new PIE concepts and techniques
4. Provide PIE at other facilities (e.g. TREAT, ATR)
5. Decrease or remove the requirement that instrument be tolerant to the in-cell environment.

### Summary

A mock-up PIE module has been designed and constructed in a non-radiological environment during this fiscal year in order to begin testing and development of examination instruments that have been identified for initial demonstration, see Figure 1. These include visual inspection, profilometry, gamma autoradiography and eddy current measurement techniques. Other techniques that would be compatible with the module are e.g. laser ablation inductively coupled plasma mass spectroscopy, laser induced break-down spectroscopy, and x-ray and neutron scattering techniques etc. Several vendors are being considered for this instrumentation. University of Idaho students were part of the initial feasibility study of the PIE module.



INL researchers have been working together with an external partner, Square-1, for the conceptual design of a state-of-the-art precision specimen positioning system. This company has previous experience manufacturing high precision robotic systems for use in nuclear environments. The sample positioning system is a key component for integrating the entire platform. The sample positioning system must be able to attach to samples with varying shapes and sizes with a flexible gripping device. The positioning system must be able to translate a 2 m long sample with very high accuracy and repeatability. The current concept considered for the sample positioning system is shown in Figure 1 below. The conceptual design of the sample positioning system has been finalized in fiscal year 2017 and include software considerations for controlling the positioning system.

The conceptual design study for the PIE has been started during this fiscal year and will continue during the next fiscal year. The current conceptual design is shown in Figure 1 and consists of gate valves, instrumentation modules, and an atmosphere control module. Each instrumentation module can be designed to accommodate the needs of each instrument in terms of size, radiation shielding requirements, and access to the specimen. A guiding principle for determining the dimensions of the examination platform is that it should be able to examine any specimen that anticipated transport mechanisms can bring to it. The complete length is 2 m long with an inner diameter of 60 cm. The inner diameter is based on the largest transport cask anticipated to couple to this platform, and the length is sufficient to accommodate most specimens available in the HFEF hot cell. Using adapter modules the PIE platform can dock to any accepting facility, e.g. HFEF hot cells, ATR, TREAT or other nuclear facilities and casks. Radiological and radiation protection aspects of the PIE platform are also being considered at this early stage of the project.

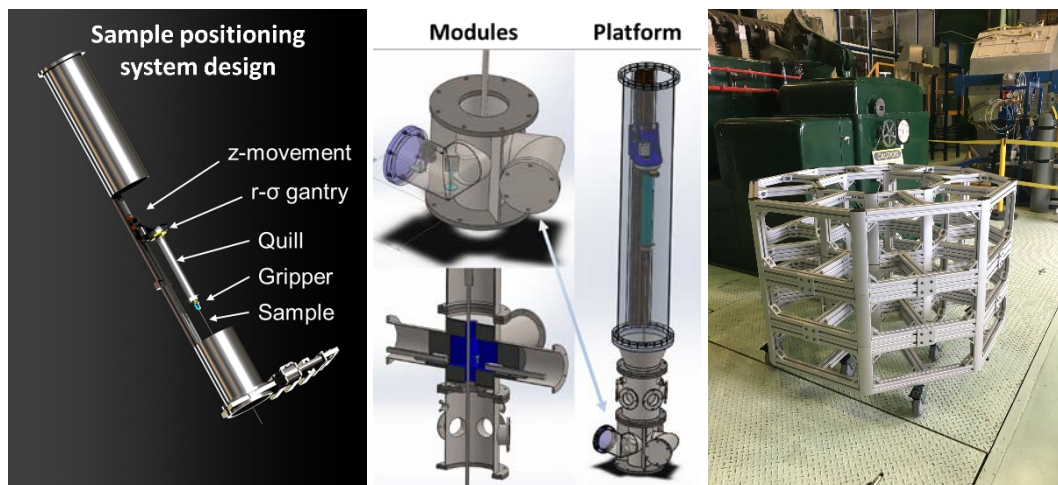


Figure 1. The sample positioning system, PIE modules and mock-up PIE platform.

## Benefits to DOE

The development of the novel and innovative PIE module proposed in this project will revolutionize the way non-destructive PIE is performed. It will substantially decrease the time and cost for non-destructive PIE while increasing the quality of the generated data. Furthermore, easy access to the specimen will allow for characterization techniques that currently cannot be performed in hot cells. The concept is also transportable and can be deployed at many different locations.

## Publications

The results from the project will be published during fiscal year 2018



## **Presentations**

Jadernas, D., A. E. Craft, S. A. Moore, N. M. Boulton, and P. B. Bragg, Patrick B, 2017, New Approach for PIE Using Modular Transportable Instrumentation – Yearly review presentation, poster presentation.  
Jadernas, D., A. Craft, S. Moore, N. Boulton, J. Giglio, and M. Meyer, 2017, New Approach for PIE Using Modular Transportable Instrumentation, poster presentation.

## **Invention Disclosures, Patents, and Copyrights**

None.

## **Interns, Postdocs, and Staff support for Graduate Studies**

Interns: Nicholas Boulton and Miranda Wachs.

## **Collaboration**

University: University of Idaho.

## 17A1-227FP: Multi-Physics, Multi-Scale Coupled Simulation of Power Impulse Experiments

Warren Jones,<sup>1</sup> Hailong Chen,<sup>1</sup> Stephen Novascone,<sup>1</sup> Benjamin Spencer,<sup>1</sup> and Wade Marcum<sup>4</sup>

### General Project Description

The response of fuel systems undergoing transient-accident-based power loading has historically been addressed via experiment, out of necessity, due to the complexity of the related interactions. Capturing fracturing of fuel, fission-gas release, pressurization and subsequent rupture of cladding, and ultimately, the interaction of the dynamic fuel system with coolant has been outside the capabilities of fuel-modeling packages. With the advent of increased computational power and efficiency, the pending addition of peridynamics capabilities to the MOOSE/BISON multi-physics solver, and application of well established finite-element (FE) /arbitrary Lagrangian-Eulerian (ALE) modeling to nuclear fuel systems, modeling these complex, interlaced physics is achievable. Capitalizing on these advances, this research project will computationally model loss-of-coolant accidents (LOCAs), reactivity-insertion accidents (RIAs), and post-accident fuel migration of a Special Power Excursion Reactor Test (SPERT)- or Power Burst Facility (PBF)-type fuel, capsule, and coolant experiment geometry. The modeling will be performed with verified codes, and validation will be performed against documented experimental results and new experiments performed at Oregon State University, experiments which will explore post-accident fuel migration and dispersion. Ultimately, the combination of these methods and simulations will provide information to feed full-core simulations such as MELCOR.

### Summary

For modeling efforts using peridynamics, following two significant accomplishments have been made so far: First, we developed a Peridynamic thermomechanical model based on irregular domain discretization, finished MOOSE-based implementation, and submitted a journal paper on this topic. Most of the current peridynamics models are based on a regular grid structure, which will result in biased or mesh-dependent crack initiation and growth for cases when the domain of interest is non-rectangular, which is the case for fuel pellet. We have demonstrated that the proposed model can handle domains of arbitrary shape without biasing or mesh configuration dependencies in the predicted fracture patterns. Second, we developed a new self-stabilized non-ordinary state-based peridynamic model, finished MOOSE-based implementation, and are in the process of submitting a journal paper on this model. Non-ordinary state based peridynamic correspondence models permit directly incorporating arbitrary continuum material models into peridynamic models, but still have the advantages of peridynamics for fracture modeling. This is important for modeling fracture behavior of nuclear fuel under long-term irradiation because both creep and fracture effects are important. This will permit including appropriate material models to include creep effects in the setting of peridynamics. One major issue with non-ordinary state-based models is that they have zero-energy modes, which can lead to instabilities unless steps are taken to remove them. We have developed a new procedure to remove this material instability, which is an essential step toward being able to use this method for creep-fracture modeling of nuclear fuels. Publications and supporting studies from this portion of the LDRD are [P1 – P4], [C1 – C3], [PD-1], and [PhD-1].

The implementation of existing multi-physics codes has made progress as well. Contact was made with Sandia National Laboratory to establish the framework necessary to develop a computational model on the Sandia HPC system. This was necessary due to the proprietary nature of certain modules in the ALEGRA framework that will enable nuclear physics feedback in the modeled system. In addition, a simplified model of a fuel/rodlet/coolant system was developed in the multi-physics program CTH, which is used for high-energy, fast transient events that include fracture modeling and phase changes. This model is being exercised to determine the appropriate modeling conditions prior to running a full 3-dimensional model of a rodlet. The results from the CTH model will

be compared to the ALEGRA model to determine whether the influence of nuclear-physics feedback significantly alters the solution.

The experimental portion of this project is conducted at Oregon State University. The experimental campaign takes place over the three year LDRD project, with explicit objectives/outcomes to be completed in year 1. The goal of the experimental campaign is to experimentally characterize, through advanced measurement techniques, the dispersion of surrogate fuel particles post-fuel failure in representative phenomenological conditions to that of a PWR. During year 1, the goal is to complete the design, and assembly of an experimental loop that is to be used during the remaining portion of the campaign. An experimental loop has been designed and is being procured and assembled; it is anticipated that all goals will be completed by the end of the project year. Additionally, preliminary tests have been performed for the purpose of scoping studies in support of the design of the loop already and demonstrated success in the metering techniques chosen to be used for this project. Publications and supporting studies from this portion of the LDRD are [C4 – C5], and [PhD-2].

### Benefits to DOE

In the interest of designing implicit safety into new reactor and fuel designs, current national and international research targeting advanced fuel concepts and accident-tolerant fuels is at the forefront of nuclear research and development [1]. INL has restarted the Transient Reactor Test Facility (TREAT) to support advanced modular reactor design and investigate the transient response of fuel to accident profiles, including LOCAs and RIAs [2]. Understanding the results of TREAT experiments is imperative to the acceptance and licensing of these next-generation reactors and fuels. Accurate modeling of these transients requires the implementation and application of detailed, coupled-physics simulations. The scope of integration across the required physics and the small time and space scales involved necessitates a significant amount of computational power, such as that available through INL's High Performance Computing (HPC) Center. The intellectual and computational resources available at INL make solving this cutting-edge problem feasible.

### References

- [1] “Nuclear Energy Research & Development Roadmap, Report to Congress”, *Department of Energy, Office of Nuclear Energy*, 2010.
- [2] *Office of Nuclear Energy*, “Resumption of Transient Testing”, <http://energy.gov/ne/articles/resumption-transient-testing>, accessed 6/10/2016

### Publications

- “A MOOSE-Based Implicit Peridynamic Thermomechanical Model”, 2016, *ASME IMECE 2016* conference proceeding, Nov. 2016.
- “Thermomechanical Peridynamic Analysis with Non-uniform Domain Discretization”, *Computer Methods in Applied Mechanics and Engineering*, under review.
- “Peridynamics using Irregular Domain Discretization with MOOSE-Based Implementation”, *ASME IMECE 2017* conference proceeding, Nov. 2017.
- “A Self-Stabilized Non-Ordinary State-Based Peridynamic Correspondence Model”, *Journal of Mechanics and Physics of Solids*, to be submitted.

### Conference Presentations

- “A MOOSE-Based Implicit Peridynamic Thermomechanical Model”, *ASME IMECE 2016* conference, Nov. 2016.

“Peridynamics using Irregular Domain Discretization with MOOSE-Based Implementation”, *ASME IMECE 2017* conference, to be presented on Nov. 2017.

“Implicit Peridynamic Thermo-mechanical Formulations for Fracture Modeling”, *EMI 2017* conference, Jun. 2017.

“Plume Progression of a Ruptured Fuel Element in a Representative 5x5 PWR Fuel Assembly”, *ANS Winter Conference*, Nov. 2017.

“Advection and Diffusion Calculations Supporting Fuel Fragmentation, Relocation, and Dispersion Experiments”, *ANS Winter Conference*, Nov. 2017.

### **Interns and Postdocs**

Interns: Haoyang Wei and Griffen Latimer.

Postdoc: Hailong Chen.

### **Collaborations**

Universities: Arizona State University and Oregon State University.

## 17P10-003FP: In-Situ Small-Scale Mechanical Testing of Neutron Irradiated Ferritic Steels

Cheng Sun,<sup>1</sup> Jian Gan,<sup>1</sup> and Mitchell K. Meyer<sup>1</sup>

### General Project Description

Development of advanced materials that can withstand harsh irradiation environments in nuclear reactors is crucial for the license extension of current and the design of future advanced nuclear reactors. Ferritic steels have been considered important fuel-cladding materials for advanced nuclear reactors. Neutron-radiation-induced changes in the microstructure of ferritic steels has a pronounced impact on mechanical properties. This project aims to study the mechanical degradation of irradiated ferritic steel using innovative small-scale testing technique in electron microscopes. Our research can be used to design the microstructure and composition of the next generation of ferritic and martensitic steels for light-water-reactor applications. This project is directed basic research in the nuclear-engineering and materials-science disciplines, and fits into INL's strategic area of advanced nuclear energy.

### Summary

**Scientific progress:** (1) we have characterized the microstructure of neutron irradiated ferritic Fe-9Cr alloy, a high density of dislocation loops were formed in the microstructure. Nanoindentation of Fe-9Cr alloy was performed to study the indentation-induced pile-ups, which is an indicator of strain hardening rate. The orientation dependent deformation behaviors of Fe-9Cr alloy before and after neutron irradiation was studied and compared. (2) In-situ compression tests in transmission electron microscope (TEM) was used to observe the dislocation activities of Fe-9Cr under mechanical loading. A clear formation of shear band start at the displacement of 300 nm, which causes the localized deformation and there the load drop at ~ 300 nm. The load-displacement curve can be obtained simultaneously and correlate to the evolution of the microstructure during loading. (3) High-dose ion irradiation of Fe-9Cr–C model alloy was performed at University of Michigan to compare the void swelling behavior of ferrite and tempered martensite phase. Tempered martensite shows a stronger void swelling resistance compared to ferrite phase due to the chemical partitioning of Cr and Si. (4) The archive and neutron irradiated 9CrYWT oxide-dispersion-strengthened steels (ODS) alloy were characterized using transmission electron microscopy, atom probe tomography and synchrotron X-ray diffraction. The results show the bimodal distribution of second phase particles ( $Y_2Ti_2O_7$ ,  $TiO_2$  and  $CrO_3$ ), the average size of large particles is ~ 50 nm, while that of small particles is ~ 5nm. Our scientific progress will provide guidance for the design and development of structural materials for advanced nuclear reactors.

**Technical progress:** We have successfully performed compression/tensile testing of TEM lamella in TEM. Push-to-pull device was used to covert compressive force into tensile force. An innovative sample preparation procedure in focused ion beam system was developed for in-situ testing experiments. This technique can be used to perform fundamental understanding of materials failure mechanisms in nuclear reactor environments and accelerate the discovery of advanced fuels and materials.

**Programmatic progress:** We has established internal and external collaborations through this project. Crystal plasticity finite element modeling was initiated with Dr. Wen Jiang, a computational materials scientist in NS&T at INL. Atom probe tomography analysis of second phase particles in ODS alloy was collaborated with Dr. Mukesh Bachhav, a material scientist in NS&T at INL. We also collaborate with Dr. Yang Ren, a physicist at Argonne National Laboratory for synchrotron X-ray diffraction on Advanced Photon Source (APS). High-dose ion irradiation experiments were performed in Michigan Ion Beam Laboratory (MIBL) at University of Michigan, collaborating with Prof. Gary Was.

## Benefits to DOE

This project will help rebuild and reestablish INL's core strength in developing both cladding and structural materials, a strategic discipline that is necessary for the development of advanced nuclear energy technology. The application of small-scale mechanical testing techniques will accelerate the research and development of nuclear fuels and materials. The rapid and efficient development of nuclear fuels and materials is essential to DOE-NE's mission and the emerging advanced reactor private sector.

## Publications

- Sun, C., F. A. Garner, L. Shao, X. Zhang, and S. A. Maloy, 2017, "Influence of injected interstitials on the void swelling in two structural variants of 304L stainless steel induced by self-ion irradiation at 500C", *Nuclear Instrumental Methods Physics Research B*, submitted 2017.
- Sun, C., J. Li, and E. Fu, 2017, "Chapter 5 Radiation damage in nanoporous metals, Radiation damage of nanostructured materials", *Progress in Materials Science*, submitted 2017.
- Sun, C., L. Malerba, M. J. Konstantinovic, F. A. Garner, and S. A. Maloy, 2017, "Microstructural characterization of high-dose ion-irradiated duplex Fe-9Cr-C model alloy", *18th International Conference on Environmental Degradation of Materials in Nuclear Power Systems – Water Reactors*, accepted 2017.
- Aydogan, E., S. A. Maloy, O. Anderoglu, C. Sun, J. G. Gigax, L. Shao, F. A. Garner, I. E. Anderson, and J. J. Lewandowski, 2017, "Effect of tube processing methods on microstructure, mechanical properties and irradiation response of 14YWT nanostructured ferritic alloy", *Acta Materialia*, 134 (2017): 116-127.

## Presentations

- Sun, C., "Emulating void swelling in stainless steels using ion irradiation", *18th International Conference on Environmental Degradation of Materials in Nuclear Power Systems-Water Reactors*, Portland, Oregon, August 2017.

## **17P11-007FP: Coupling of Modeling and Experiment to Develop Predictive Models of the Mechanical Behavior of Nuclear Fuels and Materials**

Katya Le Blanc<sup>1</sup> and Johanna Oxstrand<sup>1</sup>

### **General Project Description**

The objective of this project is to investigate the impact of high levels of automation in complex, safety critical systems and to demonstrate ways to enable optimal situation awareness for human operators in those systems. Specifically, this research will demonstrate how to design human-automation interaction to support optimal situation awareness, workload, and plant performance in a multi-unit small modular reactor.

### **Summary**

In FY 2016, INL researchers worked with NuScale personnel to design realistic scenarios for investigating operator performance under a variety of levels of automation. NuScale power has defined a preliminary human automation interaction design, where many of the plant's functions are fully automated, but some functions have an intermediate level of automation. INL researchers developed three interfaces for a boron dilution task with varying levels of automated support for the operator. The research worked with operations, engineering, and human factors staff at NuScale to design an experimental test for evaluating the effect of each of the three interfaces on human performance and situational awareness. One of the interfaces developed by the INL team has been adopted by NuScale as a template for all automation processes in the control room. This interface will be updated based on the results of this and future studies, resulting in a design that optimally supports operators in automated tasks.

INL researchers supported methodology development for the workload analysis NuScale conducted as part of their request for exemption to the Nuclear Regulatory Commission (NRC) staffing rule. We advised NuScale on how to perform and analyze several common workload measurement tools and provided several suggestions on how to develop criteria for characterization of acceptable workload. NuScale adopted several of our suggestions, including using workload at an existing operating plant as baseline criteria for workload comparison. NuScale noted that the discussions we had on workload methodology helped them develop their own expertise and enhanced their ability to successfully present their approach to NRC. The workload analysis is an important part of NuScale's request for exemption to the NRC staffing rule, which is one of the greatest challenges to licensing the NuScale design. Supporting the workload analysis directly supports NuScale's licensing efforts.

The researchers designed an experiment to test the dilution display's effect on performance, situational awareness, and workload. The researchers worked closely with NuScale operations engineers, human factors engineers, and simulator engineers to design scenarios and performance measures for the experiment. Testing of the experimental protocol and initial data collection began the week of June 13, 2016, and continued through September 20, 2016. Experimental data collection was slightly delayed due to challenges with the NuScale simulator and delays in their workload analysis for NRC that took priority over this work. Data collection will be complete by December 2016.

### **Benefits to DOE**

The results of this work support design of human automation interaction in the nuclear industry and will also inform use of advanced technologies that may be installed in existing light water reactors as part of control room upgrades and design of systems installed to support grid modernization and hybrid energy systems.

This work comprises scientifically rigorous research in close collaboration with industry. We meet several key challenges in conducting scientific research in full-scale simulator studies, thus advancing the science of human performance measurement in the nuclear context.



This work supports licensing of a small modular reactor and demonstrates an effective collaboration between INL and NuScale that benefits the entire nuclear industry and any industry that has human-automation interaction challenges:

- NuScale provides the platform, facilities, operational expertise, and operators for conducting high-quality research to understand human automation interaction
- Interfaces developed and tested in this work will be implemented in the NuScale control room and the concepts can be applied to related work in other Office of Nuclear Energy programs
- Support of NuScale's licensing directly supports the DOE mission of deploying a small modular reactor.

## Publications

The paper titled, "Measuring Workload: Consequences of Weightings when Combining NASA TLX Subscales," is in final preparation and will be submitted to *Human Factors*.

The researchers will prepare a paper summarizing the experimental results and will submit it to *Safety Science*.

## Presentations

Presented project to 2016 Nuclear Science and Technology Advisory committee on May 17, 2016.

## Interns and Postdocs

Intern: Rachael Hill.

Postdoc: Wei Zhang.

## Collaborations

University: University of Idaho.

Industry: NuScale.

## 17P11-014FP: The Influence of Irradiation on the Corrosion Kinetics and Hydrogen Pickup of Zirconium Alloys

Daniel Jadernas,<sup>1</sup> Arthur Motta<sup>16</sup>, Gary Was,<sup>1</sup> Mukesh Bachhav,<sup>1</sup> Evrard Lacroix,<sup>1</sup> Robert O'Brien<sup>1</sup>

### General Project Description

It is critical for the nuclear industry to understand the evolution of the properties of zirconium alloys during irradiation. One of the primary factors limiting the utilization of fuel rods is hydrogen pickup during oxidation. As a result of oxidation and hydrogen pickup, hydrides form and accumulate in cladding, causing embrittlement and limiting fuel lifetime. Proposed Nuclear Regulatory Commission (NRC) loss-of-coolant-accident (LOCA) criteria will be hydrogen-dependent (see Figure 1). The new rule allows less oxidation of the cladding during a LOCA as hydrogen content increases. The Electric Power Research Institute (EPRI) estimates that transitioning to the new regulatory requirements [1] will cost the U.S. nuclear industry \$100M. Other issues related to oxidation and hydrogen pickup in Zircaloy (Zry) include channel distortion in boiling water reactors (BWRs) that can lead to control blade binding, and recent BWR fuel-assembly structural failures in Asia and Europe that have potentially been traced to Zry components. In order to improve the performance of zirconium alloys in light water reactors (LWRs), this project seeks to first develop an understanding of the mechanisms governing oxidation and hydriding under irradiation in the reactor environment. Because the individual factors that can affect corrosion and hydriding are complex and can be convoluted, separate effects testing will be used to obtain a more fundamental understanding of this issue. Idaho National Laboratory, Penn State University, University of Michigan, and Westinghouse will use a combination of ion irradiation, autoclave exposure, and advanced characterization techniques to study the effect of irradiation on the corrosion kinetics of zirconium alloys. Ion irradiation has been shown to replicate the basic features of in-reactor irradiation that appear to affect most strongly corrosion behavior, including amorphization and dissolution of precipitates. This research will focus on separating the effects through which irradiation can affect corrosion, including irradiation-induced changes to the base-material microstructure and microchemistry, changes to water chemistry through radiolysis, and irradiation effects on diffusional transport through the oxide. Four types of experiments will be conducted in tailored environments using both Zry-2 and Zry-4 alloys. Advanced characterization techniques such as microbeam synchrotron (x-ray) diffraction, electron microscopy, and atom probe tomography will be used to study the microstructure of the protective oxide layer formed under different conditions and at different stages of the corrosion process to explain the mechanisms by which irradiation affects corrosion. These tools will also be used to benchmark the ion-irradiated microstructures against those known to be present in reactor-irradiated alloys.

An improved understanding of the hydrogen uptake mechanism and oxidation of zirconium will be used to improve the modeling and predictability of hydrogen-related issues affecting fuel such as LOCAs, reactivity-initiated accidents (RIA), channel and fuel-assembly distortion, hydrogen embrittlement and cracking, seismic performance, secondary fuel degradation, and dry-cask storage and transportation. This work is a free-standing component of an industry-led research framework (Mechanistic Understanding of Zirconium Corrosion Phase 3 [MUZIC-3]) that involves national and international nuclear laboratories, industry, and U.S. and international universities. In cooperation with other research groups, the data generated will be used to develop and validate models for better understanding the oxidation and hydrogen pickup mechanisms in zirconium based alloys. INL participation in a critical part of this program will increase INL's exposure and visibility to the nuclear industry and expand INL's network of research collaborators in the U.S. and internationally.

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<sup>16</sup> Penn State University

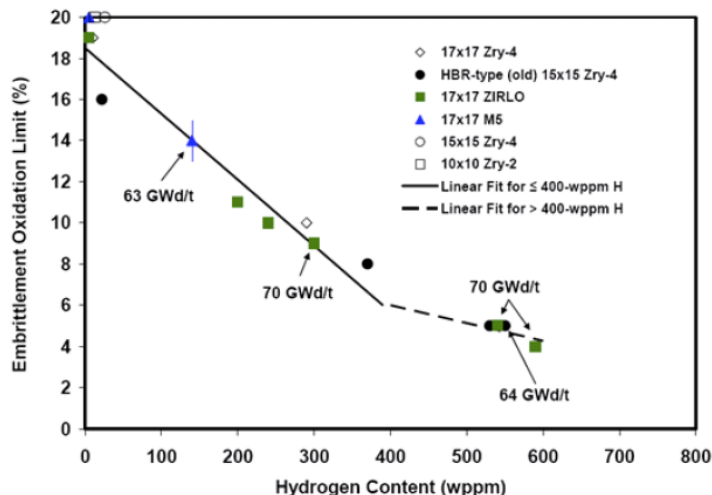


Figure 1. Ductile-to-brittle transition oxidation level (CP-ECR) as a function of pretest hydrogen content in cladding metal for as-fabricated, prehydrided, and high-burnup cladding materials [1].

## Summary

This out of cycle LDRD project started in the end of fiscal year 17 and the time has been used to acquire suitable material to use for the experiments in this project and characterize the material so that the baseline state of the materials are known before proceeding to perform further experiments. Zircaloy-2, Zircaloy-4 and ZIRLO type material have been acquired from Westinghouse and this material have been characterized using polarized light optical microscopy, scanning electron microscopy, focused ion beam sample preparation for transmission electron microscopy, atom probe tomography, combustion infrared detection, hot vacuum extraction, inert gas fusion and direct current plasma emission spectroscopy. These examinations have provided the grain size distribution, secondary phase size distribution and type, chemical composition, elemental distribution, defect and dislocation densities and distribution and crystallographic texture for the three materials. Further material characterization and data evaluations is planned before irradiation and autoclave experiments commences.

## Benefits to DOE

The research conducted in this project involves collaboration between the INL and some of the most renowned researchers in the field of irradiation damage of materials. It is also part of a bigger research effort and INL's participation in a critical part of this program will increase INL's exposure and visibility to the nuclear industry and expand INL's network of research collaborators in the U.S. and internationally.

## References

[1] U.S. NRC Draft Regulatory Guide DG-1263

## Interns and Postdocs

Intern: Evrard Lacroix

## Collaborations

University: Penn State University

## 17P11-018FP: Advanced Manufacturing of UO<sub>2</sub> Fuel Pellets with Radially and Axially Zoned Burnable Poisons and Hour-Glassing Control Features

Robert C. O'Brien,<sup>1</sup> Connie M. Hill,<sup>1</sup> Randall Scott,<sup>1</sup> Daniel Schwen,<sup>1</sup> Daniel Jadernas,<sup>1</sup> Raul Rebak,<sup>17</sup> Brian Jacques,<sup>15</sup> and James Tulenko<sup>2</sup>

### General Project Description

Gadolinia (Gd<sub>2</sub>O<sub>3</sub>)-doped UO<sub>2</sub> pellets are used widely across the light-water-reactor (LWR) industry to establish higher core fuel loadings and to help level the power of the reactor as a function of burnup on each loading. The bulk addition of gadolinia results in overall lower softening and melting temperatures, under that of bulk uranium dioxide (UO<sub>2</sub>). Bulk doped pellets are therefore challenged by their mechanical stability at operating temperatures and under irradiation, and have in practice been linked to pellet/cladding mechanical interaction (PCMI)-driven failures of fuel rods and assemblies through hour-glassing and hard-contact establishment with irradiated claddings [1]. The objective of this project is to evaluate and demonstrate advanced manufacturing (AM) techniques that can significantly improve the performance of gadolinia-doped nuclear fuels by constraining the gadolinia to outer-rim regions of pellets as a functional gradient material that 1) makes the equivalent power damping and 2) allows the hot pellet center to have a higher melting point than bulked doped pellets. Similarly, the project utilizes advanced modeling and simulation tools, specifically the Bison code coupled to benchmarked codes such as Monte Carlo N-Particle Transport Code (MCNP), to develop geometrical features on or within the pellet structure that aim to mitigate the hour-glassing behavior, for example, through the creation of an inverse hourglass structure. Neither of these approaches can be achieved with conventional manufacturing processes. Laser-additive manufacturing [2-4], stereo laser lithography (both referred to as 3D printing techniques) and spark plasma sintering [5] AM techniques show near-term viability to produce UO<sub>2</sub> structures of interest, and facilities are being commissioned and utilized at Idaho National Laboratory (INL) and collaborating institutions to support this study.

### Summary

At the inception of this project in June 2017, a parallel effort of modeling and simulation (M&S) and practical fabrication technique development was undertaken. Under the initial M&S activities, an MCNP analysis was done to determine whether or not PWR burnable poison fuels fabricated with Gadolinia on the outer rim of standard fuel pellets could achieve the same level of power damping as that of traditional pellets with 8 weight percent (wt%) Gd<sub>2</sub>O<sub>3</sub> [6] impregnated into the fuel as a homogenous bulk doping. Four compositions of interest were evaluated for a doped rim region within a pellet. Similarly, the equivalent thickness of pure Gd<sub>2</sub>O<sub>3</sub> that matches the neutronic behavior of traditional bulk doped UO<sub>2</sub> was found to be 0.3mm. Since pure Gd<sub>2</sub>O<sub>3</sub> coatings on UO<sub>2</sub> are likely to fracture and spall from the substrate under irradiation conditions, it is necessary to adopt a doped rim region to serve as a mechanically robust functional gradient transition to the bulk UO<sub>2</sub> pellet. See Table 1 for summary results. These results will be used in experimental pellet fabrication activities. In July 2017, the INL collaboration worked with the Laser Additive Manufacturing (LAM) vendor Optomec at the Materials and Fuels Complex to install and train the collaboration team members on operation of its model LENS-MR7 LAM machine. Initial training and geometric representations of doped pellets were fabricated using 316 stainless steel. The equipment is being adapted and work control is being finalized to begin operations with uranium oxide. A containment bag has been developed to contain the overspray of powder in the LAM apparatus. Work with Inert Incorporated of Amesbury MA has been initiated to co-develop a centrifugal sieve and powder re-circulator system for use with LAM. The aim of the technology development is to minimize the waste of materials in the LAM process and is especially important for fissile material handling and accountability. A CRADA and IDR are

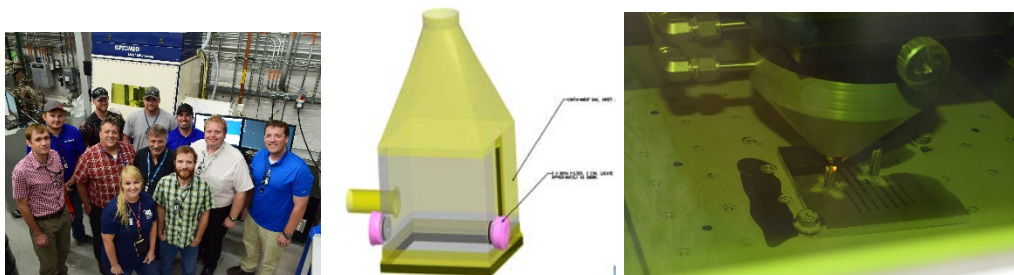
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<sup>17</sup> General Electric

being developed to facilitate this activity. This, activities will likely lead to licensable commercial technologies for the advanced manufacturing industry.

*Table 1. Equivalent rim thickness for various combinations of  $UO_2$  and  $Gd_2O_3$  applied on the rim of standard  $UO_2$  fuel material to achieve the equivalent of the nuclear reactivity performance in traditional burnable poison doped fuels.*

Doped $UO_2$ Pellet Composition	Equivalent Rim Thickness (cm)
Traditional (Bulk Doped) Gadolinia, $Gd_2O_3$ @ 8 wt.%	0.41 (full radius)
$UO_2$ Fuel, Rim Gadolinia, $Gd_2O_3$ @ 8 wt.%	0.369
$UO_2$ Fuel, Rim Gadolinia, $Gd_2O_3$ @ 15 wt.%	0.164
$UO_2$ Fuel, Rim Gadolinia, $Gd_2O_3$ @ 20 wt.%	0.113
$UO_2$ Fuel, Rim Gadolinium, $Gd_2O_3$ @ 100 wt.%	0.03



*Figure 1. Left, INL and Optomec staff with LAM machine following successful startup. Middle, initial prototype containment bag to be used inside the LAM machine enclosure to mitigate mass system contamination. Right, LAM processing that takes place inside of containment bag. Grey over-sprayed powder on substrate highlights the need for containment when processing nuclear materials.*

This project will continue in 2018 with the initial “3-D printing” of commercial type fuel pellets followed by experimental trials of functionally graded pellets. Scientific data that will be collected during these trials includes advanced spectral imaging and online elemental analysis to better understand the physical chemistry and elemental behavior during the processes.

## Benefits to DOE

This research will enable future improvements in LWR fuel performance and potentially further reduce the number of failed fuel rods during LWR operations. The DOE Nuclear Energy Advanced Modeling and Simulation Program and INL modeling and simulation tools will be used in support of specimen fabrication design, thereby demonstrating in practice some of the integral capabilities of these tools. The proposed project will nurture innovation for DOE and INL in advanced nuclear-fuel fabrication. Utilization of such specimens could establish the foundations for future advances in our understanding of fuel-performance phenomena. The project will also nurture advancement and innovation in industrial applications with potential technology-transfer opportunities at its completion. By working in collaboration with universities and industrial partners, the project leverages expertise, capabilities, and infrastructure to fast-track innovation in advanced manufacturing and nuclear-fuels development.

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## Presentations

- R. C. O’Brien, 2017, “Advanced Manufacturing of Nuclear Fuels & Materials” *Boise State University Advanced Manufacturing Meeting*, Boise, Idaho, 7<sup>th</sup> August 2017.

## Invention Disclosures, Patents, and Copyrights

- IDR Number 4521. “Advanced Manufacturing of Uranium Dioxide Fuel Pellets with radially and axially zoned burnable poisons and hour-glassing control features.”



## 17P11-022FP: Development of Nonlinear Eigenvalue Solvers in the Multiphysics Object Oriented Simulation Environment (MOOSE)

Fande Kong,<sup>1</sup> Yaqi Wan,<sup>1</sup> David Andrš,<sup>1</sup> Javier Ortensi,<sup>1</sup> and Cody Permann<sup>1</sup>

### General Project Description

This project develops fully integrated, new *nonlinear* eigenvalue solvers within the MOOSE framework to further the core capabilities of the MOOSE project. Eigenvalue problems arise in many physical simulations, such as solid mechanics and neutron transport. When modeling coupled multiphysics problems involving one of these physics types, a robust nonlinear eigenvalue-solution scheme is necessary for the efficiency of these simulations. While several numerical methods have been explored and experimented with over the past several years under different work packages, a fully integrated and robust solution method capable of handling a wide range of general nonlinear problems within the framework is not currently available. The eigenvalue problem is a methodological concern in neutron-transport physics that can be nonlinear with feedback. Existing nonlinear eigenvalue algorithms and their implementations consider problems that nonlinearly depend on the *eigenvalue* (referred to as nonlinear-in-eigenvalue) [1,2]. Solver techniques or strategies are not well established for problems that have a nonlinear dependence on the *eigenvector* (referred to as nonlinear-in-eigenvector). The proposed work fills this important gap. This work directly benefits the modeling and simulations efforts for the Transient Reactor Test Facility (TREAT) by enabling researchers to solve coupled thermal-nuclear problems with fast transients, which is a key characteristic of TREAT.

### Summary

A pluggable, fully integrated, user-friendly eigenvalue solution system has been developed and implemented within the MOOSE framework. The new system is able to solve several types of eigenvalue problems including standard linear, generalized linear, standard nonlinear and generalized nonlinear eigenvalue problems, and more importantly, nonlinear-in-eigenvector problems, which is not well established in the modeling and simulation community. We describe the new design and the new enhancements in detail as follows:

1. **Designed and implemented a unified eigenvalue system:** The old eigenvalue system in MOOSE was limited in both flexibility and capability. In the new eigenvalue system, both nonlinear and linear eigenvalue problems are handled in a unified interface and in a user-transparent way. Several linear eigenvalue solvers were added including Arnoldi, Krylov-Schur, and Jacobi-Davidson. This was done by leveraging the solution techniques from SLEPc [3]. The addition of these additional linear eigenvalue solvers enhances the solution capability of MOOSE for challenging *linear* eigenvalue problems.
2. **Implemented Nonlinear Inverse Power Iteration (NIPI):** The NIPI solver is based on SLEPc [3] and PETSc [4]. Inverse power iteration is a basic and well-understood algorithm for linear eigenvalue problems [5], and packages for these types of problems are widely available. However, an extension of the inverse power iteration for nonlinear-in-eigenvector problems is not well studied. In this work, a nonlinear version of the inverse power iteration was designed and implemented as an open-source contribution to SLEPc with a corresponding interface in MOOSE. This work provides the first open-source implementation for the NIPI approach, which is now widely available to the research community.
3. **Designed and implemented a Newton-based nonlinear eigenvalue solver (Newton):** The Newton eigenvalue solver is based on SLEPc[3] and PETSc[4]. While NIPI works well when the ratio of the minimum eigenvalue to the second smallest eigenvalue, (i.e. the dominant ratio), is sufficiently small, its performance degrades when the ratio between these two values increases. Thus, an acceleration technique is necessary for more challenging problems where the dominant ratio approaches the value one. The traditional Newton method [5] is redesigned in a creative way to accelerate the convergence of NIPI for nonlinear-in-

eigenvector problems. Compared with NIPI, Newton runs significantly faster for difficult multiphysics applications.

4. **Invented a Rayleigh-quotient constrained Newton (RQNewton):** Newton often works well, but sometimes fails to converge to the minimum eigenvalue or the fundamental mode. Instead, it may converge to the second smallest eigenvalue. Applications in neutronics usually require the fundamental mode. To overcome this difficulty, a Rayleigh-quotient constraint is applied to improve likelihood of obtaining the minimum eigenvalue. Independent applications have been used to verify the efficiency of the Rayleigh-quotient constrained Newton. This innovation improves the robustness of the Newton method greatly for certain classes of multiphysics problems.

## Benefits to DOE

By extending core MOOSE capabilities, the methods developed here make these new techniques available to every application that requires such capabilities. The implementation delivered in this project enables a superior solution for supporting the modeling and simulations of TREAT. Additionally, full core deterministic calculations for the ATR can be made more efficient through the application of these techniques while running with the mesh-refinement levels necessary to fully resolve the fuel meat and experiment details. These capabilities are of interest to ATR operations as well, and provide new capabilities to ATR LEU conversion work funded by DOE/NNSA through the INL Global Security and International Safeguards Division. Furthermore, it is anticipated that this work potentially permits further deployment of Rattlesnake-based multiphysics to other reactor-focused programs such as LWRS and ART. These techniques may also be applied to the solid mechanics capabilities within BISON and allow for development of new solid-mechanics tools for applications outside of fuel analysis. Finally, as noted earlier, this work can potentially benefit other MOOSE-based animals both within and external to the INL MOOSE biosphere.

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- Kong, F., Y. Wang, S. Schunert, C. J. Permann, D. Andrš, J. W. Peterson, R. C. Martineau, 2017, “A fully coupled two-level Schwarz preconditioner based on smoothed aggregation for the transient multigroup neutron diffusion equations”, *Numerical Linear Algebra with Applications*, 2017 (Revision).
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## 17P11-032FP: Production, Encapsulation and Process Optimization of Energy Producing Isotopes

Stephen G. Johnson,<sup>1</sup> Eric Clarke,<sup>1</sup> Kendall Wahlquist,<sup>1</sup> Jorge Navarro,<sup>1</sup> and Brian Gross<sup>1</sup>

### General Project Description

Several aspects of production, encapsulation and process optimization of energy producing isotopes were investigated using predominantly undergraduate student teams affiliated the Center for Space Nuclear Research located at the INL. Each team was led by one or more INL staff engineers or scientists. Specifically, the research centered on the following three areas: 1) modeling of isotope production in ATR using computational methods with Pu-238 used as an example isotope, 2) optimization of work flow for fueling and testing a power system device and 3) examining alternative materials for encapsulation of energy producing isotopes from a safety perspective.

### Summary

#### *Isotope production*

Plutonium is currently produced at the High Flux Isotope Reactor (HFIR) at Oak Ridge National Labs in Tennessee, but the production rate is too low to be viable for upcoming fuel demands. As a result, the Advanced Test Reactor (ATR) at Idaho National Labs (INL) has been proposed as the main <sup>238</sup>Pu production facility for the near future. This effort will reveal neutronic characteristics of the ATR, why it is a practical choice for plutonium production, and how to optimize production in the reactor based on neutronics calculations.

Two Monte Carlo codes were used to tally the neutrons, MCNP and SERPENT, which were used to characterize and optimize the neutrons for plutonium-238 production respectively. MCNP is a neutronics Monte Carlo code that was developed in the 1940s. Its intended purpose was to follow neutronics in critical bomb configurations, but it was eventually updated to include reactor physics calculations. As a result, it does have isotope tracking abilities using an internal code called CINDER, but this is not the most reliable method of tracking intricate isotope production. SERPENT is a continuous energy Monte Carlo reactor physics burnup calculation code. It was originally designed for tracking fuel depletion characteristics in reactor fuel using SCALE, so it is a better fit for tracking the isotopes of interest in the <sup>238</sup>Pu production process. Both MCNP and SERPENT are used for isotope tracking to determine the reliability of results.

#### *Optimization of work flow*

The objective of this research has been to investigate how INL can meet the challenges of ambitious future MMRTG campaigns. With regards to streamlining the fueling and testing process, two metrics are of primary interest. First, the time required to complete several RTGs should be minimized. This reduces the decay of Pu-238 fuel and therefore increases beginning-of-life power for the mission. Second, the cost of new equipment and personnel recommended to INL should be minimized. We have approached this problem according to the “Theory of Constraints”, which suggests that the throughput of a production system is typically limited by a relatively small number of constraints.

The software itself has been written in a combination of Matlab and Simulink using an add-on called “SimEvents.” It consists of a master Simulink model and numerous supporting Matlab scripts for plotting and optimization. Optimization is performed using two methods: simulated annealing and the genetic algorithm. The optimization problem is posed in two analogous forms and used to perform trade studies between the completion time of an MMRTG campaign and the cost of staff and equipment.

A sensitivity study of design parameters was also performed and is described in a separate document titled “Sensitivitystudy\_FinalVersion.docx”.

### ***Alternative materials for encapsulation of energy producing isotopes***

The objective was to investigate alternative materials to replace the carbon-carbon composite, known as Fine Weave Pierced Fabric (FWPF), currently used by NASA in their Multi-Mission Radioisotope Thermoelectric Generators (MMRTG). These MMRTGs are used as the power sources for nearly all of NASA's probes and rovers. The MMRTG produces its power using a thermocouple that utilizes the extreme thermal gradient found between the external environment and the decaying Plutonium-238 ( $^{238}\text{Pu}$ ) heat source. There are thirty two  $^{238}\text{Pu}$  pellets in each MMRTG and these are stored in pairs within eight composite housings known as the General Purpose Heat Sources, or GPHS.

During the research into cost reduction of the production, two additive manufacturing processes were found as viable production methods for the future. The first is Markforged's (Cambridge, MA) advanced 3D-Printing process, which utilizes a dual material jetting head 3D printer allowing for placement of continuous fibers within their composites. The second is Carbon, Inc.'s vat polymerization process. Their Continuous Liquid Interface Production (CLIP) and Digital Light Synthesis (DLS) processes enable them to produce composites out of the thermoplastic resins suggested in our PMC combinations. They are currently developing ways to implement a fiber reinforcement structure into these composites. As technology continues to advance, both of these processes could be options for the production of a FWPF alternative at much lower production cost and time.

### **Benefits to DOE**

The production of isotopes in a reactor is an ongoing DOE business line through both the Office of Science (SC) and the Office of Nuclear Energy (NE) and this work could be of interest to those programs going forward. There is the possibility that programmatic interest may result based on these efforts supported by LDRD this year.

### **Presentations**

There were three posters presented at the Summer 2017 session by the three teams.

### **Interns, Postdocs, and Staff support for Graduate Studies**

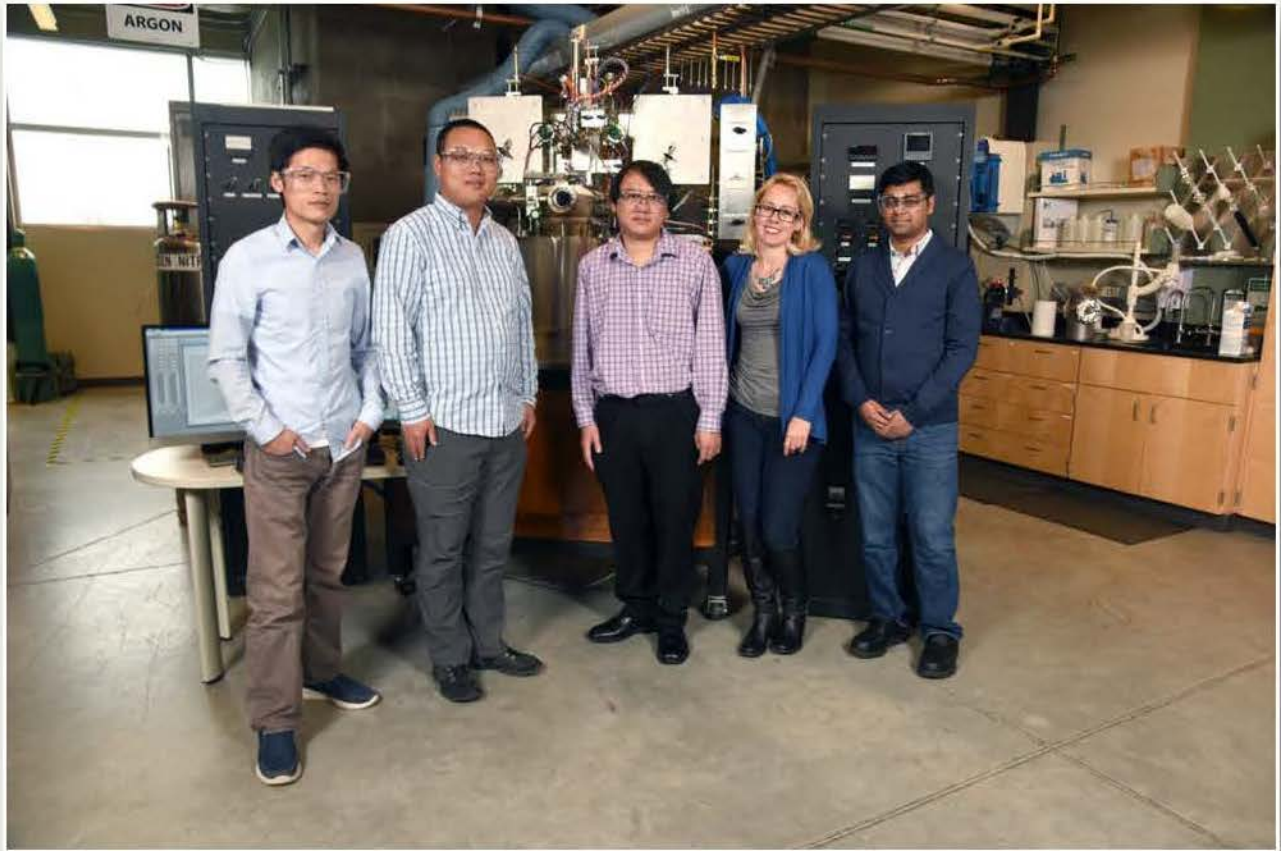
Interns: Lucas B. Beveridge, Dominik A. Fritz, Grace A. Marcantel, Ashoak N. Nagarajan, Joshua H. Rhodes, Jessica Berry, Justin Mansell, Jacob Quint, Meng-Jen Wang, Darrell Cheu, Lauara Hawkins, Syed Zameeruddin Mazhuruddin, and Matthew Wells.

### **Collaborations**

Universities: Idaho State University, Rensselaer Polytechnic Institute, Texas A&M University, Missouri University of Science and Technology, Colorado School of Mines, Purdue University, University of Nebraska-Lincoln, Virginia Institute of Technology, University of Southern California, and the University of Tulsa







# Enabling Clean Energy Deployment

- 15-039: Transient Modeling of Integrated Nuclear Energy Systems with Thermal Energy Storage and Component Aging and Preliminary Model Validation via Experiment
- 15-125: Phosphoranimines for Advanced Battery Applications
- 15-128: Microstructural Evolution and Mesoscale Coupled Flow-Reaction-Fracturing Processes in Organic Rich Nanoporous Shales
- 15-135: Dynamic Simulations for Large-Scale Electric Power Networks in a Real-Time Environment using Multiple RTDS
- 15-146: Tailoring the Kinetic Function of a Surface through Electronic Effects of Nanoscale Architecture
- 16-002: Advanced Carbon Feedstock Processing Using Ionic Liquids
- 16-176: Development of Direct Carbon Fuel Cells
- 16-187: Micro-Scale Technique to Evaluate Grain Boundary Cohesion of Irradiated Alloys
- 16-215: Electrochemical Manufacturing Processes
- 16P6-002FP: Kinetic-based Scale-Up Science for an Energy Efficient Route to Ethylene
- 17A1-007FP: High Performance Polymeric Membranes for Nano and Ultrafiltration Applications
- 17A1-055FP: Electro-Reduction of Metals in Supercritical Fluid-Room Temperature Ionic Liquids
- 17A1-166FP: Electrochemical Reduction of CO<sub>2</sub> Enriched in Switchable Polarity Solvents
- 17A1-173FP: Fractionation of Lignocellulosic Biomass with Switchable Polarity Solvents
- 17P11-001FP: Enabling Material Discovery for Waste Heat Recovery Systems using a Multimode Optical Sensor
- 17P11-030FP: CED—Investigation of Exciton Delocalization and Exciton Coherence in Chromophores and Acoustic Nanostructures



## 15-039: Transient Modeling of Integrated Nuclear Energy Systems with Thermal Energy Storage and Component Aging and Preliminary Model Validation via Experiment

Shannon M. Bragg-Sitton,<sup>1</sup> J. Michael Doster,<sup>3</sup> Stephen D. Terry,<sup>4</sup> Carol Smidts,<sup>18</sup> Qiao Wu,<sup>4</sup> Andrew Klein,<sup>4</sup> Charles Forsberg,<sup>6</sup> and Patrick McDaniel<sup>5</sup>

### General Project Description

Nuclear power systems could offset intermittent generation sources, such as wind and solar, via tight, behind-the-grid coupling in “hybrid energy systems” (HES). Diverting steam from electricity production to process steam, thermal storage, or other applications would support production of additional commodities, but will initiate a reactor transient due to the tight coupling. This research aims to develop the high-fidelity, experimentally validated simulation tools that are necessary to adequately characterize coupled system response and to optimize operational strategies for accomplishing transient maneuvers by leveraging expertise and previous research—including existing models and experimental data—within the National University Consortium partners. Research includes modeling of energy-storage systems integrated with nuclear systems, modeling of anticipated transient behavior and response of subsystems, conducting limited experiments and mining existing data to validate these models, and assessing the impact of aging and degradation of key components (e.g., valves) on system operation.

### Summary

This project leverages university partner expertise and access to previous research, with management and coordination provided by the INL PI. The overall scope focuses on transient modeling of integrated HES that would incorporate nuclear and renewable generators, electricity production, an industrial process, and energy storage. Preliminary investigation of advanced energy conversion systems that could be coupled with advanced reactor technologies as an evolutionary application for nuclear HES (NHES) was also included in FY-15 via MIT and UNM partners.

NCSU researchers developed several models that can now be incorporated into INL-developed tools for economic analysis of HES upon conversion to the Modelica modeling language. These include:

- Generalized integrated HES with sufficient detail for controls engineering to apportion energy and to evaluate system transients
- Integral PWR model that allows diversion of bypass steam to the thermal energy storage (TES) system while maintaining constant reactor power; possible connection points for the TES are upstream or downstream of the turbine control valve or from a tap off the low pressure turbine
- Several candidate TES systems have been modeled mathematically:
  - Sensible heat TES, where steam can support additional ancillary applications (e.g. a chiller)
  - Chilled water generation and storage (process or HVAC)
  - High pressure steam accumulators (primary reactor steam)
  - Low pressure steam accumulators (process steam)
  - Compressed air storage
- Various control strategies have been employed to determine control hierarchy and storage mix to produce the most economic system.

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<sup>18</sup> The Ohio State University

Operating an integrated, hybrid system introduces new duty cycles on system components due to maneuvers necessary to divert steam in response to the changing loads. Ohio State University (OhSU) researchers have designed and tested an OnLine Monitoring (OLM) system to track the impact of duty cycles on aging, control and reliability of the steam bypass and delivery system. The OLM design incorporates measurement and control components and alarm strategy. Research outcomes include:

- Created system models (structural and behavioral) of the secondary loop system for fault simulation using the Integrated System Failure Analysis (ISFA) method
- Simulated fault propagation paths and extraction of distinguishing features
- Demonstrated OLM capability to detect and diagnose faults tested; an example evaluation was performed for a Turbine Bypass Valve using degradation modeling that accounts for natural aging and usage.

OhSU will deliver the final OLM design with a database of the most effective signals (sensors) for detecting possible component faults to INL.

OhSU also demonstrated Distributed Test Facility (DTF) capabilities during the course of the research. The DTF assembles geo-distributed software and hardware components into a prototype cyber-physical control system, allowing one to test multiple “integrated” system configurations using existing facilities across multiple laboratories, universities, etc. Key accomplishments include:

- Development of DTF interface that manages and controls components, applications, and users
- Demonstration with a nuclear plant simulator and steam generator hardware-in-the-loop
- Reliability and performance of digital systems tested in possible operational environments
- OLM demonstration using the DTF, allowing for verification of the OLM system design.

As a part of the LDRD research NCSU also developed a model of the OrSU Multi-Application Light Water Reactor (MASLWR) scaled thermal hydraulic test facility for benchmarking studies. MASLWR was an integral test facility at OrSU, representing a 1/3 height scale NuScale model and capable of simulating steady state and accident transients (the facility has since been dismantled and reconfigured for testing of the current NuScale design). OrSU researchers mined data from the 2010 IAEA testing in MASLWR to provide data for HES model validation and provided a RELAP5-3D model for running simulations that can be used to valid current models. Key OrSU accomplishments include:

- Full power scaling parameters developed for MASLWR
- Modified/improved benchmark for the MASLWR facility RELAP5-3D model for use in load following studies.

The new set of scaling parameters gave reasonable values for a single-phase solution, but they cannot be extended to two-phase conditions due to limited fidelity in the experimental system (i.e. core design). Hence, the new analysis results for MASLWR are useful, but limited in application. Future extension to two-phase scaling analysis using data from NuScale may extend the model applicability.

### Benefits to DOE

Integrated, non-emitting energy systems could play a major role in future U.S. energy planning and development. This project leverages INL and university expertise to build an enhanced dynamic modeling capability for energy system design and development, supporting objectives within DOE-NE and DOE Energy Efficiency and Renewable Energy; developed methods will also be used to evaluate the probability of control system stability. Ohio State University’s advanced digital alarm system will allow real-time data processing from installed sensors

in future hardware applications to minimize the potential of component failure, and the DTF work will provide a basis for future multi-laboratory, integrated testing of simulation models and hardware to further advance NHES concepts. In the future, work could influence approaches used within the DOE Office of Electricity for energy-system planning. Follow-on work to this LDRD (modeling and experimental) could enable more rapid adoption of the proposed NHES technology by industry.

## Publications

- Frick, K., C.T. Misenheimer, J.M. Doster, S.D. Terry, and Bragg-Sitton, 2017, “TES Configurations for Small Modular Reactor Load Shedding,” *Nuclear Technology*, submitted September 2017.
- Guo, Q., M. Pietrykowski, R. Aggarwal, C. Liu, and C. Smidts, “A Distributed Test Facility for Cyber-Physical Systems: Fundamental Principles,” *IEEE Transactions on Systems, Man, and Cybernetics: Systems*, to be submitted.
- Misenheimer, C. and S. D. Terry, 2017, “Modeling Hybrid Nuclear Systems with Chilled-Water Storage,” *ASME Journal of Energy Resources and Technology*, Vol. 139, No. 1, pp. 012002-1 – 012002-9, January 2017.
- Li, H., X. Diao, X. Li, B. Li, and C. Smidts, 2017, “Fault Propagation and Effects Analysis for Designing an Online Monitoring System for the Secondary Loop of a Nuclear Power Plant Part of a Hybrid Energy System,” *selected for possible inclusion into a special issue of Nuclear Technology*, 2017.

## Presentations

- Doster, J. M. and K. L. Frick, 2016, “Coupling of Thermal Energy Storage with Small Modular Reactors,” *Transactions of the American Nuclear Society*, Winter Meeting, Las Vegas, Nevada, November 2016.
- Frick, K. and J. M. Doster, 2016, “Design of a Thermal Energy Storage System for SMRs,” *Transactions of the American Nuclear Society*, Annual Meeting, New Orleans, Louisiana, June 2016.
- Frick, K., J.M. Doster, and S. Bragg-Sitton, 2017, “Control Strategies for Coupling Thermal Energy Storage Systems with Small Modular Reactors,” *Transactions of the American Nuclear Society*, Annual Meeting, San Francisco, CA, June 2017.
- Guo, Q., M. Pietrykowski, and C. Smidts, 2015, “Dynamic Data Transmission Frequency Decision for Distributed Control Systems,” *NPIC-HMIT 2015*, Charlotte, North Carolina, February 23-26, 2015.
- Hoover,\* K., Q. Wu, and S. Bragg-Sitton, 2016, “SMR Re-Scaling and Modeling for Load Following Studies,” *Transactions of the American Nuclear Society*, Las Vegas, Nevada, November 2016.
- Ibekwe, R. T. and C. W. Forsberg, 2015, “Firebrick Resistance-Heated Energy Storage: Existing Technology Base,” *Transactions of the American Nuclear Society*, Winter Meeting, Washington D.C., November 8-12, 2015.
- Li, H., S. Bragg-Sitton, and C. Smidts, 2016, “Failure Diagnosis of the Holdup Tank System via ISFA Technique,” *Transactions of the American Nuclear Society*, Winter Meeting, Las Vegas, Nevada, November 2016.
- Li, H., X. Diao, X. Li, B. Li, and C. Smidts, 2017, “Fault Propagation and Effects Analysis for Designing an Online Monitoring System for the Secondary Loop of a Nuclear Power Plant Part of a Hybrid Energy System,” *International Topical Meeting on NPIC & HMIT 2017*, San Francisco, California, June 11-15, 2017.
- Mikkelsen, D., C., Chang, S. M. Cetiner, A. L. Qualls, J. M. Doster, and T. N. Dinh, 2015, “Small Modular Reactor Modeling Using Modelica for Nuclear-Renewable Hybrid Energy Systems Applications,” *Transactions of the American Nuclear Society*, Winter Meeting, Washington, D.C., November 8-12, 2015.
- Misenheimer, C., S. Terry, J.M. Doster, and S.M. Bragg-Sitton, 2017, “Analysis of a Nuclear Hybrid Energy System using Absorption Chillers and Stratified Chilled-Water Storage with an mPower Reactor,” *Transactions of the American Nuclear Society*, Annual Meeting, San Francisco, CA, June 2017.

- Schneider, E. and C. W. Forsberg, 2015, “Variable Electricity from Base-Load Nuclear Power Plants Using Stored Heat,” *Proceedings of International Congress on Advanced Nuclear Power Plants*, Nice, France, May 3-6, 2015.
- Stack D. C., 2015, “Improving Nuclear System Economics Using Firebrick Resistance-Heated Energy Storage (FIRES),” *Transactions of the American Nuclear Society*, Annual Meeting, San Antonio, Texas, June 7-11, 2015.
- Stack, D. C., 2015, “Impact of Firebrick Resistance-Heated Energy Storage (FIRES) on Electricity Prices in a Nuclear Renewable Grid,” *Transactions of the American Nuclear Society* Winter Meeting, Washington D.C., November 8-12, 2015.
- Teeter, L., F. Teng, W. Marcum, J. Kruzic, M. Anderson, and J. Tucker, 2015, “Supercritical Carbon Dioxide System for Materials Corrosion Testing,” presentation at *Minerals, Metals & Materials Society Annual Meeting*, Orlando, Florida, March 2015.
- Zhu, M., R. Aggarwal, S. Bragg-Sitton, and C. Smidts, 2016, “Effect of Aging and Demand for Reliability Analysis of Degrading Components,” *Transactions of the American Nuclear Society*, Winter Meeting, Las Vegas, Nevada, November 2016.

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- C.T. Misenheimer, *Modeling Chilled-Water Storage System Components for Coupling to a Small Modular Reactor in a Nuclear Hybrid Energy System*, PhD Dissertation, Department of Mechanical Engineering, North Carolina State University, July 2017.
- M.T. Daniels, *Integration of Large-Scale Steam Accumulators for Energy Storage in Nuclear Hybrid Energy Systems*, MS Thesis, Department of Nuclear Engineering, North Carolina State University, August 2017.
- K. Hoover, *SMR Full-Power Scaling Analysis and Numerical Simulations for Nuclear Hybrid Energy System Testing*, Master of Science Thesis, Department of Nuclear Engineering, Oregon State University, December 2016.
- K. Frick, *Coupling and Design of a Thermal Energy Storage System for Small Modular Reactors*, MS Thesis, Department of Nuclear Engineering, North Carolina State University, August 2016.
- M. Zhu, *Design of an Online Monitoring System for Degrading Hardware Components Using Failure Modes and Effects Analysis*, Undergraduate Honors Thesis, Department of Mechanical and Aerospace Engineering, The Ohio State University, Ohio, April 2016.
- A. Odeniyi, *Hybridization of a Gas Turbine for Compressed Air Energy Storage*, Department of Mechanical & Aerospace Engineering, North Carolina State University, July 2016.
- Q. Guo, *A Distributed Test Facility for Cyber-Physical Systems*, PhD Dissertation, Department of Mechanical and Aerospace Engineering, The Ohio State University, Columbus, Ohio, August 2015.
- J. Nickels, *Optimization of Turbine and Heat Exchanger Stages For the Expansion Process of a Compressed Air Energy Storage System*, Department of Mechanical & Aerospace Engineering, North Carolina State University, 2015.

### Interns, Postdocs, and Staff

Interns: Daniel Mikkelson, Corey Misenheimer, Konor Frick, John Nickels, Adefolaoluwami Odeniyi,

M. Tucker Daniels, Qingti Guo, Cheng Liu, Michael Pietrykowski, PhD, Huijuan Li, Rachit Aggarwal, Muzhi Zhu, Bobak Rashidnia, Jonathon Huang, Edillower Wang, Kyle Hoover, Lucas Teeter, BenAdam, Marco Teeter, Bjorn Westmen, Daniel Stack, Nima Fathi, and David Weitzel

Postdoc: Xiaoxu Diao

## Collaborations

Universities: North Carolina State University, Ohio State University, Oregon State University, Massachusetts Institute of Technology, and the University of New Mexico

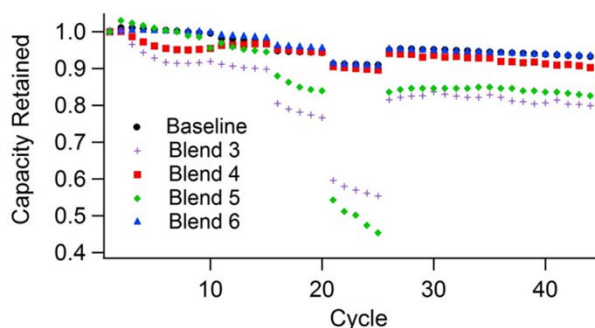
## 15-125: Phosphoranimines for Advanced Battery Applications

Eric Dufek,<sup>1</sup> John Klaehn,<sup>1</sup> Josh McNally,<sup>1</sup> Harry Rollins,<sup>1</sup> Kevin Gering<sup>1</sup>

### General Project Description

Organic carbonates are the principal solvent component in electrolytes for Li-ion batteries (LIBs) and for Li metal batteries (LMBs). For most applications, these compounds are effective, yet they suffer at high voltages, and there are questions regarding their safety and long-term stability. At relatively low temperatures, carbonate electrolytes and the primary salt in LIBs, lithium hexafluorophosphate (LiPF<sub>6</sub>), start to break down and form products which impact the performance of other materials in the battery. The ability to maintain performance for a wide range of applications thus relies on components which minimize degradation and improve the overall safety of the battery. In addition to performance improvement, there is a need to understand performance and create toolsets that allow better understanding of degradation. The work performed thus far under “Phosphoranimines for Advanced Battery Applications” has focused on routes to enhance performance and to identify the scientific shortcoming of different electrolyte blends.

### Summary



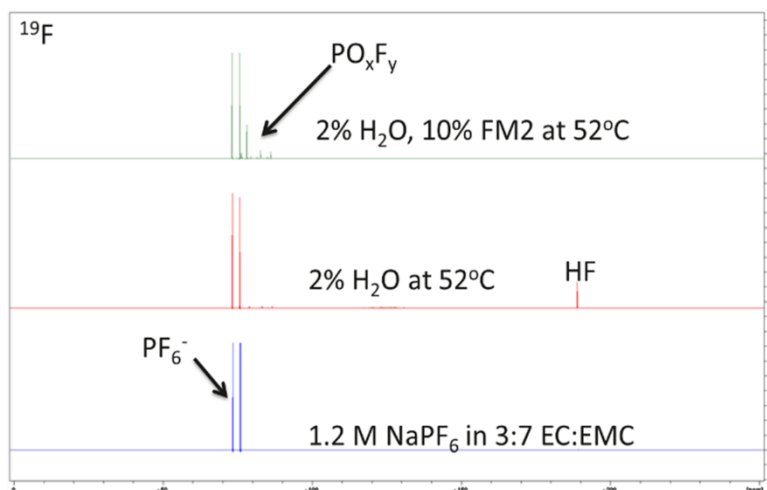
*Figure 1: Performance characterization between baseline and phosphoranimine blends of 9-20% which showed performance on par with standard electrolytes. All phosphoranimine blends increased safety through elevated flashpoints and decomposition temperatures.*

Following on success in FY-15 and FY-16, FY-17 activities have continued to explore the use of phosphoranimines as battery electrolytes and on understanding fade mechanisms which are related to electrolytes. Previously published work relating to the use of phosphoranimines showed that it was possible to attain performance on par with standard battery electrolyte while increasing the overall safety of the electrolyte (Figure 1). This work was further advanced and published in work which detailed the synthesis of novel ionic liquids which display a high degree of positive charge delocalization on the phosphoranimine backbone. This delocalization is seen as crucial to improving the overall stability of the potential electrolytes while maintaining safety enhancing features associated with the Lewis base nature of the P=N unit. The other benefit of the ionic liquids is that they provide the opportunity to selectively include low concentrations of crucial anions in the electrolyte composition which have been shown to aid in the overall deposit morphology and performance for LMBs. The ionic liquids have been found to have better conductivity and viscosity and provide more flexibility when blending electrolytes as evidenced by data obtained using the Advanced Electrolyte Model.

In addition to understanding the performance in battery systems, research has continued looking at the chemical stability of the phosphoranimines and other phosphazenes. This work is geared toward understanding degradation



pathways and has involved collaboration with Boise State University (Figure 2). The premise of the work is that it is possible to follow the degradation of the hexafluorophosphate using nuclear magnetic resonance (NMR) spectroscopy. This line of research has shown that the anion degradation is altered by alkali metals (Li or Na) in the electrolyte and by the presence of a phosphazene/phosphoranimine. Understanding this degradation is key to improving safety, durability and reliability of advanced batteries.



*Figure 2: Comparison of NMR data showing the degradation products of battery electrolytes containing phosphazenes (FM2) after exposure to water and elevated temperatures. The phosphazenes inhibited hydrofluoric acid formation thus improving battery performance.*

Combined the work related to phosphoranimines has generated two peer reviewed publications, one patent, a second patent application and an invention disclosure. The work has also led to multiple presentations at national/international meetings and currently a book chapter has been accepted and multiple manuscripts are in varying degrees of preparation.

## Benefits to DOE

Battery manufacturers, DOE, and other government entities such as the Department of Defense have signaled significant recent interest in new classes of electrolytes and electrolyte additives that improve the safety and performance of LIB and LMB chemistries. Improving battery performance is a key concern and a necessity for increasing electrification of the transportation sector in the United States. This move, which is a key focus of DOE, will decrease demand on foreign energy sources and reduce carbon emissions. From a military perspective, interest in safer electrolytes is tied directly to keeping soldiers and other military assets safe. Recent discussions with members from the automotive and general battery industries have highlighted the need to more thoroughly validate electrolyte chemistries prior to inclusion in the manufacturing process for batteries. Currently, the deployment process is impeded by the enormous quantity of new electrolyte possibilities and a desire by researchers and inventors to see their contributions succeed. A major focus of industry interest is the ability to perform standardized, high-quality validation that is directly tied to performance-driven metrics. Current research provides a novel electrolyte additive that deviates from the purely carbonate-based line of thinking, which is an approach that DOE is interested in. This project also directly looks at metrics to understand scientific needs for improving battery performance directly in line with the scientific mission of DOE.



## Publications

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- Klaehn, J. R., H.W. Rollins, J.S. McNally, N. Arulsamy, E.J. Dufek, 2017 “Phosphoranimines containing cationic N-imidazolium moieties” *Inorganica Chimica Acta* 466, pp. 254-265.
- Xiong, H., E.J. Dufek, K.L. Gering, 2017, “Batteries-Materials for Rechargeable Lithium-ion Batteries”, accepted book chapter, part of Comprehensive Energy Systems. – Listed in *STIMS* under Title “Batteries”

## Presentations

- Dufek, E. J., J. R. Klaehn, J. S. McNally, and H.W. Rollins, 2016, “Phosphoranimine Electrolytes for Alkali Ion Batteries,” *18<sup>th</sup> International Meeting on Lithium Batteries*, June 2016.
- Dufek, E. J., J. R. Klaehn, J. S. McNally, and H. W. Rollins, 2015, “Phosphorus-containing electrolytes – Expansion to include phosphoranimines for Li-ion Batteries,” *228<sup>th</sup> Electrochemical Society Meeting*, Phoenix, Arizona, October 2015.
- Parrish, R., 2015, “Electrolyte Performance for Na-ion Batteries,” *2015 Northwest Regional Meeting of the American Chemical Society* (support for hosting a SULI intern from Boise State University).
- Klaehn, J.R., McNally, J.S., Arulsamy, N., Rollins, H.W., Dufek, E.J., 2017 “Cationic N-Phosphoranimine Ionic Liquids” *253<sup>rd</sup> American Chemical Society Meeting*, San Francisco, CA, April 2017
- McNally, J.S., Klaehn, J.R., Dufek, E.J., Rollins, H.W., Harrup, M.K., 2015 “Computational studies of phosphoranimine electrolytes for Li systems” *249<sup>th</sup> American Chemical Society Meeting*, Denver, CO, March 2015
- Smith, K, Parrish, R., Barnes, P., Savva, A. Karsann, D., Deng, C., Dufek, E.J. Xiong H., 2017, “Interactions of Nanostructured TiO<sub>2</sub> with Nonaqueous Electrolytes for Na-ion Batteries” *232<sup>nd</sup> Meeting of the Electrochemical Society*, National Harbor, MD, Oct. 2017

## Invention Disclosures, Patents, and Copyrights

- BA-892, “Using Hybrid Arrangement of Li-ion and Na-ion Cells to Achieve Better Power Performance in Batteries.”
- BA-846, “Phosphoranimine Compounds, Electrolyte Solutions including a Phosphoranimine Compound, and Energy Storage Device including Same,” Patent Application No. 14/817,511; August 8, 2015.
- Postdocs: Birendra Adhikari and Joshua S. McNally

## Collaborations

University: University of Connecticut

## 15-128: Microstructural Evolution and Mesoscale Coupled Flow-Reaction-Fracturing Processes in Organic Rich Nanoporous Shales

Hai Huang,<sup>1</sup> Earl Mattson,<sup>1</sup> Travis McLing,<sup>1</sup> Darryl Butt,<sup>19</sup> Milind Deo,<sup>1</sup> and Paul Leonard<sup>20</sup>

### General Project Description

This project brings together a multi-institutional, interdisciplinary team of computational geoscientists, experimentalists, and material scientists in a focused effort to better understand the fundamental physics that controls the behaviors of organic-rich nanoporous shales and the fluids within them. The project coordinates an array of state-of-the-art characterization and imaging tools, including x-ray, SEM, TEM, FIB-SEM, combined with nano-indentation testing, to characterize and image the evolutions of the microstructures of nanoporous shales in detail and at the highest possible resolution. The computational component of the proposed project—mesoscale models of coupled diffusion-reaction-fracturing processes—aims to develop multiphysics models that will provide physics-based predictions of microstructure evolutions in the shales induced by changes of fluid chemical compositions, temperature, and pore pressure.

### Summary

During FY-17, a number of important research milestones, and critical experimental and modeling capabilities, impactful research results were achieved:

1. The modeling team successfully applied a reactive force field molecular dynamics model to successfully build realistic kerogen cross-linked polymeric molecule models, which revealed great amount of sub-nanometer porosities that could potentially transform our perception of in-place resource estimates the fundamental understandings of transport mechanisms in shales. Further, the modeling team was also able to characterize the polar/nonpolar/hydrogen-bonding solvent-induced swelling of kerogen where the kerogen swelling may result in stresses that are sufficient to generate additional fractures in nanoporous shales.
2. The experimental team at University of Utah successfully milled our micron size pillars from our shale samples using focused ion beam (FIB) milling technique and then successfully crushed these micro-pillars to understand the failure mechanisms of shales at the microscopic scale.

### Benefits to DOE

Research into areas such as microstructural changes of nanostructured organic-rich shales, coupled with fluid flow and volume changing/stress generating processes such as chemical transformations, swelling/shrinking, sorption/desorption and thermal expansion/contraction is of strategic importance to the nation's energy security and environmental sustainability, and these are basic science areas that promise new scientific discoveries with high economic and societal impact. The proposed research has important implications for sustainable and environmentally friendly recovery of shale gas and oil, geological storage of CO<sub>2</sub> in depleted shales, and underground storage of nuclear and other hazardous wastes

### Publications

Xia, Y., J. Goral, H. Huang, I. Miskovic, P. Meakin, and M. Deo, 2017 “Many-body dissipative particle dynamics modeling of fluid flow in fine-grained nanoporous shales”. *Physics of Fluids*, 2017, 29(5).

<sup>19</sup> University of Utah

<sup>20</sup> Pioneer Natural Resources

Zhou, J., H. Huang, J. McLennan, P. Meakin, and M. Deo, 2017, “A Dual-Lattice Discrete Element Model to Understand Hydraulic Fracturing in Naturally Fractured System”. *Hydraulic Fracturing Journal*, 2017, 4(2).

Pathak, M, H. Kweon, M. Deo and H. Huang, 2017, “Kergoen Swelling and Confinement: Its implication on Fluid Thermodynamic properties in Shales”, *Nature: Scientific Reports*, 2017

Pawar, G., P. Meakin, and H. Huang, 2017, “Reactive Molecular Dynamics Simulation of Kerogen Thermal Maturation and Crosslinking Pathways”, *Energy and Fuels*, 2017, 31(11). Manuscripts in preparation and ready for submission during FY-17

Pawar, G., P. Meakin, and H. Huang, 2017, “Evaluation of the Adequacy of the General-Purpose DREIDING Force Field for Simulation of Kerogens”, *Energy and Fuels*, 2017 (ready to submit)

Pawar, G., P. Meakin, and H. Huang, 2017, “Solvent induced swelling of kerogens: A molecular dynamics and thermodynamic integration approach”, *Nature: Scientific reports*, 2017 (in preparation)

### **Presentations**

Pawar, G. and H. Huang, 2017, “An atomistic investigation of hydrocarbon behavior confined in kerogen nanopores”, AIChE annual meeting 2017, Minneapolis, MN, Oct 30–Nov 3, 2017

Pawar, G. and H. Huang, 2017,” Modeling adsorption and transport processes in kerogen”, AIChE annual meeting 2017, Minneapolis, MN, Oct 30–Nov 3, 2017

### **Interns, Postdocs, Staff**

Interns: Jan Goral.

Postdocs: Gorakh Pawar and Jing Zhou.

### **Collaborations**

Universities: University of Utah.

Industry: Pioneer Natural Resources.

## 15-135: Dynamic Simulations for Large-Scale Electric Power Networks in a Real-Time Environment using Multiple RTDS

Manish Mohanpurkar,<sup>1</sup> Rob Hovsopian,<sup>1</sup> and Siddharth Suryanarayanan<sup>1</sup>

### General Project Description

This LDRD aims to establish a vendor-neutral distributed real-time simulation (RTS) platform to utilize geographically dispersed power-system assets by interconnection of real-time simulators over a wide area network. This connectivity will aid in conducting dynamic and transient analysis of large and complex power systems in real-time. It will also help to bridge the existing gaps in modeling and simulation of newer hardware such as power converters with an operational resolution in the seconds-to-minutes time scale. The project will also serve as a test bed to evaluate the performance, efficiency, and effectiveness of these power devices with their integration in geographically distributed test power systems. This enabled characterization of the devices under real-world operating conditions. Challenges in developing decoupled power system models that can be distributed and simulated on multiple real-time simulators in synchronism from multiple vendors across long distances are addressed. Prediction of transients (microseconds to seconds) under increased proliferation of distributed renewable energy sources at the regional and national level was addressed.

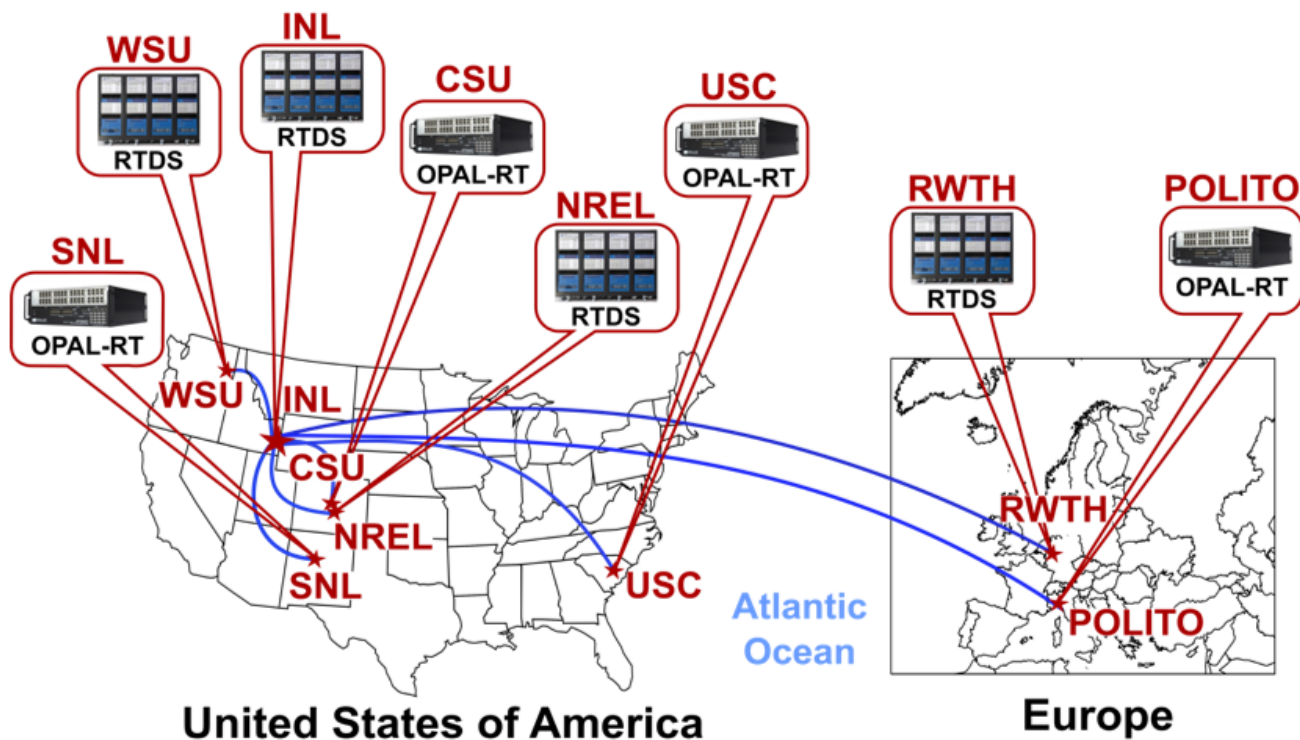


Figure 7: Distributed large scale power system simulation using RT-SuperLab

### Summary

From the beginning, the focus has been on data latency mitigation by development of prediction-correction techniques in geographically distributed RTS. To this end, a linear predictor has been developed for transmission-distribution real-time co-simulation. Success with the first-of-its-kind distributed RTS between INL and National Renewable Energy Laboratory (NREL) has enabled to advance the power-hardware-in-the-loop (PHIL)

experimental setup spatially. Main challenge associated with geographically distributed RTS is to ensure simulation fidelity of the same degree as in the case when the entire simulation is performed at the same location. Simulation fidelity in geographically distributed RTS is investigated and an empirical characterization is provided in this paper. Fidelity degradation caused by different values of time delay and sending rate of data exchange between two digital real-time simulators is presented. Two methods for representation of interface quantities in co-simulation interface algorithms are developed and published.

As a part of this LDRD, distributed RTS has been successfully conducted on a global scale between INL and its partners, NREL, University of South Carolina (USC), Colorado State University (CSU), Rheinisch-Westfälische Technische Hochschule (RWTH) Aachen University in Germany, Politecnico di Torino University in Italy as shown in Figure 1. In one simulation scenario, reactive power compensation in the test bed system by application of controller-hardware-in-the-loop (CHIL) has been successfully integrated in distributed RTS between INL and USC. Simulation results show that the power hardware mitigates the reactive power losses in the system once a control signal is actuated. In the same scenario, high voltage direct current link had been simultaneously simulated between INL and RWTH that resulted in a successful large-scale multi-lab simulation setup. New data communication optimization techniques in collaboration with RWTH Aachen University are under development to co-simulate power system assets from Sandia National Laboratory (SNL) and Washington State University (WSU). These capabilities have further advanced the research on addressing data latencies to improve simulation fidelity and also enable local and geographically distributed RTS using PHIL and CHIL, electrical/thermal/mechanical subsystem co-simulation at different computation time steps. These research collaborations will result in development of power grid network equivalence techniques on geographically distributed test systems. This research will culminate in the development of a plug and play distributed power system RTS testbed for rapid integration and testing of distributed geographically power hardware for dynamic and transient simulation studies. This LDRD has resulted in over 10 peer reviewed conference and journal publications. Many program activities under EERE such as FCTO, VTO, WPTO, WETO and grid modernization has derived benefits from this multi-lab connectivity. On 26<sup>th</sup> September 2017, LDRD will demonstrate the first-of-its-kind geographically distributed real-time simulations leveraging DOE and academics with a total of eight participants as mentioned above.

### Benefits to DOE

The project enables assessment of large-scale deployment of distributed renewable energy and smart-grid technologies for safe integration with the existing electric grid. Simulation of cascading failures in the next generation of interconnected power grids can be studied. This is achieved through both high-fidelity RTS and testing in real-world conditions. It is further achieved by using resources available through collaborations and interconnectivity between geographically distributed experimental facilities.

### Publications

- M. Mohanpurkar, M. Panwar, S. Chanda, M. Stevic, R. Hovsopian, V. Gevorgian, S. Suryanarayanan, and A. Monti, "Distributed real-time simulations for electric power engineering," *Cyber-physical social systems and constructs in electric power engineering*, Pages 451-486, *The Institution of Engineering and Technology (IET)*, London, UK (October 2016)
- Liu, R., M. Mohanpurkar, M. Panwar, R. Hovsopian, A. Srivastava, and S. Suryanarayanan, 2017, "Geographically distributed real-time digital simulations using linear prediction," *International Journal of Electrical Power & Energy Systems*, Volume 84, January 2017, Pages 308-317, ISSN 0142-0615
- Panwar, M., S. Suryanarayanan, and R. Hovsopian, 2017, "A multi-criteria decision analysis-based approach for dispatch of electric microgrids," *International Journal of Electrical Power & Energy Systems* 88, Pages 99-107, 2017.

- Luo, Y., M. Panwar, M. Mohanpurkar, and R. Hovsopian, 2016, "Real Time Optimal Control of Supercapacitor Operation for Frequency Response," *2016 IEEE Power and Energy Society General Meeting (PESGM)*, Boston, Massachusetts, pp. 1–5, 2016.
- Chanda, S., M. Mohanpurkar, R. Hovsopian, and A. Srivastava, 2016, "Quantifying Power Distribution System Resiliency Using Code Based Metric," *IEEE International Conference on Power Electronics, Drives and Energy Systems (PEDES)*, pp. 6, December 14-17, 2016.
- Md Hossain, R., Md. K. Hossain, Md. A.Hasan, L. Yusheng, and R. Hovsopian, 2017, "Synchronous Generator Stabilization by Thyristor Controlled Supercapacitor Energy Storage System," *SoutheastCon*, 2017, Charlotte NC, pp. 1-6.
- Osorio, J., R. Hovsopian, and J. Ordonez, 2016, "Dynamic Analysis of Concentrated Solar Supercritical CO<sub>2</sub>-based Power Generation Closed-Loop Cycle," *Applied Thermal Engineering*, 93.C (2016): n. pag. Web. doi:10.1016/j.applthermaleng.2015.10.039.
- Stevic, M., M. Panwar, M. Mohanpurkar, R. Hovsopian, and A. Monti, 2017, "Empirical Study of Simulation Fidelity in Geographically Distributed Real-Time Simulations," *North American Power Symposium 2017*, pp. 1-6, under print.
- Stevic, S., V. Tuyen, M. Mohanpurkar, C. Edrington, and R. Hovsopian, "Real-time Co-simulation of Advanced Power Electronics Inverters for Studying Grid Integration of Renewable Energy Systems," *Applied Power Electronics Conference (APEC) 2018*, pp. 1-5, under review.
- Luo, Y., S. Srivastava, M. Mohanpurkar, S. Stevic, and R. Hovsopian, "Real Time Impact control in Pulsed Power load For Shipboard Power Systems," *IET Power Electronics*, pp. 1-12, under review.

## Presentations

- Mohanpurkar, M., 2015, "Distributed Real Time Simulations Using RTDS®," *RTDS User General Meeting*, San Francisco, California, May 5 through 7, 2015.
- Hovsopian, R., 2015, "Laboratory of the Future," for the project titled, *Dynamic Modeling and Validation of Electrolyzers in Real Time Grid Simulation*, demonstration during Dr. David Danielson's INL visit, Idaho Falls, Idaho, June 30, 2015, available: <https://vimeo.com/131928051>.
- Hovsopian, R., 2015, "DRTS-DRTS Link for Distributed Real Time Simulation," presentation as part of U.S. delegation visit, *Aalborg Symposium on Microgrids*, Aalborg, Denmark, August 27 and 28, 2015.
- Hovsopian, R., 2015, "LDRD review," *BEA Board of Science and Technology Committee Meeting*, July 21, 2015.
- Hovsopian, R., 2015, "Dynamic Simulations for Large Scale Electric Power Networks in Real Time Environment using Multiple RTDS," *DOE-NE Review Germantown Meeting*, September 22, 2015.
- R. Hovsopian, "DRTS-DRTS Link for Distributed Real Time Simulation," Presentation, *Workshop on cyber-physical systems application to power grid*, Boston, MA, July 16-17, 2016.
- R. Hovsopian, "Laboratory of the Future," for project – Dynamic Modeling and Validation of Electrolyzers in Real Time Grid Simulation, *Demonstration during Dr. David Danielson's INL visit*, Idaho Falls, ID, June 30, 2015. [Online], available: <https://vimeo.com/131928051>.



## 15-146: Tailoring the Kinetic Function of a Surface through Electronic Effects of Nanoscale Architecture

Rebecca Fushimi,<sup>1</sup> Michael Glazoff,<sup>1</sup> and Gregory Yablonsky<sup>1</sup>

### General Project Description

Nearly 90% of the industrial processes that provide food, fuel, and consumer products rely on catalysis. Many of today's leading chemical-transformation technologies remain highly energy intensive, complex, and expensive. In addition, poor selectivity results in waste production and high CO<sub>2</sub> emissions. The U.S. shale-gas industry has entered a period of sustained low natural gas prices and growing supply. We may now envision a paradigm shift away from the historical chemical process starting from heavy petrochemical feedstocks. This project is motivated by the need to shift the focus of industrial processes to build chemical intermediates from more abundant shale-gas resources.

The surface of a solid catalyst orchestrates the making and breaking of chemical bonds in a complex reaction mechanism. While an endless variety of catalytic architectures can be created, only a few chemical bonds must be broken or formed in the interest of energy transformations: e.g. C-H, C-C, C-O, O-H, etc. This work is focused on the selective dehydrogenation of light alkanes, the first step in upgrading abundant domestic gas resources to higher value alkenes, which serve as the building blocks of vitally important petrochemicals such as polypropylene and polyacrylonitrile.

While platinum is an excellent metal for C-H bond activation, it binds too strongly to unsaturated intermediates, leading to the formation of coke and deactivation. A general strategy is to alloy Pt with another metal to reduce the bonding strength of unsaturated hydrocarbons. New synthetic advances allow precise engineering of multicomponent metal architectures. When combining two different metals at the nanoscale, a material with *emergent* electronic properties—i.e., new properties that are distinct from the summation of individual parts—is created. For example, the surface electronic states will vary widely when two metals are arranged in an alloy configuration, from a core-shell configuration to an assembly of discrete nanoparticles. This work utilizes a unique, low-pressure transient kinetic technique to understand how nanoscale bimetallic architectures, particularly core-shell configurations of different precious metals (Pt, Pd, Re, Au) and base metals (Co, Ni, Sn), can be used to direct the activation of light alkanes.

### Summary

This project has established INL leadership in the area of transient kinetics for gaining fundamental understanding of how catalytic surfaces control complex multistep reaction mechanisms. The acquisition of the TAP (Temporal Analysis of Products) reactor technology is unique in the DOE complex and distinguishes INL with expertise to address the interfacial chemical reactions at a basic science level. Early on in the project, TAP was used to investigate a series of nanostructured Pt/Mo<sub>2</sub>C catalysts prepared via atomic layer deposition by collaborators at the University of Wyoming. Since Mo<sub>2</sub>C and Pt exhibit very similar geometric and electronic properties this combination enabled the study of strain-ligand effects similar to those exhibited in composite and bimetallic systems. In this work conventional temperature dynamic experiments were compared with a pulsed-variant in the TAP system. This unique experimental format yielded new understanding for how the material controlled the decomposition of CO and the generation of CO<sub>2</sub>. It was found that the presence of platinum acted to enable the storage of carbon at low temperatures which extended the activity of molybdenum adsorption sites. These features were highly dependent on the size and structural features of the platinum domains. This work was presented at the annual meeting of the American Institute for Chemical Engineering (AIChE) and is published in one peer-review publication with another presently in preparation.



Platinum nanoscale architecture was further exploited utilizing electroless deposition methods to create bimetallic core-shell structures in similar sized domains (<2 nm); this time supported on inert SiO<sub>2</sub>. Using the TAP pulse response technique the thermodynamic and kinetic properties of ethane and ethylene were collected on these materials. Experimental measurements on real systems were compared with theoretical predictions for well-defined systems through DFT (density functional theory) calculations. For example the calculation in Figure 1 shows the transition state structure for the  $\pi$ -C<sub>2</sub>H<sub>4</sub> → di- $\sigma$  C<sub>2</sub>H<sub>4</sub> step in the adsorption of ethylene on a bimetallic Pd@Pt surface. While Pd@Pt systems only revealed a dilution effect, a synergistic effect was observed for Ru@Pt mixtures both experimentally and theoretically. Investigations of Ni@Pt and other bimetallic compositions are ongoing. TAP is being used to track changes in ethylene adsorption/desorption and decomposition with respect to metal species, domain size and shell thickness. Corroboration of experimental/theoretical results on simple systems supports the reliability of measurements on complex materials. This work enables us to extend the precise kinetic measurements associated with atomistic modeling to real systems with compositional and architectural complexity using the TAP pulse response measurement.

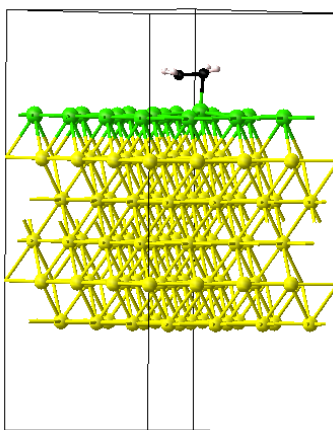


Figure 1: Calculated structure for the  $\pi$ -C<sub>2</sub>H<sub>4</sub> → di- $\sigma$  C<sub>2</sub>H<sub>4</sub> transition state on a single Pt overlayer on Pd, transition state energy barrier 13.87 kJ/mol.

## Benefits to DOE

New catalytic technology is needed that can utilize abundant shale gas resources to replace the conventional production of fuels and chemicals that are presently based on petroleum. This work contributes to fundamental understanding of how catalytic materials can be improved to control a desired sequence of chemical reaction at reduced energy consumption.

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### Invention Disclosures, Patents, and Copyrights

One step synthesis of Ethane to Ethylene Oxide, Invention disclosure, August 28, 2017.

### Interns and Postdocs

Interns: Christian Reece, Shuai Tan, Ken Lim,

Postdocs: Weijian Diao, Chinmoy Baroi, Soe Lwin

### Collaborations

Universities: Cardiff University, United Kingdom, University of Wyoming, and University of California, Berkeley.

## 16-002: Advanced Carbon Feedstock Processing Using Ionic Liquids

Luke Williams,<sup>1</sup> Chenlin Li,<sup>1</sup> Hongqiang Hu,<sup>1</sup> Haiyan Zhao<sup>1</sup>

### General Project Description

This project is focused on developing efficient ionic liquid (IL)-based dissolution processes to transform coal and biomass into fuels and chemicals. Development of these processes addresses national concerns over energy security and environmental sustainability. Both coal and biomass have a complex cross-linked macromolecular network that requires efficient depolymerization to be transformed into clean fuels, chemicals, and high-value materials. ILs are salts that exist in liquid form at temperatures below 100°C and are generally non-flammable with negligible volatility. Some past research has investigated biomass dissolution in IL for bio-ethanol production; however, application as a solvent, catalyst, or reaction media in coal depolymerization and upgrading are still in their infancy. Additionally, IL dissolution of coal and biomass with a focus on recovery of value-added chemicals and materials (like rare earth elements from coal), along with IL purification and recovery, is still limited. This project will develop and demonstrate laboratory capabilities pertaining to IL-based carbon-conversion processes targeting low-rank Wyoming coal and commercially relevant lignocellulosic biomass feedstocks.

### Summary

This project began in early December of 2015 and significant progress has been made in the following 21 months, including:

- Initial experiments studied the dissolution of a sub-bituminous coal and a pine feedstock with 10 different imidazolium based ILs with varying anions and functional groups.
- Down selection from the 10 initial ionic liquids to the two most effective ILs allowed for the study of feedstock extensibility to six different biomass and coal samples, while optimizing IL recovery.
- The effect of IL dissolution on sugar release during enzymatic hydrolysis for six different commercially harvested biomass samples is being compared with traditional dilute acid hydrolysis.
- IL dissolution of coals spanning the range of quality from lignite to anthracite has been investigated to see the effects of depolymerization and demineralization on the quality of heat generated during combustion, and to explore the potential extraction of rare earth elements.

Experimental results from the IL screening and pretreatment of a recalcitrant biomass sample (pine) and a mid-grade coal can be seen in Figure 1. The results from these initial experiments indicates that IL pretreatment can improve fermentable sugar yields, and ultimately fuel production, from biomass by over 500% from the untreated case (Figure 1A). It is also apparent that the peak combustion temperature of a mid-grade coal can be increased by about 50 °C (Figure 1B). Other experimental investigations have revealed that IL dissolution alters physical structure and reduces ash content.

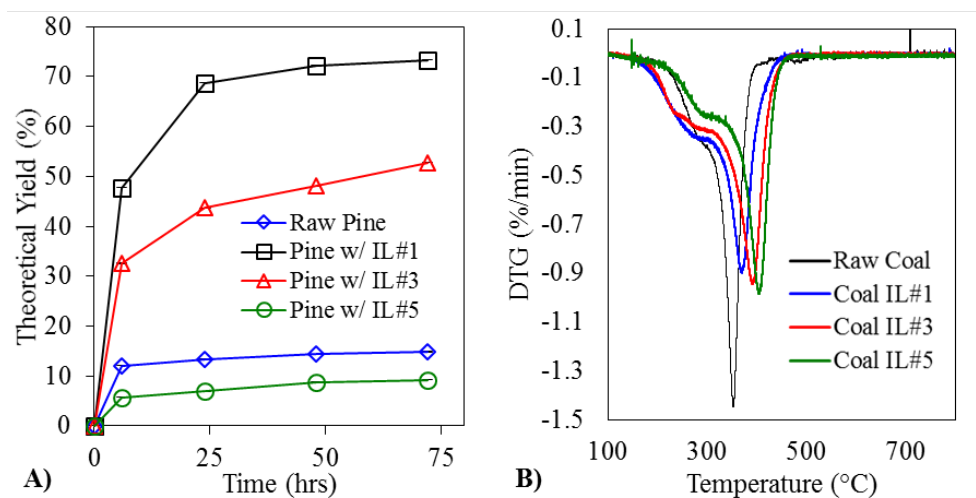


Figure 8. IL pretreatment increases fermentable sugars yields from pine (A) and the increases the peak combustion temperature (and quality of heat) for coal (B).

## Benefits to DOE

This research aims to enable an advanced approach to materials and fuels production from domestic biomass and coal resources that supports the mission of two DOE offices, Energy Efficiency and Renewable Energy and Fossil Energy. The efficient utilization of domestic energy resources, such as the available billion tons of lignocellulosic biomass and domestic coal resources, through advanced carbon engineering, will promote both clean energy and national energy security. This new research direction will also strengthen INL's sustainable biomass-feedstock development program and advanced separation capabilities.

## Publications

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## **Interns and Postdocs**

Interns: Jared C. Allen and Kelli R. Nelson.

Postdoc: Shuai Tan.

## **Collaborations**

Universities: University of Wyoming, University of Idaho, and University of Utah.

## 16-176: Development of Direct Carbon Fuel Cells

Ting He<sup>1</sup> and Maohong Fan<sup>1</sup>

### General Project Description

This project aims at fundamentally changing the coal industry's paradigm from combustion to electrochemical oxidation so that carbon, derived from coal (or biomass or bio-wastes, eventually), can be used as a clean energy source to generate electricity cleanly and efficiently. This project focuses on developing robust, reduced-temperature direct carbon fuel cells (DCFCs) by integrating expertise in coal or carbon engineering, ceramic fabrication and characterization, corrosion mitigation, system modeling, and integration with fast ionic conductors as electrolytes as well as surface modifications for fast electrode kinetics. The success of this project will impact not only regional, national, and global coal industries, but also the human vision of energy and the energy future.

### Summary

A well-equipped lab has been established with the capability of materials synthesis, processing, cell fabrication and assembly as well as electrochemical characterizations. Novel DCFCs have been developed at intermediate temperatures (500–600°C) and demonstrated extremely high power density (higher than those reported at 700–850°C). The reduction of operating temperature will drastically mitigate problems associated with the high temperature operation, such as fast degradation, sealing issues, utilization of expensive materials, slow response to rapid start-up, and poor thermal cycling. In our cell configuration (Figure 1a), gadolinium-doped ceria (GDC)-Li/Na<sub>2</sub>CO<sub>3</sub> composites were used as electrolyte. The composite electrolyte showed the conductivity of 15 and 235 times higher than GDC itself and the conventional electrolyte, yttria stabilized zirconia (YSZ) at 500°C, respectively (Figure 1b). The high conductivity enables fast transport of the charge carrier, CO<sub>3</sub><sup>2-</sup> and O<sup>2-</sup>. Samarium doped strontium cobaltite (SSC) was employed as the cathode, due largely to its favorable oxygen reduction reaction kinetics, especially at low temperatures. Most importantly, a novel carbon-ceramic textile was incorporated as hybrid anode. The anode consists of a number of hollow fibers with diameter of 3–4 μm (Figure 1c), allowing the facile penetration of solid carbon when mixed with carbonate. Consequently, the anode/electrolyte interface provides intimate contact between solid carbon and electrolyte when assembled, thus playing a key role in the performance enhancement. The peak power densities of 143, 196 and 325 mW cm<sup>-2</sup> were achieved at 500, 550 and 600°C, respectively, at the presence of CO<sub>2</sub> and O<sub>2</sub> mixture, as shown in Figure 1d. A comparison of peak power densities (Figure 2) clearly depicts how this work stands out from those reported in literature, and provides a remarkable evidence for direct electrochemical oxidation of carbon. Our research towards low temperature DCFCs establish a benchmark below 600°C, suggesting a great prospective in developing high performance DCFCs at reduced temperatures. Noted that a new fabrication technique along with good sinter ability has been developed with this project, allowing for assembling electrochemical cells at a temperature as low as 700°C, compared to the conventional temperature of above 1400°C, resulting in a great energy saving and capital reduction in the manufacturing of electrochemical cells and stacks.

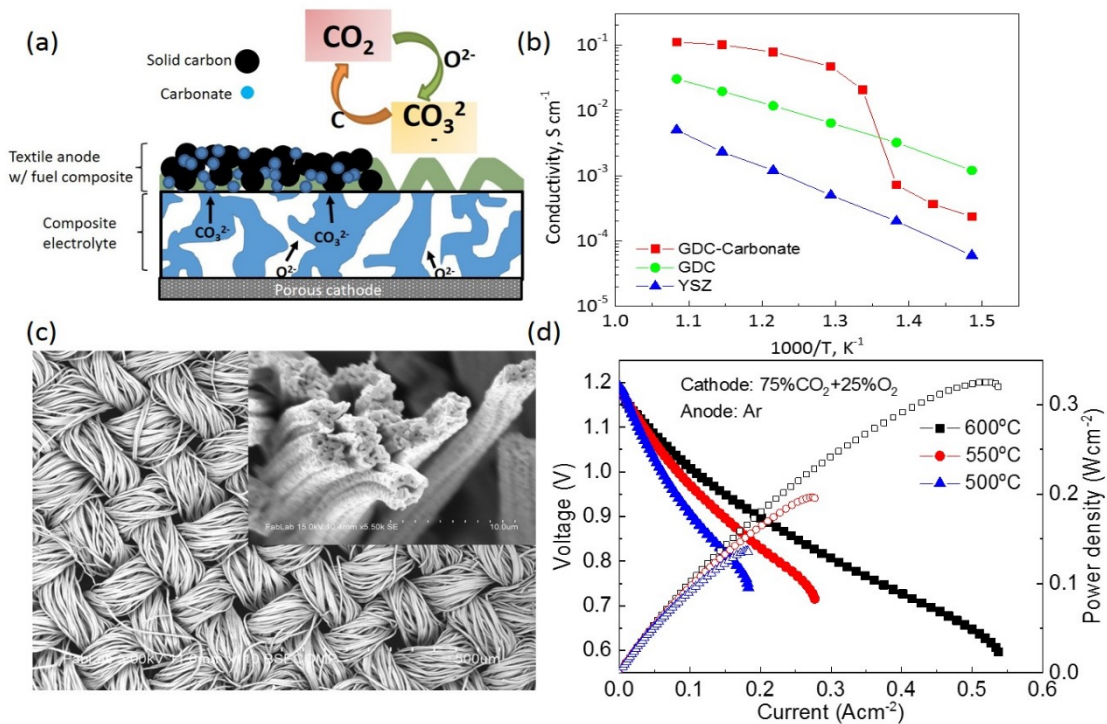


Figure 1. a) Schematic of the DCFC electrochemical process in this work with special emphasis on anode structure, charge carrier in electrolyte and fuel composite b) Arrhenius plot of the total conductivities of GDC-carbonate composite, GDC, and YSZ electrolytes as a function of temperature, c) Ceramic textile anode material consist of hollow fibers, d) I-V and I-P characteristics of the DCFC at 500–600°C.



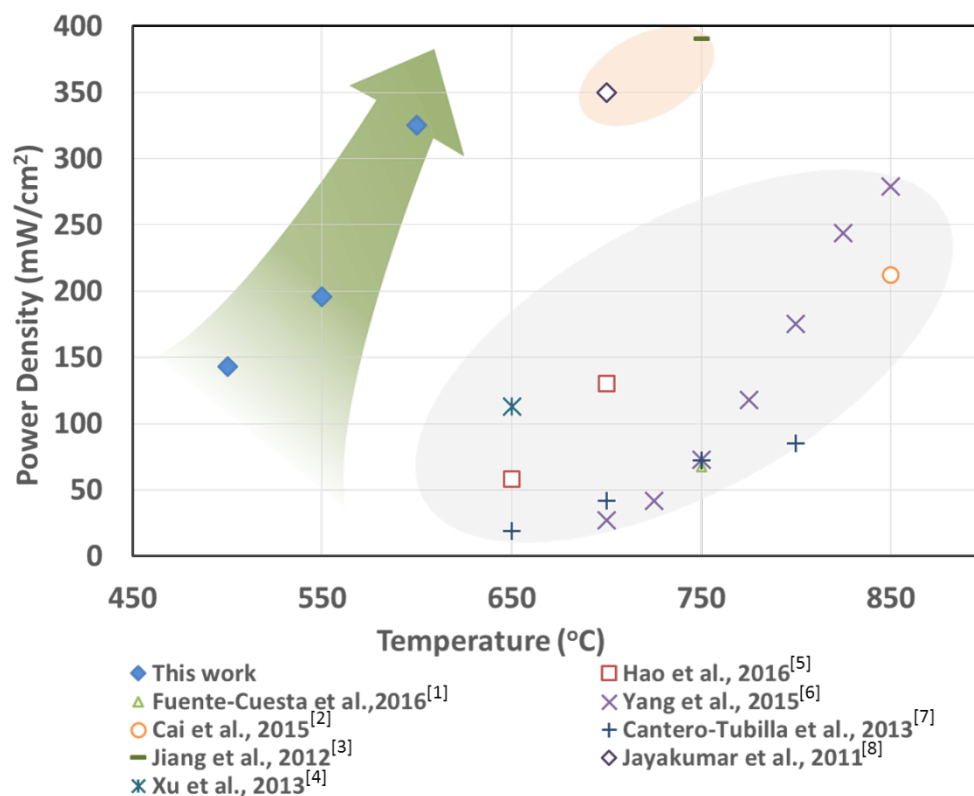


Figure 2. Comparison of maximum power densities of the state-of-art DCFC technologies at different temperatures.

In addition, a cost-effective catalytic pyrolysis process for producing high-quality oil and carbon from coal with low CO<sub>2</sub> emission has been developed at University of Wyoming. Catalytic pyrolysis of the Powder River Basin coal using Na<sub>2</sub>CO<sub>3</sub> and FeCO<sub>3</sub> catalysts has been investigated in a fixed bed reactor between 500 and 800°C under atmospheric pressure to evaluate effects of catalyst on quantity and quality of the resulting oils, gases and solids. The results indicated that Na<sub>2</sub>CO<sub>3</sub> as a catalyst can lower the O and S in oil by as high as 36.1% and 50.6%, respectively. The heating value of oil can be increased from 4,056 kcal/kg to 4,245 kcal/kg. Also, Na<sub>2</sub>CO<sub>3</sub> can change the reaction pathway of pyrolysis, resulting in a decrease of the contents of furan and esters and an increase of the contents of phenols, ketones, straight-chain olefins, and alicyclic hydrocarbons. Moreover, Na<sub>2</sub>CO<sub>3</sub> can reduce CH<sub>4</sub> concentration in the gas by 23.11% and increase H<sub>2</sub> and CO by 70.22% and 6.54%, respectively. All these results demonstrate that Na<sub>2</sub>CO<sub>3</sub> is a promising coal pyrolysis catalyst.

## Benefits to DOE

This project addresses the CAES mission of accelerating nation's transformation to sustainable energy self-reliance through collaborative research. It addresses the INL mission of discovering and demonstrating innovative clean energy options. Great engagement with regional educational institutions and industry sectors would benefit regional economies and also advance INL's national missions. The DCFC technology developed by this project will not only leverage the CAES core capabilities, but also build new capability in high-efficiency energy conversion and distributed generation that can complement the CAES institutional portfolio, exceed stakeholder requirements, and address DOE current and future needs. The technology will help the regional, national and global coal and power industries to dramatically reduce their carbon footprints, meet EPA's Clean Power Plan target, and reduce environmental impact.

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- Wu, W., Y. Zhang, D. Ding, and T. He, 2017, "A High-Performing Direct Carbon Fuel Cell with 3D Architected Anode Operated Below 600°C", *Advance Materials*, DOI: 10.1002/adma.201704745.
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- Xu, B., W. Lua, Z. Sun, T. He, A. Goroncy, Y. Zhang and M. Fan, 2017, "High-quality fuels/chemicals from catalytic pyrolysis of Powder River Basin coal". *Fuel Processing Technology*, 167 (2017) 334-344.
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- Tang, T. He, H. Adidharma, G. Tan and M. Fan. "Coal-derived carbon materials: a modern approach to unlock nature's complexity and nurture the gift from the past". *Progress in Materials Science*, submitted.

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Wu, W., D. Ding, and T. He, IDR# 4437. “Textile-architected 3D hollow framework for energy conversion and storage systems”

**Interns and Postdocs**

Postdoc: Wei Wu

## 16-187: Micro-Scale Technique to Evaluate Grain Boundary Cohesion of Irradiated Alloys

Chao Jiang,<sup>1</sup> Wen Jiang,<sup>1</sup> Brian Jaques,<sup>15</sup> Indrajit Charit,<sup>121</sup> and Ray Fertig<sup>22</sup>

### General Project Description

Metallic alloys are widely used, or planned for use, as structural and cladding materials in current and future reactors. Under irradiation, grain-boundary (GB) cohesion strength decreases due to interaction with defects and impurities, leading to intergranular fracture and embrittlement of alloys. The objective of this project is to develop a technique for quantifying GB cohesion and its impact on fracture behavior in irradiated alloys by utilizing transmission electron microscopic (TEM) in situ cantilever testing in concert with multi-scale modeling. The TEM in situ cantilever testing is a novel approach for studying the real-time mechanical response of materials. It will be used in this work for studying intergranular fracture behavior in several irradiated iron-based ferritic alloys and for providing key information to link atomistic-level events with mesoscale/macroscale mechanical properties. The Multi-Physics Object-Oriented Simulation Environment (MOOSE)-based cohesive zone model (CZM) and extended finite-element method (XFEM) for intergranular fracture of irradiated ferritic alloys will be developed in this work by utilizing atomistic results as inputs and experimental results for validation.

### Summary

Under neutron or ion irradiations, many point defects and their clusters will be directly formed during collision cascades. Diffusion of interstitials or vacancies towards sinks such as GBs can lead to redistribution of solute concentrations, so-called radiation-induced segregation effect. In ferritic Fe-Cr alloys, both radiation-induced depletion and enrichment of Cr at GBs have been observed. Due to super-saturation of point defects created under irradiation, radiation-enhanced diffusion can also greatly accelerate the segregation of impurity elements to GB. According to present density functional theory (DFT) calculations (see Table 1), sulfur (S) and phosphorus (P) in steels and helium (He) produced by nuclear transmutation reactions all have a strong tendency to segregate to GB. An important consequence of the local enrichment of impurities at GBs is that they can drastically weaken GB cohesion strength and induce intergranular fracture and embrittlement. Present DFT calculations reveal a dramatic reduction of GB cohesion energy due to the segregation of S, P and He (see Table 1). In contrast, Cr segregation does not seem to have a detrimental effect on GB cohesion in bcc Fe.

*Table 1. DFT calculated segregation energies ( $E_{seg}$ ) of impurities to a  $\Sigma(310)[001]$  symmetric tilt GB in bcc Fe. The change of the GB cohesion strength ( $dE_{coh}$ ) due to impurity segregation is also shown.*

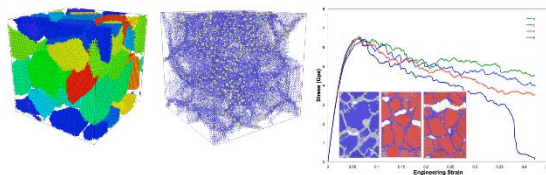
Impurity	S	P	He	Cu	Si	Al	Mo	Ni	Cr
$E_{seg}$ (eV)	-1.25	-0.87	-1.51	-0.56	-0.44	-0.38	-0.40	-0.40	-0.25
$dE_{coh}$ (eV)	-2.25	-1.30	-3.21	-0.33	-0.48	-0.22	+0.90	+0.04	+0.47

In FY-17, molecular dynamics (MD) simulations with empirical embedded atom method (EAM) potential have also been performed using LAMMPS code to predict the effects of He loading on the GB cohesion strength in bcc metal molybdenum (Mo). Here Mo-He is used as a surrogate system for Fe-He due to the lack of EAM potential for the latter. Nanocrystalline (nc) bcc Mo sample containing 32 grains and around a half million atoms has been generated using the Voronoi tessellation method. He gas atoms are then randomly loaded at GBs (yellow spheres in Figure 1). Due to the replacement of strong metallic bonding with repulsive He-Mo bonds, He segregation at

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<sup>22</sup> University of Wyoming

GB significantly reduces the strength of nc bcc Mo by promoting intergranular fracture. During uniaxial loading simulations, complete failure of the nc Mo sample is observed when local He concentration at GB exceeds 6%.



*Figure 1. MD simulation of the effects of He on mechanical strength of nc bcc Mo.*

On the continuum scale, implementation of CZM in the MOOSE Framework has been realized by utilizing ElemElem constraint in XFEM based on a phantom node method: the element containing a crack is deleted and replaced by two partial elements at the same location. Mode-I implementation of CZM was compared with a commercial finite element package, Abaqus for a benchmark data set. The traction-separation obtained from MOOSE and Abaqus are in very good agreement. Future work will be aimed towards combining crystal plasticity with CZM to simulate the response of polycrystalline BCC Fe when loaded.

During FY 2017, experimental efforts have been focused on developing capabilities for measuring GB cohesion strength using focused ion beam (FIB) for sample fabrication, electron back scatter diffraction (EBSD) for GB quantification, and in situ TEM mechanical testing. Multiple nanometer-scale geometries have been investigated, including; 4-point bend testing, cantilever testing, and tensile testing in order to investigate the mechanical response of induced stresses on grain boundaries. Each of the geometric designs allows for the isolation of single grain boundaries on the scale of a few micrometers and the samples can be fabricated within micrometers of the surface of the specimens. Accordingly, the experimental work allows for accurate representation of damage incurred during neutron irradiations using ion-induced damage (which has a small penetration depth). Using high energy ball milling followed by spark plasma sintering (SPS), Fe-9Cr alloy has also been synthesized. Iron and chromium powders were mixed in the right proportion in a glove box under argon environment and then ball milled for different milling times. For SPS, different sintering time, temperature and pressure have been used to achieve the best density. X-ray diffraction was carried out on the sintered samples and showed essentially peaks of bcc iron indicating that the material was ferritic. EBSD performed on the Fe-9Cr sample showed the presence of grains with size of  $1.8 \pm 0.5 \mu\text{m}$  and preponderance of high angle grain boundaries. TEM characterization showed grain size to be 1-4  $\mu\text{m}$  with approximately 100 nm intra- and intergranular precipitates, which appeared to be chromium oxide. The Fe-9Cr samples have been sent to Texas A&M Ion Beam Laboratory for proton irradiation with doses up to 5 dpa at 300°C and 475°C. Irradiated alloy samples will be used to study the radiation-induced segregation behavior and its effect on grain boundary cohesive strength.

### Benefits to DOE

The radiation-induced degradation of mechanical material properties poses serious limitations to nuclear energy applications. The capabilities of TEM in situ mechanical testing and MOOSE-based fracture models developed for this work will help elucidate and predict the performance of materials in reactors. In turn, it would enable safer and more economical nuclear energy in the future. Results from this project will contribute to the DOE's leading role on research of materials behavior and performance in radiation environments.

### Publications

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## Presentations

- Kundu, A. and I. Charit, 2017, “A study on high energy ball milling and spark plasma sintering of Fe-9Cr model alloys”, *Materials Science & Technology (MS&T) 2017*, Pittsburgh, PA, Oct 2017.
- Watkins, J., B.J. Jaques, A. Bateman, Y. Wu, I. Charit, J.P. Wharry, K.H. Yano, W. Jiang, and C. Jiang, 2018, “Irradiation effects on Fe-9%Cr grain boundary strength via in-situ TEM testing”, *The Minerals, Metals & Materials Society (TMS) 2018*, Phoenix, AZ, March 2018.
- Kundu, A., I. Charit, B. Jaques, and C. Jiang, 2018, “A study on the high energy ball milling and spark plasma sintering of Fe-Cr based alloys”, *The Minerals, Metals & Materials Society (TMS) 2018*, Phoenix, AZ, March 2018.

## 16-215: Electrochemical Manufacturing Processes

Ting He<sup>1</sup>

### General Project Description

This project focuses on the most energy-intensive activation process in manufacturing chemicals, plastics, and fuels from natural gas and natural-gas liquid feedstocks by developing electrochemical processes to replace conventional thermal processes. It aims at fundamentally changing the petrochemical manufacturing paradigm from widely used thermal practices (fossil-energy combustion) to a clean energy regime. It is an enabling technology in initiating INL's position in advanced manufacturing. The electrochemistry platform will also support and leverage existing EES&T programs in clean energy integration and advanced transportation as well as new initiatives at INL.

### Summary

Upon our well-established fabrication and electrochemical test labs, we are able to promptly implement our research. So far, we have successfully demonstrated the two types of advanced electrochemical manufacturing technologies: co-production of chemicals/fuels and hydrogen (CPCH) and co-generation of chemicals/fuels and power (CGCP) at 400–500°C. Figure 1a schematically depicts the principal of CPCH based on an electrochemical cell when ethane used as the feedstock. The electrochemical membrane reactor was fabricated by advanced ceramics fabrication techniques with a porous electrode-support (400 μm), a dense thin electrolyte (10 μm) and a porous counter electrode (7 μm), as shown in Figure 1b. The electrolyte is Y- and Yb-doped barium zirconate-cerate perovskite (BZCYYb), having two orders of magnitude higher conductivities at 400–500°C and lower activation energy, compared to the yttria-stabilized zirconia (YSZ) oxygen ion conductor (Figure 1c), allowing for fast proton migration through the membrane, thus decreasing overpotential drastically at reduced temperatures. Figure 1d shows the electrical consumption, 0.408 V, corresponding to an electrochemical overpotential of ~0.140 V at a current density of 1 A cm<sup>-2</sup>, equivalent to a proton flux of 10.37 μmol cm<sup>-2</sup> s<sup>-1</sup> or a hydrogen production rate of 0.448 mol cm<sup>-2</sup> per day at 400°C. Also, the selectivity of ethylene is as high as 94.1%. By infiltrating more active nano-structured catalysts and optimizing the interfaces and microstructure of electrodes, overpotential can be further reduced to minimize the electrical energy consumption.



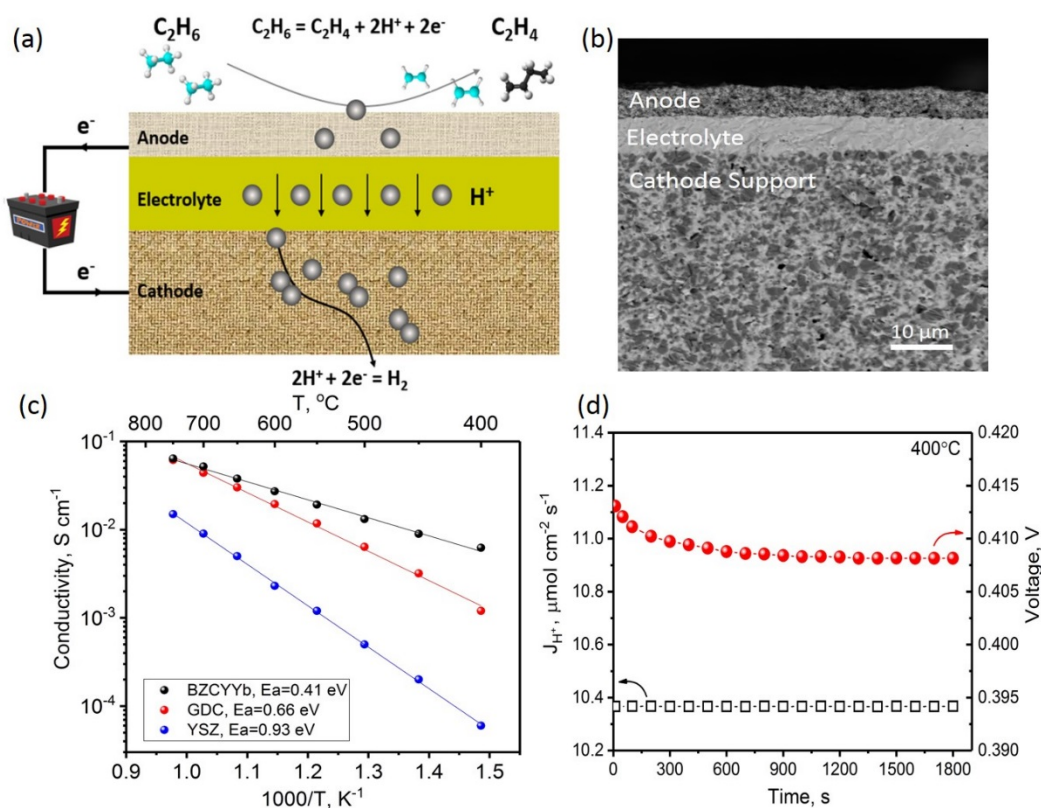


Figure 1. a) Schematic of an electrochemical cell for the co-production of chemicals/fuels and hydrogen; b) A cross-sectional SEM of an actual electrochemical membrane reactor; c) Conductivity of BZCYYb, GDC and YSZ; d) The electrical energy consumption and the hydrogen production rate of our electrochemical process at  $400^\circ C$

Our electrochemical process exhibited a significant process energy saving when compared to industrial steam cracking in ethylene production, as shown in Figure 2a. Taken the smallest energy consumption from the public sources as an example [1], as much as 65% of process energy could be reduced by replacing industrial steam cracking with our technology. When taken into account of the hydrogen energy generated, the electrochemical process actually has a net energy gain (hydrogen energy output minus process energy input) due to the extremely high heating value of hydrogen (LHV of  $240\ kJ\ mol^{-1}$ ) while the steam cracking burned out all generated hydrogen due to the cost for separation [2]. Our electrochemical process also exhibited remarkable advantage of a low carbon footprint. Figure 2b compared  $CO_2$  emission in our electrochemical process with the industrial steam cracking in ethylene production. It is clearly shown that our electrochemical process led to a 72.8% reduction in carbon footprint when grid electricity was used. Further, it will result in a 89.1% reduction, or about one tenth of carbon footprint associated with the industrial steam cracking process, when renewable energy is used to provide power. Eventually a 98.6% reduction in carbon footprint will be obtained when renewable energy is used for both heat and electricity.

The CGCP has been successfully realized at  $400\text{--}600^\circ C$  using an oxygen-ion conducting electrolyte when ethane being used as feedstock and air as oxidant. The peak power density of the cell is  $0.60$  and  $0.25\ W/cm^2$  at  $600$  and  $500^\circ C$ , respectively. The performance obtained is among the top of the fuel cells using ethane as fuel [3]. The ethylene is produced by controlling the current density (e.g. oxygen ion flux), whose selectivity increases with reduced current density. At  $400^\circ C$ , the ethylene is still generated at low current density.

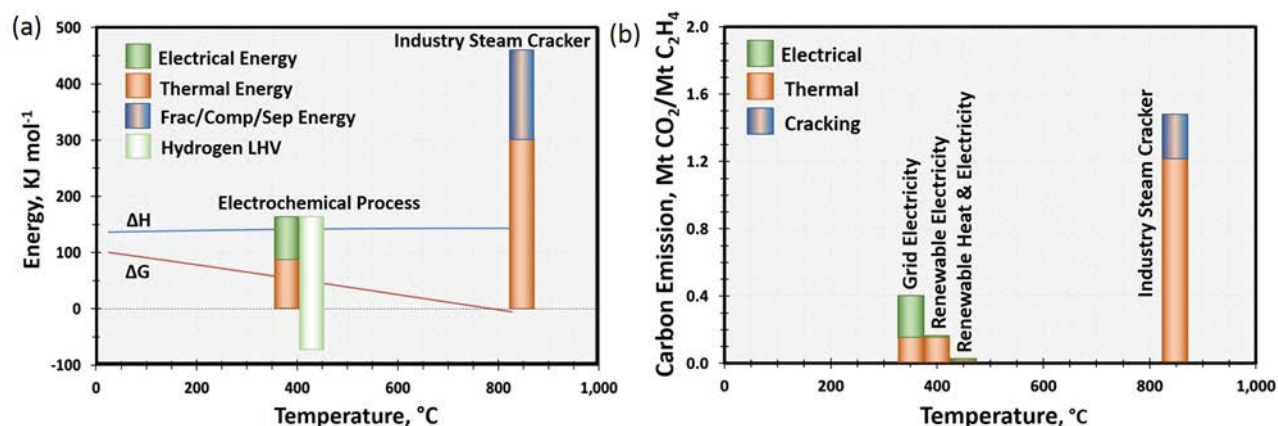


Figure 2. a) A comparison of the process energies for ethylene production from ethane; b) A comparison of the carbon footprint for ethylene production from ethane;

## Benefits to DOE

This project contributes directly to a reduction of energy intensity in petrochemical manufacturing. Improving efficiency and lowering energy intensity will not only reduce greenhouse gas emissions and carbon footprint, but also increase the efficiency of deployed capital investment for a wide-deployment of clean energy resources, including nuclear-derived heat. This project addresses the INL mission of discovering and demonstrating innovative clean energy options. The novel electrochemical processes developed by this project will enable INL's position in advanced manufacturing and help advance small modular reactor deployment through market, particularly manufacturing pull. A core electrochemical capability will be established that can support and leverage both the existing programs, such as the hybrid energy systems where the co-generation of power and products is the key to manage large-scale renewable electricity grid, and new initiatives at INL, such as the regional partnership that stewards enormous carbon reserves.

## Reference

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## Publications

- Tang, Q., Z. Shen, L. Huang, T. He, H. Adidharma, A.G. Russell and M. Fan, 2017, "Synthesis of methanol by CO<sub>2</sub> hydrogenation promoted by dissociative adsorption of hydrogen on Ga<sub>3</sub>Ni<sub>5</sub>(221) surface", *Physical Chemistry Chemical Physics* 19, (2017) 18539-18555
- Xu, X., Y. Chen, P. Wan, K. Gasem, K. Wang, T. He, H. Adidharma and M. Fan, 2016, "Extraction of lithium with functionalized lithium ion-sieves". *Progress in Materials Science* 84, 276 (2016).
- Wu, W., D. Ding and T. He, *ECS Transactions*, 80 (2017) 167-173.
- Ding, D., Y. Zhang, W. Wu and T. He, *Energy Environmental Science*, under review.

## Presentations

- He, T., 2016, "Engineering Platinum Alloy Electrocatalysts in Nanoscale for Fuel Cell Application", *ACS 251<sup>st</sup> National Meeting & Exposition*, San Diego, March 2016.
- He, T., 2016, "Performance and Durability of PtTi Catalyst for Oxygen Electroreduction", *PRiME 2016*, Honolulu, October 2016.
- He, T., and D. Ding, 2017, "Perovskite Proton Conductors for Energy Conversion and Storage at Intermediate Temperatures", *20<sup>th</sup> Topical Meeting of the International Society of Electrochemistry*, Buenos Aires March 2017.
- He, T., D. Ding, Y. Zhang and W. Wu, 2017, "Electrochemical Activation of Natural Gas Liquids in Petrochemical Manufacturing", *68<sup>th</sup> Annual Meeting of the International Society of Electrochemistry*, Providence, August 2017,
- Wu, W., D. Ding, and T. He, 2017, "Development of high performance intermediate temperature proton-conducting solid oxide electrolysis cells", *232<sup>th</sup> Meeting of the Electrochemical Society (ECS)*, National Harbor, October, 2017.

## Invention Disclosures, Patents, and Copyrights

- IDR # 4104. "Process intensification for light hydrocarbon gases"
- IDR # 4276, Patent Application filed (2017). "Hydrogen production via water electrolysis at intermediate temperatures"
- IDR # 4327, Patent Application filed (2017). "Carbon dioxide electrochemical hydrogenation/protonation to produce functional molecules"
- IDR # 4334, Patent Application filed (2017). "Electrochemical Activation of Ethane for Co-production of Chemicals/Fuels and Hydrogen"
- IDR # 4478, "Non-oxidative activation of methane via electrochemical processes"

## Interns, Postdocs and Staff

Postdoc: Yunya Zhang and Wei Wu

Staff: Dong Ding

## 16P6-002FP: Kinetic-based Scale-Up Science for an Energy Efficient Route to Ethylene

Chinmoy Baroi,<sup>1</sup> Weijian Diao,<sup>1</sup> and Soe Lwin<sup>1</sup>

### General Project Description

This project focuses on a new, energy-efficient catalytic route to produce ethylene from ethane based on oxidative dehydrogenation (ODH) of ethane using a novel composition of the M1 catalysts.

### Summary

The project dealt with different composition of M1 catalysts prepared by dry-up method followed by post-treatment of the catalysts and testing their activity in ODH of ethane to ethylene. In a typical synthesis, solutions of components is mixed together to form a mixed metal-oxide by precipitation (Fig.1). Then water from the precipitated solution is removed by evaporation, and the recovered solid is dried overnight. Finally, the M1 catalyst is obtained by calcination at 600°C. As a post-treatment, the catalyst is treated with oxalic acid, and then liquid nitrogen is poured into the catalyst, which was ground (cryo-ground) using a mechanical grinder.



Figure 1. M1 catalyst synthesis by dry-up method.

The novelty of this project is a new composition of M1 catalysts followed by post-treatment. The catalytic test indicates that a certain composition of M1 catalyst (DRU-2) is very active (Table 1).

Table 1. Catalyst activity testing at 360 °C.

Catalyst Samples	C <sub>2</sub> H <sub>6</sub> conversion (%)	C <sub>2</sub> H <sub>4</sub> selectivity (%)	CO selectivity (%)	CO <sub>2</sub> selectivity (%)	O <sub>2</sub> conversion (%)	C <sub>2</sub> H <sub>4</sub> yield (%)
MoV <sub>0.4</sub> Nb <sub>0.15</sub> Te <sub>0.1</sub> O <sub>X</sub> (DRU-5)	49.1	73.6	26.4	-	51.4	36.1
MoV <sub>0.2</sub> Nb <sub>0.15</sub> Te <sub>0.15</sub> O <sub>X</sub> (DRU-1)	69.4	87.9	12.0	-	66.7	61.1
MoV <sub>0.3</sub> Nb <sub>0.15</sub> Te <sub>0.15</sub> O <sub>X</sub> (DRU-2)	61.2	94.5	5.5	0	55.1	57.8
MoV <sub>0.4</sub> Nb <sub>0.15</sub> Te <sub>0.15</sub> O <sub>X</sub> (DRU-3)	51.0	74.7	25.2	0	54.3	38.3
MoV <sub>0.4</sub> Nb <sub>0.15</sub> Te <sub>0.20</sub> O <sub>X</sub> (DRU-4)	53.7	89.6	10.4	0	74.6	48.1
MoV <sub>0.2</sub> Nb <sub>0.15</sub> Te <sub>0.20</sub> O <sub>X</sub> (DRU-6)	2.3	100	0	0	4.9	2.3
MoV <sub>0.1</sub> Nb <sub>0.15</sub> Te <sub>0.15</sub> O <sub>X</sub> (DRU-7)	4.2	100	0	0	5.5	4.2
MoV <sub>0.1</sub> Nb <sub>0.15</sub> Te <sub>0.2</sub> O <sub>X</sub> (DRU-8)	3.6	100	0	0	1.4	3.6
MoV <sub>0.3</sub> Nb <sub>0.15</sub> Te <sub>0.15</sub> O <sub>X</sub> (DRU-2) - Cryo-grinded	40.4	85.4	14.6	0	69.6	34.5
MoV <sub>0.3</sub> Nb <sub>0.15</sub> Te <sub>0.15</sub> O <sub>X</sub> (DRU-2) - oxalic acid treated	20.5	100	0	0	47.4	20.5
MoV <sub>0.3</sub> Nb <sub>0.17</sub> Te <sub>0.21</sub> O <sub>X</sub> (DRU-9) - oxalic acid treated	40.6	70.6	11.1	18.3	100	28.6

MoV <sub>0.3</sub> Nb <sub>0.17</sub> Te <sub>0.21</sub> O <sub>x</sub> (DRU-9) - oxalic acid treated + Cryogrinded	65.8	84.4	7.0	8.5	100	55.6
MoV <sub>0.3</sub> Nb <sub>0.17</sub> Te <sub>0.21</sub> O <sub>x</sub> (DRU-9)- oxalic acid treated + Cryogrinded – 5 bar operating pressure	52.6	79.2	8.6	12.2	86.5	41.7

The results (Table 1) indicate that post-treatment methods would not improve catalytic activity. In addition it is also found that operating at higher pressure would not improve catalytic activity.

## Benefits to DOE

Shale gas is a major source of ethane. An abundant supply has led to a recent decline in shale-gas pricing, making shale gas an attractive source of ethane for ethylene production. The domestic chemicals industry invested \$15 billion from 2008 to 2012 in ethylene production, increasing capacity by 33%. As these investments take hold, yielding more supply, the United States could become a major global low-cost provider of energy and feedstocks (i.e., ethylene) to the chemicals industry. Dow, Chevron Phillips, and Shell, the major ethylene-producing companies in the US, could directly benefit from this novel catalytic route and would be expected to invest in this research. This proposal matches the goals of the Department of Energy–Advanced Manufacturing Office (DOE-AMO). This work directly supports concepts included in Rapid Advancement in Process Intensification Deployment (RAPID).

## Publications

- Baroi, C., A. Gaffney, and R. Fushimi, 2017, “Process economics and safety considerations for the oxidative dehydrogenation of ethane using the M1 catalyst,” *Catalysis Today*, 2017, article in press
- Lwin, S., W. Diao, C. Baroi, A. Gaffney, and R. Fushimi, 2017, “Characterization of MoVTeNbO<sub>x</sub> Catalysts during Oxidation Reactions Using In Situ/Operando Techniques: A Review,” *Catalysts* 7 (4), 109, (2017)

## Presentations

- Baroi, C., R. Fushimi, A. Gaffney, and G. Maffia, 2016, “Techno-economic and process safety analysis of ethane to ethylene production process through oxidative dehydrogenation (ODH) route”, *2016 Annual AIChE Meeting*, November 13-18, 2016, San Francisco, California, USA

## Invention Disclosures, Patents, and Copyrights

- IDR #4266 “Oxidative Dehydrogenation (ODH) of ethane to ethylene using CO<sub>2</sub> and a novel composition of M1 catalyst”.
- IDR #4464, “One-step synthesis of ethane to ethylene oxide”.



## 17A1-007FP: High Performance Polymeric Membranes for Nano and Ultrafiltration Applications

John R. Klaehn,<sup>1</sup> Christopher J. Orme,<sup>1</sup> Harry W. Rollins,<sup>1</sup> Aaron D. Wilson,<sup>1</sup> and Birendra Adhikari<sup>1</sup>

### General Project Description

The goal of this research is to create high-performance (HP) polymeric membranes that are able to withstand aggressive water feed streams for nanofiltration (NF), ultrafiltration (UF), reverse osmosis (RO) or forward osmosis (FO) applications. These HP membrane technologies must be economical but also endure aggressive conditions, such as high temperatures, organic solvents, as well as high or low pH. This project satisfies the advanced separations techniques for water purification, materials separations, and other aspects of industrial process efficiency (e.g. acid/base processes that make salted solutions). Also, the proposed HP membranes will improve processes for water treatment or chemical product purification and enable aspects of existing processes and capabilities. These HP membranes will incorporate materials that increase hydrophilicity and improve liquid throughput, selectivity, and membrane stability at higher temperatures. The project will build upon HP polymer membrane capabilities at INL and develop new methods to introduce porosity that will enable high flow rates in challenging water separations.

### Summary

Our research this year focused on benchmarking NF commercial membranes at high temperatures ( $\geq 70^{\circ}\text{C}$ ) and fabricating new high performance (HP) polymer membranes with induced porosity. Several paths forward were developed to create NF membranes with several HP polymers including polyimides, fluoropolymers, block copolyamide, and polyphosphazenes. Membrane designs focused on the nanostructured fugitive fillers (carbon nanotubes (CNT), ceramic particles, nanocrystalline cellulose (NCC)) to induce porosity. The aim is creating a hydrophilic interface to our membranes so that the feed streams are able preferentially permeate water through the membrane, while rejecting other components, such as salt and organics. Currently, new polymeric membranes are being examined with polymeric and fugitive fillers that have hydrophilic properties. Currently, we are showing positive results in forming micro to nanoporous polymer membranes with our analytical methodologies. We have confirmed that we have created porous membranes by SEM, water permeation and gas permeation. However, it will take further research and development to create successful porous polymer membranes for high temperature water separations.

The water filtration apparatus was upgraded for the benchmarking performance of sheets to membrane module at high temperatures ( $\geq 70^{\circ}\text{C}$ ). This benchmarking performance with our modified water filtration apparatus was a major milestone for our project. Several commercial NF membranes, including cellulose acetate (CA), polyamide thin film composite (PA-TFC), and polyamide (PA) membranes, were examined for their rejection of organic dyes and magnesium salts. Our data showed that the tested commercial membranes will not be able to perform adequately above  $60^{\circ}\text{C}$ , which provides evidence that better NF membranes are warranted. Currently, we are successfully making new NF membranes with HP polymers, and we are examining the permeability and separation efficiency. Various micro to nanostructured fugitive fillers were introduced to the various HP polymers, and we tested them for NF capabilities. From our preliminary results we found that these fabricated membranes perform well by successfully rejecting organic dyes from aqueous solutions. Also, we are forming phased inverted membranes for greater water throughput with the ability to create thin film composite on the surface of these membrane. The goal is to create as uniform a pore size distribution as possible to gain the greatest selectivity. Other technical accomplishments include a journal article (Title-“The role of water activity (aw) in water transport through membranes”) was submitted to the *Journal of Membrane Science* and several poster presentations were given at the International Congress on Membranes and Membrane Processes (ICOM2017) at

San Francisco, CA. In addition, we are collaborating with National Renewable Energy Laboratory (NREL) with NCC fugitive fillers, and we had an intern working on water chemical potential using polyethylene glycols.

## Benefits to DOE

Within DOE, interest in water technology, such as high-performance filtration and membrane separations, is pervasive. DOE-EERE, NE, and FE, to name a few, have technical needs in water purification. Water and energy are inextricably linked, and energy production consumes large amounts of water that is difficult to recycle and costly to dispose. This project will develop filtration membranes suitable for use in environments with aggressive feed streams, which can degrade conventional filtration materials. Therefore, this work places INL as a leader in the development of new HP filtration membranes that will be custom designed to fit various industrially relevant applications, such as high temperature NF. In addition, this technology fits into the Advanced Manufacturing platform where industrially critical chemical separations are sought. Further, there are new initiatives within DOE for cross-cutting platforms on energy and water, such as the expected clean-water hub. Advances from this work, combined with existing water filtration/recovery (e.g., critical material recycling efforts), gives INL a compelling position in which to meet this new opportunity. Additionally, several industrial manufacturers have expressed interest in working with INL on this research.

## Publications

Wilson, A.D., J.R. Klaehn, C. M. Hrbac, C.J. Orme, and D. L. Daubaras , 2017, “The role of water activity (aw) in water transport through membranes,” *Journal of Membrane Science* on Apr 11, 2017. INL/CON-17-41157

## Presentations

Orme, C.J., B. Adhikari, J.R. Klaehn, and A.D. Wilson, 2017, “Dewatering High Osmotic Potential Produced Water Using SPS FO”, *2017 International Congress of Membranes and Membrane Processes (ICOM) 2017*, Jul 29-Aug 4, 2017, San Francisco, CA.

Orme, C.J., J.R. Klaehn, A.D. Wilson, J.S. McNally, and J.J. Kane, 2017, “Gas Permeability of Mix Matrix Phosphazene Polymer Blends,” *2017 International Congress of Membranes and Membrane Processes (ICOM) 2017*, Jul 29-Aug 4, 2017, San Francisco, CA.

Wilson, A.D., J.R. Klaehn, C.M. Hrbac, C.J. Orme, D.L. Daubaras, 2017, “The role of water activity (aw) in water transport through membranes,” *2017 International Congress of Membranes and Membrane Processes (ICOM) 2017*, Jul 29-Aug 4, 2017, San Francisco, CA.

Barnes, J. M., J.R. Klaehn, and A.D. Wilson, 2017, “Investigation of the material osmotic density of aqueous poly(ethylene glycol) solutions,” poster session at INL Summer Intern Expo/Poster Session, Aug 10, 2017, Idaho Falls, ID.

## Interns and Postdocs

Intern: Joseph M. Barnes

## Collaborations

University: Benedictine College



## 17A1-055FP: Electro-Reduction of Metals in Supercritical Fluid-Room Temperature Ionic Liquids

Donna Baek,<sup>1</sup> Robert Fox,<sup>1</sup> and Tedd Lister<sup>1</sup>

### General Project Description

Clean energy deployment is reliant on a secure source of rare earth elements (REEs). REEs make up the key components found in high-tech devices, electric vehicles, and devices which convert renewable energy resources to electricity. Lanthanide metal ions are currently reduced to the metallic state by using a molten-salt electrochemical process at high temperatures. That energy-intensive process gives rise to considerable quantities of toxic fluoride-salt waste. An immediate improvement over the state-of-the-art is to replace the high temperature molten-salt process with a low temperature (<100°C) electrochemical process in an inherently waste-minimizing solvent system. This work explores and develops a supercritical fluid/electrochemical coupled technique to electrochemically reduce lanthanide metal ions to their metallic state from room temperature ionic liquids (RTILs) for use in consumer electronic products. This research will lead to a novel, innovative, sustainable metal-reduction technique that will lower energy consumption, produce less secondary waste, and reduce the hazard of the waste that is produced.

### Summary

REE was successfully reduced from REE<sup>3+</sup> to REE<sup>0</sup> from a RTIL at ambient temperatures and pressures in a glovebox. Experiments are conducted in a glovebox because the metal deposit oxidizes rapidly when exposed to the environment. Scanning Electron Microscopy-Energy Dispersive X-Ray Spectroscopy (SEM-EDX) and Inductively Coupled Plasma-Mass Spectroscopy (ICP-MS) data have been obtained to verify the oxidation state and quantitate the metal deposited, respectively. The oxidized REE:O ratio is 0.667; however, from the EDX results the REE:O ratio was >1. This provides evidence that metallic REE was produced. ICP-MS data revealed that a deposition rate of 0.67 mg per cm<sup>2</sup> per hour was achieved, with a 64% current efficiency for the targeted REE in Figure 1.

An important aspect in addition to studying the reduction reaction for REE, is the oxidation reaction. An oxidation species is required to protect the integrity of the RTIL. A sacrificial oxidation species has been examined to understand and characterize electrochemically driven oxidation and reduction reaction behavior as it will occur in a RTIL.

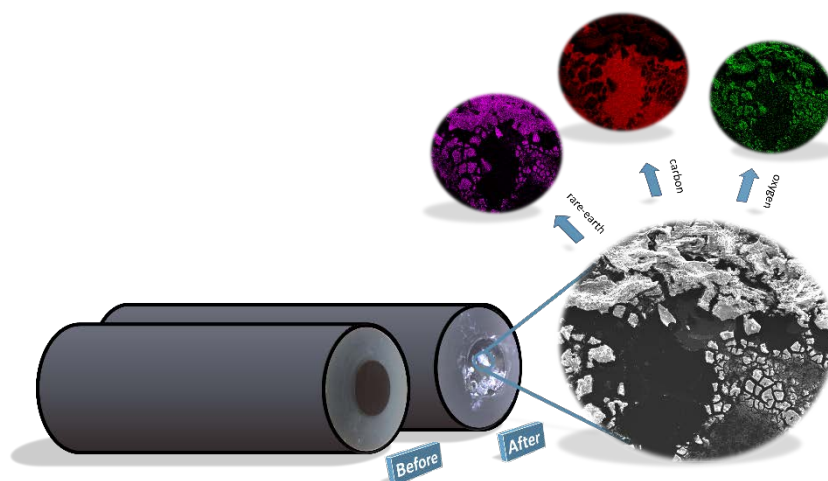


Figure 1. Left: Working electrode tip before and after electrochemistry was performed. Metal deposition was observed. Right: A SEM image of rare earth metal (REM) deposited on the electrode. Color representations of the REM (purple), carbon (red), and oxygen (green).

## Benefits to DOE

The objective of this work is to develop a market-disruptive metallurgical technology targeted at the electrochemical reduction of metal ions to their metallic state in a RTIL that has been augmented with a supercritical fluid. Deployment of clean energy technologies by US companies in US and world markets will be hindered without a secure supply of REEs and refined REE materials. REEs are used in so many different products that impact key energy-production industries (e.g., petroleum and natural-gas refining catalysts) that REE materials shortages could have significant detrimental impact on multiple industrial sectors beyond micro-electronics, magnets, electric vehicle batteries, solid-oxide fuel cells, and LEDs. This work aligns with the Advanced Manufacturing Office's goal of expanding the nation's clean energy technology and manufacturing competitiveness.

## Presentations

Day, B. C. and D. L. Baek, 2017, "Oxidation of Formic Acid in a Room Temperature Ionic Liquid," *2017 INL Intern Expo*, Idaho Falls, ID, August 10, 2017.

Higgins, C. J. and D. L. Baek, 2017, "Investigation of  $\text{Ln}(\text{H}_2\text{O})_x(\text{Tf}_2\text{N})_x$  complexes in MPPyTf<sub>2</sub>N (Ln = Ho, Pr)," *2017 INL Intern Expo*, Idaho Falls, ID, August 10, 2017.

Mitchell, J. M. and D. L. Baek, 2017, "Electrodeposition of Rare-Earth Elements Using Ionic Liquids," *2017 INL Intern Expo*, Idaho Falls, ID, August 10, 2017.

Higgins, C. J. and D. L. Baek, 2017, "Investigation of  $\text{Ln}(\text{H}_2\text{O})_x(\text{Tf}_2\text{N})_x$  complexes in 1-methyl-1-propyl pyrrolidinium bis(trifluoromethylsulfonyl)imide (Ln = Ho, Pr)," *UNLV*, Las Vegas, NV, September 1, 2017.

## Invention Disclosures, Patents, and Copyrights

BA-975, "An Electrowinning Process for Recovering High Purity Rare Earth Metals from Room Temperature Ionic Liquids," accepted on 7/10/2017.

## **Interns and Post Docs**

Interns: Brandon Day, Cassara Higgins, and Jason Mitchell.

## **Collaborations**

Universities: University of Utah, University of Nevada Las Vegas, and Idaho State University.

## 17A1-166FP: Electrochemical Reduction of CO<sub>2</sub> Enriched in Switchable Polarity Solvents

Luis A. Diaz Aldana,<sup>1</sup> Aaron Wilson,<sup>1</sup> Tedd Lister,<sup>1</sup> Birendra Adhikari,<sup>1</sup> and Eric Dufek<sup>1</sup>

### General Project Description

This project aimed to develop a process to efficiently convert CO<sub>2</sub> to value products or intermediates, with syngas as first target. The impetus is to improve carbon efficiency, improve biorefinery economics, and reduce greenhouse gas emissions. To achieve this goal, switchable polarity solvents (SPS) are used as capture-electrolyte media to facilitate the delivery of CO<sub>2</sub> to the electrocatalyst. The electrochemical reduction of CO<sub>2</sub> should be driven by electricity obtained from clean power-generation units. As the electrochemical reduction can be performed at mild conditions of pressure and temperature, biomass treatment facilities can take advantage of distributed renewable-energy sources, such as nuclear energy, solar panels, and wind turbines to supply the process-energy requirements. This work produced a technology link between clean electricity generation and manufacturing of sustainable fuels and chemicals.

### Summary

The following have been achieved:

1. Technical feasibility for the reduction of CO<sub>2</sub> present in SPS have been verified.
2. A new cathode electrode architecture than enhance the release and reaction of the captured CO<sub>2</sub> was developed.
3. For the first time captured CO<sub>2</sub> has been reduced to CO with conversions and yields over 70 % and at current densities over 100 mA cm<sup>-2</sup>. The produced syngas is a non-diluted product with H<sub>2</sub>:CO ratios between 2 and 4.
4. A provisional patent has been filed.
5. One summer intern and one postdoctoral researcher were involved in the project.
6. One peer review publication has been accepted.
7. The project is currently being consider to apply for TCF.

### Benefits to DOE

This technology directly contributes to the INL energy mission through the advancement of a technology that could transfer renewable electrical energy into a high-grade fuel compatible with the existing transportation infrastructure. Advances in this area of study are needed to provide ways to utilize energy from distributed power sources such as nuclear, wind, and solar.

### Publications

Diaz, L. A., N. Gao, B. Adhikari, T.E. Lister, E.J. Dufek, and A. D. Wilson, “Electrochemical Production of Syngas from CO<sub>2</sub> Captured in Switchable Polarity Solvents”, *Green Chemistry*, accepted manuscript; DOI: 10.1039/c7gc03069j

### Presentations

“Assessment of the use of switchable polarity solvents for delivery of CO<sub>2</sub> for electrochemical reduction”, 232<sup>nd</sup> *Electrochemical Society meeting*, October 1-6 2017.

“Electrochemistry as a Sustainable Alternative for Distributed Processing of Biomass”, *2017 Annual AIChE* meeting, October 29 to November 3, 2017.

### **Invention disclosures, Patents, and Copyrights**

BA-908 Electrochemical Reduction of CO<sub>2</sub> Enriched in Switchable Polarity Solvents.

### **Interns and Postdocs**

Intern: Ningshengjie Gao.

Postdoc: Birendra Adhikari.

### **Collaboration**

University: Oregon State University.

## 17A1-173FP: Fractionation of Lignocellulosic Biomass with Switchable Polarity Solvents

Carter Fox,<sup>1</sup> Aaron Wilson,<sup>1</sup>

### General Project Description

Switchable polarity solvents will be used to selectively fractionate lignocellulosic biomass into primary chemical components, namely cellulose, hemicellulose, and lignin. Switchable polarity solvents are a relatively new class of chemicals that can reversibly change from water-immiscible, non-polar form to water miscible, polar form in the presence of a chemical “switch.” INL has developed deep expertise in fundamental SPS chemistry through efforts to couple SPS with forward osmosis for water treatment. In their polar form, switchable polarity solvents have chemical characteristics similar to those of room-temperature ionic liquids (RTILs), which are known to be highly effective materials for fractionating biomass. Recently published research on switchable-polarity-solvent systems similar to those studied at INL bolsters the idea that switchable polarity solvents can be used to effectively fractionate biomass. Using the fundamental principles gained from biomass fractionation research with RTILs and the reported switchable-polarity-solvent systems, the research project proposes to apply INL expertise in SPS and biomass chemistry to develop a new, low-cost method to fractionate biomass for commercial biorefining. A defined set of process variables will be investigated to determine optimized systems for selectively extracting cellulose, hemicellulose, and lignin from different biomass sources (herbaceous agricultural residues, hardwoods, and softwoods). The ability to recover the extracted materials and recycle switchable-polarity=solvent chemicals will also be tested. The data obtained from these experiments will be used to produce a techno-economic model to determine whether switchable-polarity-solvent fractionation would be an economically competitive biomass treatment for a commercial biorefinery.

### Summary

No progress to report. The principle investigator left INL, and the project was closed.

## 17P11-001FP: Enabling Material Discovery for Waste Heat Recovery Systems using a Multimode Optical Sensor

David Hurley,<sup>1</sup> Robert Schley,<sup>1</sup> and Marat Khafizov<sup>1</sup>

### General Project Description

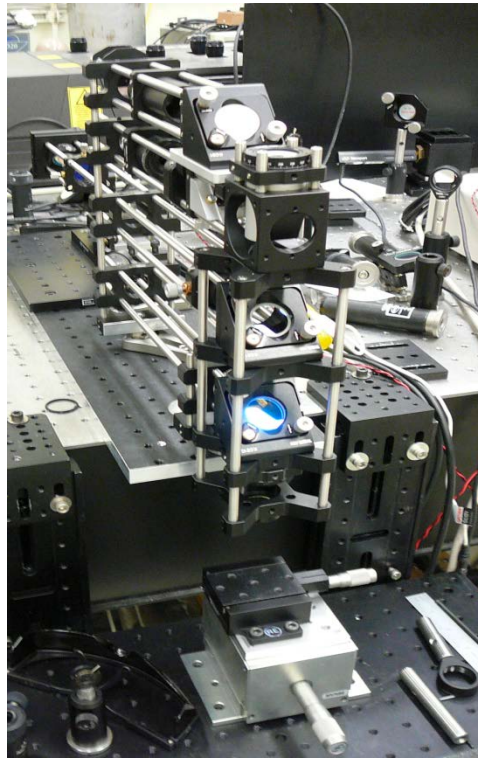
The work outlined in this project involves the development of a multimode optical sensor that will facilitate the creation of new materials for hybrid energy systems. Specifically, coherent acoustic phonon spectroscopy will be combined with diffusive wave microscopy to simultaneously image grain-boundary structure and function in  $\text{UO}_2$ ,  $\text{CdTe}$  and  $\text{PbTe}$ —three model ceramic materials envisioned for use in the hybrid energy industry. A notable aspect of the proposed research is that the measurement methodology can provide critical insight into the development of new sensors for in-situ, operando, in-pile characterization of system performance. A single measurement approach that can aid in material discovery and monitor system performance will provide a disruptive change for the development of hybrid energy technology.

### Summary

There were two main focus areas for the work conducted in FY-17. The first involved performing picosecond ultrasonic experiments on  $\text{CdTe}$ .  $\text{CdTe}$  is a very important photovoltaic material with unusual properties. The polycrystalline form of  $\text{CdTe}$  exhibits greater photovoltaic efficiency than the single crystal form. The role of grain boundaries is not well understood. One theory contends that the built-in field near boundaries is sufficient to screen recombination centers, thereby increasing carrier lifetime. Our investigative approach involves using Brillouin scattering experiments to measure the electric field near grain boundaries. Our preliminary results show that Brillouin oscillations are readily produced without a transducer film by using a blue pump and a red probe. Specifically, we found that the damping is greatly reduced by using a pump tuned to be slightly above the bandgap of  $\text{CdTe}$ . We have also demonstrated that the oscillation frequency has a strong dependence on crystal orientation. Currently we are working on synthesizing a large grained sample by annealing at high temperatures. This sample will be used to measure the orientation of the grain boundary and the built-in field associated with the grain boundary.

The second focus involved design and construction of an optical cage system to improve optical stability and ease of use. From our experience with a similar optical instrument, Thermal Conductivity Microscope, this is important for attracting new customers. The cage system uses off-the-shelf optical components and incorporates the delivery of both the pump and probe beam as well as providing a white light image used for sample positioning. The pump can be scanned relative to the probe at the sample surface by changing the input angle into the microscope objective. This optical system also has a modular common path interferometer that can be used to measure out-of-plane motion caused by the propagation of ultrasonic waves. A picture of the completed system is shown in Figure 1.





*Figure 9. Optical cage system used for pump and probe delivery as well as microscopic white light imaging.*

## Benefits to DOE

Hybrid energy systems offer great potential to recover waste heat associated with both the manufacturing and energy sectors. However, materials development for hybrid energy is complicated by multi-component, multi-element systems that often have competing performance characteristics. Expediting materials development will require new characterization techniques that can rapidly measure multiple properties in multiple samples having variable composition. As an example, consider waste heat recovery using a hybrid photovoltaic and thermoelectric device. A multimodal characterization tool that could measure carrier recombination time and thermal conductivity would (1) greatly accelerate material development by enabling a new, combinatorial approach to materials discovery and (2) provide an effective non-intrusive method to actively measure the integrity of materials in complex geometries. Moreover, the use of embedded sensors for active health diagnostics of hybrid systems components (that may include radioactive heat-transfer media) can help accelerate their development and licensing. The work outlined in this proposal involves the development of a multimode optical sensor that will facilitate the creation of new materials for hybrid energy systems. A notable aspect of the proposed research is that the measurement methodology can provide critical insight into the development of new sensors for in-situ, operando, in-pile characterization of system performance. A single measurement approach that can aid in material discovery and monitor system performance will provide a disruptive change for the development of hybrid energy technology.

## 17P11-030FP: Investigation of Exciton Delocalization and Exciton Coherence in Chromophores and Acoustic Nanostructures

David Hurley,<sup>1</sup> Bernard Yurke,<sup>1</sup> William Knowlton,<sup>1</sup> Paul Simmonds<sup>15</sup>

### General Project Description

Exciton delocalization and coherence will be investigated in dye molecule (chromophores) networks and acoustic nanostructures, two promising systems for the realization of universal quantum computers. This will be a joint effort between faculty members in the Micron School of Materials Science and Engineering and the Physics Department at Boise State University (BSU) and scientists and engineers at Idaho National Laboratory (INL). The BSU component of the study investigates Frenkel excitons associated with dye molecules. The INL component investigates manipulation of Wannier-Mott excitons in semiconductor materials using ultrahigh-frequency surface acoustic waves (acoustic nanostructures). Exciton delocalization and coherence in both systems will be examined using time-resolved spectroscopy.

This is a fundamental materials-science project that explores the manipulation of excitons in condensed matter and molecular systems. It aligns squarely with INL's emerging core competency in condensed-matter physics and applied materials science. This project brings together researchers from a wide range of backgrounds to investigate two complementary excitonic systems. The effort is deliberately organized to promote interaction between scientists and engineers at INL and BSU, as well as to promote the flow of ideas between research components. Studying differences and similarities between the two systems will introduce valuable new perspectives and allow researchers more effectively to test the efficacy of new system designs.

### Summary

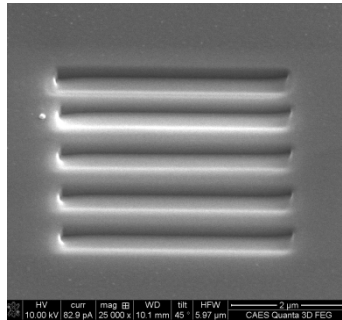
The primary focus of this project is to demonstrate exciton delocalization and coherence in two complementary excitonic systems.

*Molecular Excitonic Systems:* Work at BSU is underway to develop laboratory capability and hire technical specialist to assist in sample synthesis and preparation as well as 2D spectroscopy. Personnel augmentation at BSU is discussed in the following section. The following is a list of new laboratory capability acquired at BSU:

- Purchased optical equipment for pump probe and 2 D spectroscopy experiments to be conducted under the LDRD and have identified optical components to purchase before FY end.
- Designed an H-aggregate exciton transmission line. Purchased the DNA for the transmission line.
- Purchased heavy water and sodium tungstate to see if changing the medium mass density can give rise to longer coherence lifetimes in Cy5 dye complexes due to acoustic impedance mismatch of the dyes with the surrounding medium. Natalya will perform the experiments.

*Solid State Excitonic Systems:* David Hurley and Paul Simmonds have initiated a literature search on how static and dynamic strain fields influence Wannier-Mott excitons. David Hurley is also starting to develop analytical expressions for the magnitude and spatial distribution of the strain and associated static electric field caused by surface acoustic phonons. A subcontract was set up with Assel Aitkaliyeva from the Materials Science

Department at University of Florida to fabricate high frequency absorption gratings using focused ion beam techniques. Initial efforts applying this approach to a silicon sample are shown in Fig1.



*Figure 10. Scanning electron microscope image of grating fabricated using focused ion beam techniques.*

From the project start date until now, Paul Simmonds' molecular beam epitaxy system has been down for its annual maintenance cycle. This cycle allows his group to complete any necessary repairs to the system, install new pyrolytic boron nitride crucibles, replenish the ultrahigh purity source metals, and carry out preventative maintenance tasks. This summer's maintenance cycle has been a little longer than usual as he has also upgraded certain parts of the system, and added interlocking on process-critical components so that in the event of an emergency such as a power outage, the machine would be much better protected against serious damage. We anticipate that his molecular beam epitaxy chamber will be back on line and ready to grow material by the end of September, 2018.

Paul Simmonds has also been working to build a photoluminescence spectroscopy measurement system in the laboratory of a faculty colleague at Boise State, Dr. Dmitri Tenne. Dr. Tenne's expertise is in the area of Raman spectroscopy and he has generously agreed to let us use his optical tables, lasers and cryostat to build this crucial measurement system. The system Paul Simmonds is constructing is based around silicon and InGaAs photodetectors, which will allow him to investigate materials emitting light from visible wavelengths out to 1700 nm in the infrared, easily covering the wavelength range of interest for this project. Photoluminescence allows interrogation of the semiconductor band gaps of our materials to assess crystalline quality and alloy composition. In addition, Paul Simmonds we will be able to accurately characterize the quantum wells at the heart of the proposed work to study the excitonic spectra.

## **Benefits to DOE**

The work outlined in this proposal seeks to uncover new paradigms for realizing quantum computation systems. This is a fundamental materials-science project that explores the manipulation of excitons in condensed matter and molecular systems. It aligns squarely with INL's emerging core competency in condensed-matter physics and applied materials science. Disruptive projects like this will help researchers at INL gain a fresh, basic science perspective on current materials-based programs. Enhanced understanding of the fundamental physical principles that are the foundation of materials science will be a key element in INL's strategy to more effectively interact with DOE's, Basic Energy Science Program under the Office of Science. Basic physical-sciences research is necessary to understand, predict, and control energy at the electronic, atomic, and molecular levels in order to provide the foundations for new technologies that support INL missions in energy and national security. In collaboration with scientists from Boise State University, this project seeks to investigate new methods to drive and manipulate quantum effects in materials. By building a strong and lasting relationship with faculty members at BSU involved in quantum-computation-systems research, this project will bolster INL's foundation in condensed-matter physics and applied materials science.

## **Interns, Postdocs, and Staff Support for Graduate Studies**

Interns: Robin McCown, Allison Christy, and Paul Simmonds.

Staff Support for Graduate Studies: Dr. Ryan Pensack, Robin McCown, and Natalya Hallstorm.

## **Collaboration**

Universities: Princeton University and Boise State University.



# Critical Infrastructure Protection



- 15-094: Risk-Informed Safety, Security, and Safeguards by Design Guidance for Advanced Reactor Concepts
- 15-100: RTPS Real-Time Process Simulator
- 15-111: Adversary Signature Development and Threat Analysis
- 16-081: Modeling Thermite Reactions
- 16-085: Production of Fluoroanion Targets for Accelerator Mass Spectrometry
- 16-098: <sup>14</sup>C Analysis by Accelerator Mass Spectrometry: N&HS Capability Development
- 16-106: ICS-CAPE: Industrial Control Systems  Cyber Attacks and their Physical Effects
- 16-129: Application of Radioactive Isotope Dilution Technique to Measurement of Molten Salt Mass for Electrochemical Recycling Process
- 16-133: Secure SCADA Communications System
- 16-152: Wireless radio Frequency signal Identification and protocol Reverse Engineering (WiFIRE)
- 16P6-007FP: Consequence-driven Cyber-informed Engineering (CCE) Methodology Pilot
- 17A1-079FP: Affixing Inert Dissimilar Materials to Structural Materials for High Performance Armor Systems
- 17A1-101FP: Nuclear Instrumentation and Methods for Emergency Response
- 17A1-106FP: A Study of Fission Modes to Improve Nuclear Forensics
- 17A1-109FP: Scalable Binary Analysis
- 17A1-114FP: Resilient, Scalable Cyber State Awareness of Industrial Control System Networks to Threat
- 17A1-142FP: Modeling and Spatial-Temporal Analysis of Cyber-Physical Impacts
- 17A1-152FP: Building Systems: Access, Management, & Automation
- 17A1-156FP: Nuclear Safety Systems Cyber Security
- 17A1-160FP: Mass Storage Equipment Protection
- 17A1-162FP: Securing Electronic Control Unit Communication
- 17A1-178FP: Forensics of Embedded Devices
- 17A1-183FP: V2X Communications Security
- 17A1-206FP: Large Scale Log Analysis for Control System Networks

## 15-094: Risk-Informed Safety, Security, and Safeguards by Design Guidance for Advanced Reactor Concepts

Jeff Sanders,<sup>1</sup> Jay Disser,<sup>1</sup> and Janine Lambert<sup>1</sup>

### General Project Description

The 3S by Design (3SBD) concept is designed to capture and potentially optimize the relationships between safety, security, and international safeguards of a nuclear facility. This project intends to provide nuclear reactor operators and designers with both a cost-effective method of integrating safety, security, and safeguards considerations into reactor design and a risk-informed decision making platform for safety, security, and safeguards personnel. Because the pebble bed fast high-temperature reactor (PB-FHR) design is in its initial stages that reactor system was chosen as a test case for a quantitative application of the 3SBD approach. Insights resulting from analysis are expected to be relevant to other advanced reactor designs, e.g. the gas-cooled pebble modular reactor and, potentially, low-pressure coolant reactor designs like the sodium-cooled fast reactor.

The 3SBD framework used for this research is notionally shown in Figure 1 (a complete 3SBD analysis of the PB-FHR would require an expanded framework that is beyond the scope of this project). The first step defines the pre-conceptual design of the facility of interest. The next step identifies off-normal scenarios, which covers potential initiating events and vulnerabilities across the 3S spectrum. During this project, RELAP5-3D was used to evaluate the response of the PB-FHR passive decay heat removal system while a simplified nuclear material accountancy model was developed to analyze the pebble fueling strategy. Prior efforts focused on safety analysis of the PB-FHR concept; for FY-17, efforts focused on the nuclear material accountancy issues. Aspects of security were not studied independently, but were identified in both the safety and safeguards analysis.

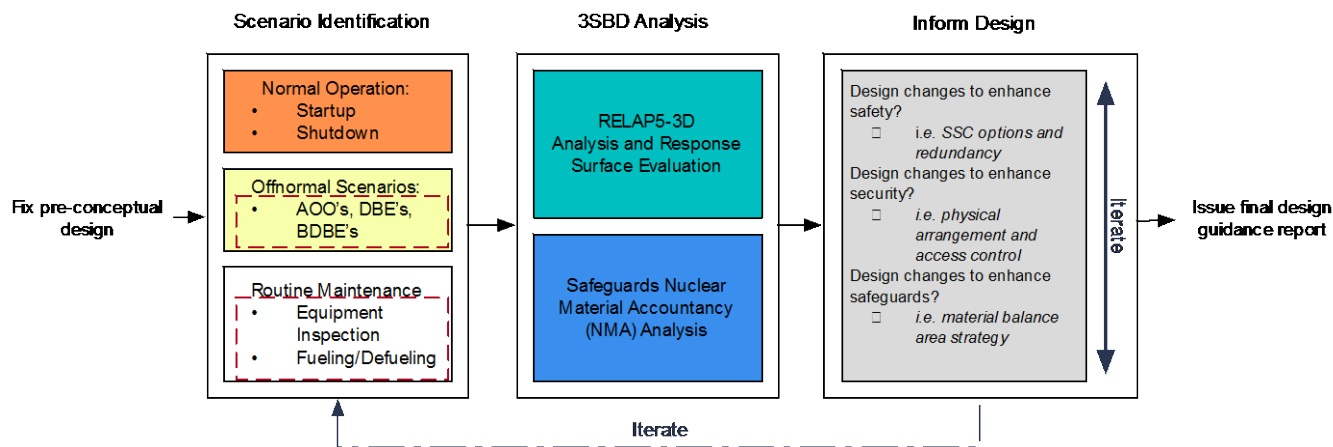


Figure 1. Notional schematic showing 3SBD approach.

### Summary

In order to evaluate the impact of safeguards of the PB-FHR, a nuclear material accountancy analysis was performed by using the projected material flows through the reactor system and the published uncertainties for existing instrumentation. This activity was initiated in FY-16 and continued and refined in FY-17. Preliminary analysis indicated that the most sensitive areas of the plant in regards to measurement uncertainty are fresh fuel storage and spent fuel storage, where the inspector and operator



are going to be making measurements on large containers that contain thousands of pebbles in order to determine the mass of the nuclear material inside. As part of this study, four facility misuse scenarios were examined:

1. Diversion and removal of spent fuel
2. Diversion and removal of partially-spent fuel
3. Diversion and removal of fresh fuel
4. Misuse of the PBMR for undeclared feed, irradiation, and withdrawal of spent fuel [3]

An in-depth assessment of the conceptual PB-FHR reactor with regards to international safeguards was completed. Two possible accountancy structures were designed and analyzed. The main differences between the two is the location of the Inventory Key Measurement Point (IKMP) for the active fuel area and the existence of an Other Strategic Point (OSP) in structure 2. Figures 2 and 3 show accountancy structures #1-2.

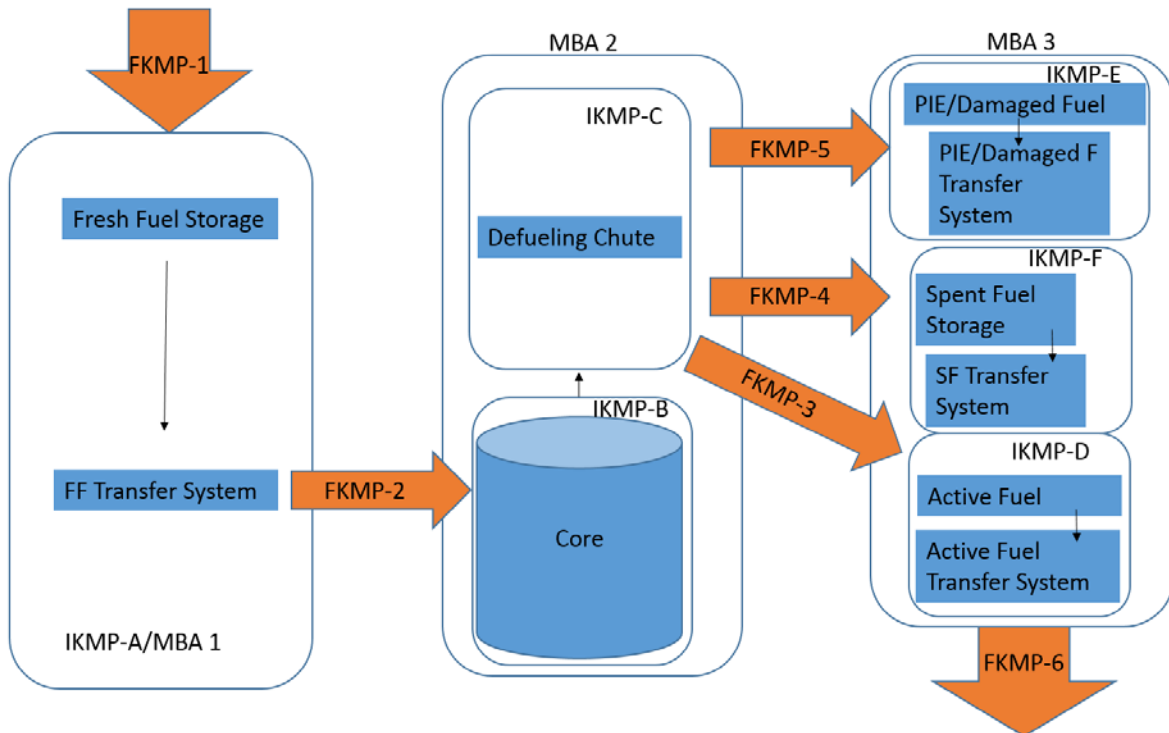


Figure 2: Accountancy Structure Possibility #1

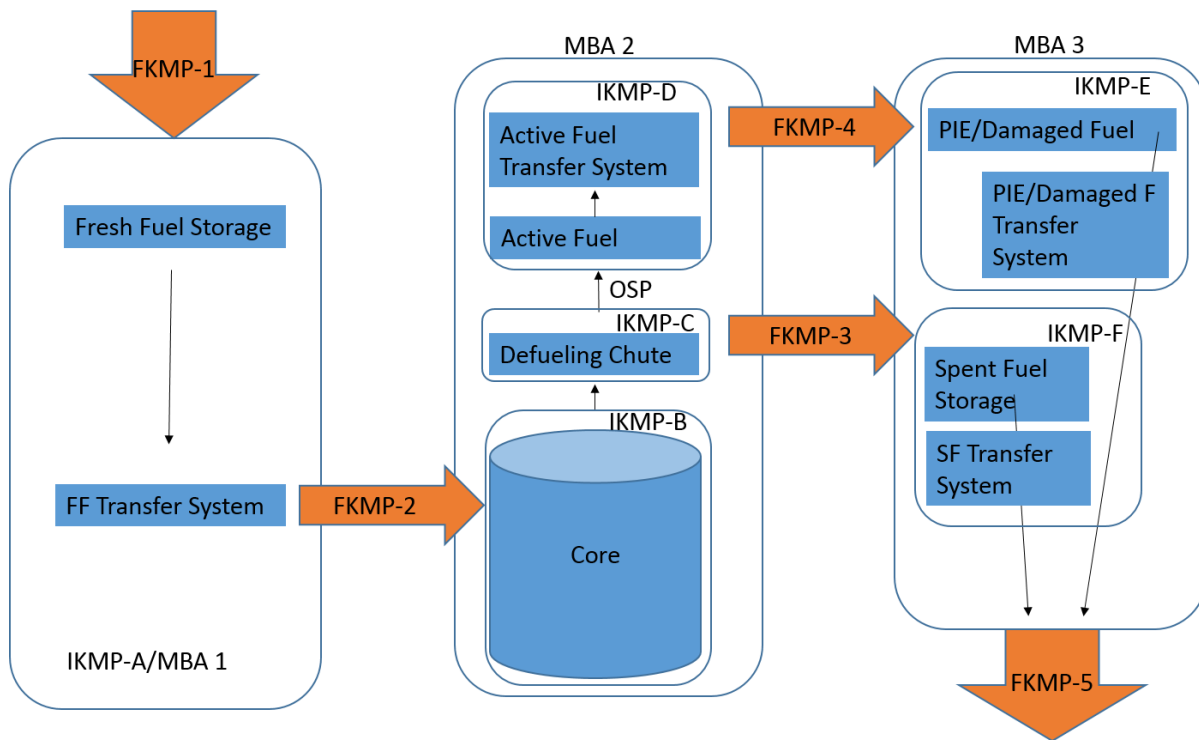


Figure 3: Accountancy Structure Possibility #2

The primary motivation for implementation of these accountancy structures will be determined by the ability of a pebble counting technology. System #1 assumes that an effective counting and burnup verification system for input and output pebbles can be developed. System #2 has additional OSP, and IKMPs to mitigate potential limitations of this system. Either approach can be applied to the PB-FHR, but if an effective pebble counting and burn-up technology cannot be developed, individual unit size and scale of multi-unit installations may be limited. Detailed evaluation of security diversion scenarios and timelines were not within the scope of this study, but the safeguards accountancy approach and MBA structure will define the basis of the security system.

### Benefits to DOE

This project will place the United States in a stronger position when engaging other countries on 3SBD for critical nuclear infrastructure by providing a more objective method for 3SBD evaluation. This project will also establish a foundation to move 3SBD from concept to practice. China is actively developing and demonstrating two pebble-bed reactors. The Chinese PB-FHR is being developed by the Chinese Academy of Sciences and is expected to start construction in 2017. Although a cooperative research and development agreement between the Chinese Academy of Science and Oak Ridge National Laboratory was signed, very little effort in the research and development process has focused on safeguards or security considerations. INL's leadership in thinking critically about using safety, security, and safeguards insights early in the design process can improve next-generation nuclear infrastructure.

## References

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- Johnson, Shirley, 2017, “Thoughts on the Safeguards Approach for A Selected Pebble Bed Reactor”, Tucker Creek Consulting PLLC (September 2017 Revision 1).
- Durst, Philip Casey et al., 2009, “Nuclear Safeguards Considerations for the Pebble Bed Modular Reactor (PBMR)”, Idaho National Laboratory, (2009).
- Boyer, Brian D. and David H. Beddingfield, 2010, “Pebble Bed Modular Reactor Safeguards: Developing New Approaches and Implementing Safeguards by Design”, Los Alamos National Laboratory, (2010).

## Publications

- Arthur, E., E. Blandford, J. Disser, et al., 2016, “Demonstration of the 3SBD Concept for the Pebble Bed Fluoride Salt-Cooled High Temperature Reactor (PB-FHR),” INMM Annual Meeting Proceedings, July 2016.
- Disser, J., E. Arthur, and J. Lambert, 2016, “Preliminary Safeguards Assessment for the Pebble Bed Fluoride Salt-Cooled High Temperature Reactor (PB-FHR) Concept,” Advances in Nuclear Nonproliferation Technology & Policy Conference Proceedings, American Nuclear Society, September 2016.

## Interns, Postdocs, Staff

Intern: Janine Lambert

## Collaborations

University: University of South Florida

## 15-100: RTPS Real-Time Process Simulator

Jared Verba<sup>1</sup> and Gordon Rueff<sup>1</sup>

### General Project Description

The purpose of the Real-Time Process Simulator (RTPS) Project is to generate a proof-of-concept simulation framework for industrial control systems (ICSs). This research creates a more open and robust ICS remote input/output (IO) simulation framework for devices outside of the IT network. This will enable current and future research efforts to produce more holistic and innovative cybersecurity solutions for ICS. By developing a field IO simulation framework that requires hardware in the loop for logic, researchers can look at solutions for protecting a system at the field-device level, i.e., programmable logic controller (PLC) or remote terminal unit (RTU) level. A side effect of this research is better understanding and simulation of ICS proprietary protocols, devices, and sensors.

### Summary

This project accomplished all planned tasks for each funded year. Many resources in FY-17 has been focused on making the system more robust, scalable and usable for researchers. The Real Time Process Simulator (RTPS) currently works with the Siemens WinCC control system software and several Siemens PLCs. Additional development areas include integration of Visio diagrams, Asynchronous injection of testing events and a more scalable architecture.

Users are able to use Microsoft Visio to generate a process control diagram and connect all components together as they would be in a real process control system. A new Visio add-on is able to determine how pieces are connected and transform that information into something the simulation can understand. This is a big step forward as previous methods involved making the connections manually via text file.

RTPS now has a ground truth web interface that is able to view the simulation components in real time and inject commands into the simulation. This can be used to verify a component's status as well as inject testing scenarios into the simulation. A user can now force a pump or valve to fail or stick in a particular state without any significant programming or low level knowledge of the simulation.

The current simulation system is able to run on a single computer host and makes the most of the processing power available. It is also able to be deployed onto a Linux cluster to achieve maximum scalability for very large systems. This allows for very high component count and complex simulations.

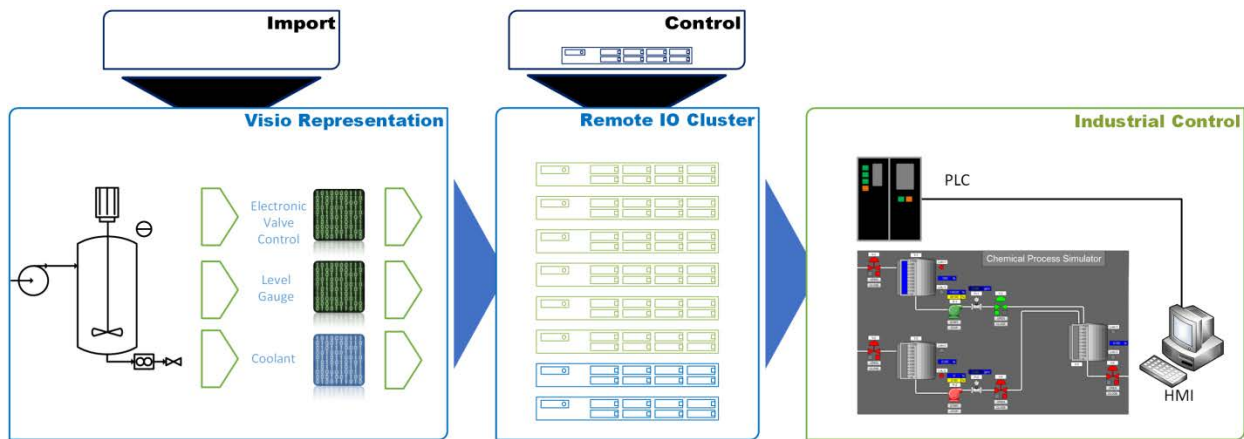


Figure 1. RTPS overview.

## Benefits to DOE

An additional year of research was used to build a capability that aligns with CIC technology goals. An Invention Disclosure Record was created from the research in the LDRD. Additional work with INL Nuclear Cyber Group has started, possibly to use the simulation aspect in a training environment.

## 15-111: Adversary Signature Development and Threat Analysis

Sarah Freeman<sup>1</sup> and Katya Le Blanc<sup>1</sup>

### General Project Description

Cyber security is most effective before an attack. However, the development of adequate proactive protection remains a challenge. Recent years have seen an explosion of threat-focused research aiming to meet the needs of an ever-evolving cyber landscape. Organizations, both public and private, have sought to advance threat analysis processes, methodologies, and capabilities in order to improve capabilities and training for the next generation of defenders. This research will improve our understanding of the cyber community by developing additional structured analytical techniques and a corresponding model to address the current challenges facing complex threat analysis.

### Summary of Scientific, Technical, and Programmatic Progress

This research blends the current concepts of behavioral economics with the analytical procedures used in law enforcement and the intelligence community in order to fill the current gap in threat analysis capabilities. The goal of this work is greater understanding of how hackers interact, share information, approach problems, and use technology. Central to this process is the development of a model that more fully describes attack scenarios and campaigns. The model is supported by a collection of indicators (such as exploits and malware used), which serve as the basis for attribution. The research conducted during FY 2015 covered two related, but uniquely focused, phases for the identification, development, and verification of a new collection of indicators. Data collected from these two phases has been combined into a single model, which will serve as a library of information for the development of cyber adversary profiles (see **Error! Reference source not found.**).

A critical component of Phase I included development and analysis of cyber incidents. The goal of this process was two-fold. First, it ensured a wider perspective was considered for both this research and the development of the combined model, as it was assumed that the cyber researcher participants were not representative of the complete hacker culture. Second, post-mortem analysis of cyber incidents assisted with the aggregation of ‘typical’ indicators (i.e., the components most often tracked and recorded following a cyber incident). During the second year of research, this work incorporated input from researchers from the Graduate School of Public and International Affairs at the University of Pittsburgh.

The experimental design for Phase II included two vetted psychological assessment tools (i.e., the Need for Cognition Scale and the Big Five Inventory), as well as an INL-designed structured interview protocol to investigate the experiences, skills, and technology preferences of the cyber security community. By expanding quantitative data beyond that traditionally collected post-incident, the research team was able to develop a more comprehensive picture of the personal motivations and thought processes of these individuals. By the same token, the inclusion of cyber incident data allowed the research team to evolve the ontology further than would be possible with the interviews alone, especially given the size of the potential sample pool. The end result of this holistic approach is a more comprehensive picture of potential signature components that can be expanded in the future.

During the third year (FY2017), the project work focused on expanding both the participants within the interview process, as well as the incidents in the database. Additionally, the University of Pittsburgh team has also developed a number of different reports on current events that have emerged this year (e.g. Industroyer/CrashOverride).

## Benefits to DOE

This research contributes directly to DOE's goal of securing critical infrastructure from cyber attacks by evaluating the existing cyber researcher community's methods and capabilities. This novel threat analysis approach will allow organizations to more accurately characterize the modern cyber threat actor, promoting creation of evolved industrial control systems protection systems. Additionally, findings from this work will allow us to more fully define the necessary skills for developing the next generation of cyber defenders.

## Publications

Le Blanc, K. and S. Freeman, 2016, "Investigating the Relationship between Need for Cognition and Skill in Ethical Hackers," publication in *Advances in Intelligence Systems and Computing, proceedings of the 7th International Conference on Applied Human Factors and Ergonomics*, Orlando, Florida, July 2016.

## Presentations

Le Blanc, K., 2017, "Adversary Signature Development and Threat Analysis," *2017 LDRD Poster Session*, Idaho National Laboratory, August 30, 2017.

Freeman, S., 2017, "Adversary Signature Development and Threat Analysis," *Strategic Advisory Committee Poster Session*, Idaho National Laboratory, June 29, 2017.

Le Blanc, K. and S. Freeman, 2016, "Investigating the Relationship between Need for Cognition and Skill in Ethical Hackers," *7<sup>th</sup> International Conference on Applied Human Factors and Ergonomics*, Orlando, Florida, July 29, 2016.

Freeman, S., 2016, "Adversary Signature Development and Threat Analysis," *Strategic Advisory Committee Poster Session*, Idaho National Laboratory, June 30, 2016.

Freeman, S., 2015, "Expanding the Cyber Portfolio," *RCTCon2015*, Baltimore, Maryland, December 9 and 10, 2015.

Freeman, S., 2015, "Adversary Signature Development and Threat Analysis," *Strategic Advisory Committee Poster Session*, Idaho National Laboratory, June 25, 2015.

Freeman, S., 2015, "Expanding the Cyber Portfolio," *Early Career Researcher Symposium*, Idaho National Laboratory, July 30, 2015.

## Interns, Postdocs, and Staff support for Graduate Studies

Interns: Rachael Hill, Andrew McClusky, Cynthia Chavez, Brendan Lyle, Kevin Pollock, Abby Waliga, Michael Goldstein, Alex Lin, Brian Liston, Luis Alonso, Eric Jackson, Kevin Jeong, Harsheen Sethi, Lin Wang,

Postdoc: Wei Zhang



## 16-081: Modeling Thermite Reactions

Ron Heaps,<sup>1</sup> Hai Huang,<sup>1</sup> Jing Zhou,<sup>1</sup> Bryan Curnutt,<sup>1</sup> Michelle Pantoya,<sup>23</sup> and Ryan Bratton<sup>1</sup>

### General Project Description

This project built a model, under the MOOSE framework, that describes the propagation of an exothermic reaction and tracks the reaction wave in a material compact. This model encompasses the reaction rate of the material as well as phase changes during the reaction. Research efforts continue focus on the addition of more complexity to the model by incorporating density, porosity, particle-size effects, and boundary conditions. This MOOSE application, referred to as Raptor, is built on a 2D mesh (10 × 400) and generates an output file that tracks the reaction. Preliminary results demonstrate that the model is following what is observed in experimental data and publications.

### Summary

Heat transfer is the primary driver for the combustion wave in highly exothermic thermite reactions. The heat transfer modules, specifically the heat conduction and heat conduction time derivative kernels are readily available in the MOOSE framework. Steady state heat conduction is given by:

$$-\rho C_p \delta T / \delta t + \nabla \cdot (-k \nabla T) - Q = 0$$

The weak form of the equation is then input in MOOSE syntax. Similarly, heat convection, radiation heat transfer, and a number of other applicable heat transfer boundary conditions, are already utilized by Raptor are available in the MOOSE framework. The current approach utilized in Raptor is to quickly input the adiabatic temperature ( $T_{ad}$ ) and the ignition temperature ( $T_{ig}$ ) of the reaction, or the temperature at which the exothermic reaction takes place into the Raptor input file rather than being calculated by Raptor. These values are then passed to Raptor's forcing function. An additional materials kernel has been added to assign the material properties for both the products and reactants.

We have also set up the model to work with the  $Fe_2O_3$ -Al reaction system and incorporated methods to deal with phase changes in the material during the reactions. The model follows the reaction quite well. As the model progresses original assumptions will be narrowed to better reflect actual conditions. We also are investigating methods to incorporate how to address other physical properties of the compact such as particle size, porosity, and density, surface area and their effects on the reaction.

INL/DOE has used thermite reactions in a variety of projects over the past years. This research will help to understand these reactions better and to be able to use them more efficiently and safely.

### Benefits to DOE

Thermally energetic materials also known as thermite reactions, are used in DOE projects as well as commercially. DOE has used them in a number of projects for national security missions, as well as nuclear research. For example because of the high temperatures they generate the reactions have been used to test a reactor vessel's ability to withstand a meltdown event. Modeling these reactions will allow efficient development of novel thermite materials and prediction of their behaviors to optimize future applications. A good model also reduces the inherent risk of handling and using thermite mixes.

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<sup>23</sup> Texas Tech University

## Publications

“Peering through the flames: imaging techniques for reacting aluminum powders”, *Applied Optics*, Vol 56, No.9, 2017, pg 2535-2541

## Interns and Postdocs

Intern: Ryan Bratton

Postdoc: Jing Zhou

## 16-085: Production of Fluoroanion Targets for Accelerator Mass Spectrometry

Christopher Zarzana,<sup>1</sup> Gary Groenewold,<sup>1</sup> Michael Benson,<sup>1</sup> Rika Hagiwara<sup>24</sup>

### General Project Description

Detection of nuclides of the actinide elements is critical for verifying the compliance of nuclear facilities with international nonproliferation treaties. Current analysis methods require time-consuming and expensive sample preparation to achieve results acceptable to decision makers. Future analytical performance with markedly improved accuracy, precision, sensitivity and faster sample throughput will be required to keep up with an increasingly complex nuclear proliferation environment. Accelerator mass spectrometry (AMS) offers an order-of-magnitude increase in sensitivity for actinide analysis, but the current state of the art still requires exacting separations, limiting throughput. Additionally, actinides are currently analyzed as oxides, which introduce isobaric interference due to the minor isotopes of oxygen, limiting abundance sensitivity and precision. The objective of this project is to develop the technology for rapid production of sample targets for actinide analysis using AMS through the use of actinide fluoroanion salts produced using novel fluorinating ionic liquids and extracted using supercritical CO<sub>2</sub>. Actinide analysis using fluoroanion salts will increase sensitivity and precision through the elimination of oxygen isobars. Additionally, manipulation of the degree of fluorination offers the potential for actinide separation in the ionization source, further reducing the need for chemical separation. The results of this project will be novel methods for the rapid analysis of actinides using AMS, increasing the nation's capabilities in the nuclear nonproliferation sphere.

### Summary

Uranium fluoroanions have been produced by dissolving UO<sub>2</sub> in the fluorinating ionic liquid 1-ethyl-3-methylimidazolium fluorohydrogenate (EMImFHF) (Figure 1). The EMImFHF ionic liquid was provided through our university collaborator Prof. Rika Hagiwara (Kyoto University). Fluoroanion production was successfully verified by electrospray-ionization mass spectrometry. Prof. Hagiwara synthesized three more fluorinating ionic liquids: 1-butyl-3-methylimidazolium fluorohydrogenate (BMImFHF), 1-butylpyridinium fluorohydrogenate (BPyFHF), and 1-butyl-1-methylpyrrolidinium fluorohydrogenate (BMPyrFHF). All three ionic liquids dissolve UO<sub>2</sub> but to significantly different degrees, suggesting the structure of the ionic liquid cation plays a large role in dissolution chemistry.

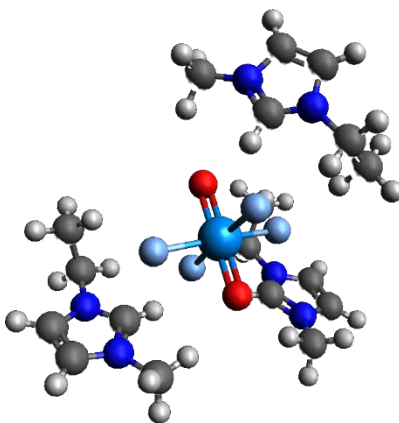


Figure 1. UO<sub>2</sub> dissolved in EMImFHF.

<sup>24</sup> Kyoto University, Kyoto, Japan

To examine the influence of cation on dissolution, the structures of EMIm cation-fluoroanion clusters were probed in collaboration with the FELIX laboratory in Nijmegen, the Netherlands, using infrared multi-photon dissociation (IRMPD). Studies of clusters containing  $\text{UF}_6^-$ ,  $\text{UO}_2\text{F}_3^-$ ,  $\text{UO}_2\text{F}_4^{2-}$ ,  $\text{ZrF}_5^-$ , and  $\text{ZrF}_6^{2-}$  revealed that the anions and cations bind in specific ways depending on structure (Figure 2), which suggests the fluorination chemistry could be controlled by varying structure, one of the main hypotheses of the proposal. We will continue to test this hypothesis with the three newly synthesized ionic liquids, and anticipate returning to the FELIX laboratory to conduct more gas-phase IRMPD measurements. Additionally, these results have suggested further experiments that could provide new insight into the mesoscopic ordering of ionic liquids, an area that is challenging to study, and thus open to further exploration. We also made the first measurements of the IR absorption frequencies of several fundamental vibrational modes of  $\text{UF}_6^-$ ,  $\text{UF}_5^-$ ,  $\text{UO}_2\text{F}_3^-$ , and  $\text{ZrF}_5^-$  as part of our experimental campaign at the FELIX laboratory. Our analysis of the measured experimental spectra suggests that the ionic liquid cations and fluoroanions interact in structurally specific ways.

Therefore, we have begun to develop separation schemes based on differences in solubilities of a cation/metal fluoroanion pairs in supercritical carbon dioxide ( $\text{SC-CO}_2$ ), which can be exploited to effect facile and efficient metal separations. Evaluations of  $\text{SC-CO}_2$  solubility of a wide variety of ion pairing salts have been initiated to identify the optimum ion pairing agent for extracting uranium fluoroanions.



*Figure 2. Gas-phase structure of  $\text{UO}_2\text{F}_4^{2-}$  stabilized by three  $\text{EMIm}^+$  cations. The structure was calculated using density functional theory and matches well with the experimental IRMPD data.*

## Benefits to DOE

This project is developing novel methods for rapid actinide analysis that are urgently needed by DOE and other National Security customers. Rapid, inexpensive actinide analysis methods will greatly enhance the ability of the international community to ensure compliance with international treaties, increasing global security. Additionally, this project also explores the fundamental actinide chemistry needed to develop these methods, furthering the Department of Energy's basic science mission.

## Presentations

Zarzana, C. A., G. S. Groenewold, M. Benson, K. Johnson-Roscioli, J. Martens, J. Oomens, R. Hagiwara, T. Tsuda, 2016, “Spectroscopic and Mass Spectral Characterization of Uranium Fluoroanions Formed from an Ionic Liquid”, INL/CON-16-38799, *Plutonium Futures – The Science 2016*, September 18<sup>th</sup>-22<sup>nd</sup>, 2016, Baden Baden, Germany.

Zarzana, C. A., G.S. Groenewold, M. Benson, J. Martens, J. Oomens, R. Hagiwara, T. Tsuda, 2017, “Gas-Phase Spectroscopic Characterization of Ionic Liquid-Hexafluorouranate Clusters”, INL/CON-17-41447, *Actinides 2017*, July 9<sup>th</sup>-14<sup>th</sup>, 2017, Sendai, Japan.

## 16-098: $^{14}\text{C}$ Analysis by Accelerator Mass Spectrometry: N&HS Capability Development

Mathew Snow,<sup>1</sup> John Olson,<sup>1</sup> Matthew Watrous,<sup>1</sup> Mary Adamic<sup>1</sup>

### General Project Description

The objectives of this LDRD are to develop and demonstrate the capability to measure ultra-trace  $^{14}\text{C}$  within samples analyzed for environmental protection and nuclear nonproliferation verification. These methodologies, intended to enable enhanced use of accelerator mass spectrometry (AMS) technology now available at INL, will also enable further research in a wide range of scientific fields relying upon radiocarbon dating measurements. This project is pursuing advances in technologies for analyzing sample matrices including organic, inorganic, and air samples.

### Summary

Achievements to date include: 1) establishment and significant improvement in  $^{14}\text{C}$  measurement precision at INL, 2) development and validation of sample pretreatment methods for vegetation and soil samples, and 3) demonstration of INL  $^{14}\text{C}$  analysis capabilities via two publishable case studies. Future work for FY-18 includes continued refinement in measurement precision,  $^{14}\text{C}$  detection limits, and development of analysis techniques for air samples ( $\text{CO}_2$ ,  $\text{CH}_4$ ).

#### 1. Initial Capability Establishment and Measurement Refinements:

In FY-16 the INL team established a preliminary capability to analyze  $^{14}\text{C}$  from simple organic compounds at the 1-2% ( $1\sigma$ ) measurement precision level. This capability was established with considerable advice from collaborators at the University of California-Irvine (Dr. Southon, Dr. dos Santos, and Dr. Xu). In FY-17 the INL team refined its  $^{14}\text{C}$  measurement precision to its current value of 0.3-0.5% ( $1\sigma$ ). These refinements were brought about by improvements in the sample preparation chemistry and AMS instrumentation and enable significant enhancement in INL's capability to quantify and attribute  $^{14}\text{C}$  from non-background sources within samples.

#### 2. Environmental Sample Pretreatment Method Development (soils and vegetations):

Accurate assessment of the  $^{14}\text{C}$  composition in soil and vegetation samples requires specific pretreatment techniques. These techniques remove unwanted forms of carbon (e.g. lignins, humic/fulvic acids, inorganic carbonate species, etc) and isolate the specific chemical form(s) of  $^{14}\text{C}$  representing the source term(s) of interest (e.g. cellulose for vegetation samples and organic/elemental carbon for soil samples). In FY-17 the INL team established 1) a vegetation pretreatment method utilizing a two step Soxhlet extraction process followed by sodium chlorite treatment and 2) a soil sample treatment method utilizing an acid digestion followed by a two stage combustion process. The effectiveness of these pretreatment processes is currently being demonstrated through analyses of tree and soil samples taken near the INL site and at the Nevada National Security Site.

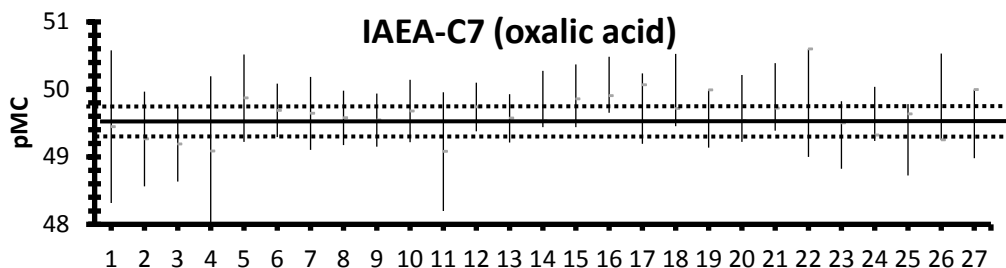


Figure 1. FY-17  $^{14}\text{C}$  replicate analyses of standard material IAEA-C7 (oxalic acid), demonstrating INL's current  $^{14}\text{C}$  measurement accuracy and precision.

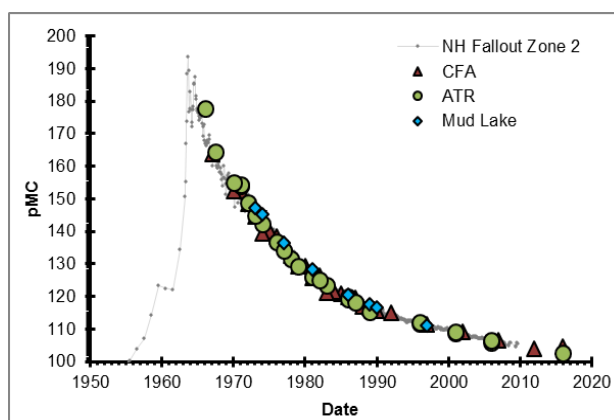


Figure 2. (left) Intern Jessica Ward collecting a tree core sample under the direction of INL scientist Mary Adamic. (right) Analyses of tree ring samples collected from the CFA, ATR, and Mud Lake. INL data correlates quantitatively with northern hemisphere global nuclear weapons testing fallout backgrounds.

### 3. Case Study Demonstrations of INL $^{14}\text{C}$ Measurement Capabilities:

$^{14}\text{C}$  emitted from nuclear facilities has the potential to be uptaken in the vegetation and soils surrounding these facilities. The INL team collected tree and soil samples from several locations around the INL site to determine the local  $^{14}\text{C}$  backgrounds and historic airborne  $^{14}\text{C}$  levels (Figure 2). These analyses reveal that historic annual, integrated  $^{14}\text{C}$  concentrations at CFA, ATR, and Mud Lake areas were consistent with regional background levels, suggesting that average integrated  $^{14}\text{C}$  emissions from the INL site were indistinguishable from global fallout levels. Results from this work are currently being prepared for publication in the Journal of Nuclear Instruments and Methods B.

Surface soil samples taken from the Nevada National Security Site provide a second case study for demonstrating INL's  $^{14}\text{C}$  capabilities. Unlike the INL site, increases in  $^{14}\text{C}$  of up to 3,000 pMC (> 30x increase over regional backgrounds) is observed in surface soils beneath above ground testing areas. Analyses of inorganic, organic, and elemental carbon fractions and correlations between  $^{14}\text{C}$  concentrations and venting operations and test yields are ongoing. Publication of this work is anticipated in early FY-18.



## Benefits to DOE

The  $^{14}\text{C}$  AMS analysis capability being established under this LDRD has led to two full proposals currently under consideration (NNSA Office of Defense Nuclear Nonproliferation R&D MINOS venture, biota and effluent portfolios). These proposals represent collaborative efforts between scientists at INL and Pacific Northwest National Laboratory, and INL and Savannah River National Laboratory, where INL's  $^{14}\text{C}$  AMS analysis capability represents a key component in each research project.

## Publications

Ward, J.W., M.S. Snow, J.E. Olson, D. Ball, D, M.L. Adamic, 2017, “Carbon-14 Content in Tree and Soil Samples at the Idaho National Laboratory Nuclear Site”, *Nuclear Instruments and Methods in Physics Research*, B. 2017 (in submission)

Snow, M.S., J.W. Ward, J. E. Olson, D. C. Snyder, “Carbon-14 Content in Surface Soils Near Atmospheric and Below Ground Nuclear Detonations”, *Journal of Radioanalytical and Nuclear Chemistry* (in preparation, expected submission Jan 2018)

## Presentations

Snow, M.S., (2017), “C-14 Analysis Capability Development” at Idaho National Laboratory. Presented at the Office of Science Laboratory Directed Research and Development 2017 Program Review, Idaho Falls, Aug 2, 2017.

Snow, M.S., M.L. Adamic, J.E. Olson, 2017, “Modern  $^{14}\text{C}$  Sample Preparation and Analyses” at Idaho National Laboratory. AMS-14 Conference, Ottawa, CA. Aug 14, 2017.

## Interns and Postdocs

Intern: Jessica Ward

Postdoc: Mathew Snow

## 16-106: ICS-CAPE: Industrial Control Systems—Cyberattacks and their Physical Effects

Mary Klett,<sup>1</sup> Dale Christiansen,<sup>1</sup> and Tim Klett<sup>1</sup>

### General Project Description

ICS-CAPE is focused on the expansion and improvement of the nation’s capability to identify and understand the physical impacts of a cyberattack on an industrial control system and to categorize data points at both a general and industry specific level in order to identify functional consequences. Diving into the inner workings of a component, system, or asset will enable a robust assessment of a specific facility or collection of industry assets. This assessment will, in turn, lead to a more accurate understanding of what the potential functional consequence of a cyber-attack on an ICS network may be. Building the component profiles on an established platform will allow the analysis to be conducted within a facility and then taken one level out to identify potential impacts to supported infrastructure, resulting in a cumulative consequence.

Many models and methodologies that are used to determine the best way to protect or attack an ICS network exist, and these approaches oftentimes consider the worst-case scenario; in actuality, a gap exists in methods to understand the physical effects of a cyberattack. The goal of this research is to create an architecture for a base structure that can be used to develop a library of infrastructure-specific process maps and identify key data points to be collected at each connection or component in order to determine functional impacts. This research will assess and enhance the use of a universal model and living algorithms to delve into the components typically used within an industry:

- Profile: develop a library of network mapping profiles for various infrastructure types
- Assess: select the closest profile and apply it to a specific facility or asset. Answer applicable data points for each critical component
- Analyze: determine the potential functional consequence of a successful cyberattack
- Expand: link to known downstream dependencies in order to explore the cumulative consequence or cascading impacts of an attack.

### Summary

**Profile**—An assessment of existing component libraries and mapping profiles was completed. Additional network mapping profiles were developed based on schematics for proposed substations that were never built. Initial translators were developed to allow for a common ontology to be able to be used for components and extensible and available beyond the profiles.

**Analyze**—Initial functional consequence calculations were developed and during review it came to light that redundancy data points needed to be restructured in order to adequately determine functional consequence. A corrected calculation is currently being finalized and reviewed. While these algorithms are intended to be “living” and evolve as additional data is collected and identified, the base calculation must be sound before any true assessment can begin. Another outcome of the functional consequence calculation is the concept of how structural complexity relates to redundancy, resilience, and functional consequence.

## Benefits to DOE

The research undertaken in this project supplements the Department of Energy's role as the sector-specific agency and national leader in energy/electric-grid security against cyberattacks. The methodology stemming from this work will benefit Department of Homeland Security personnel, to include protective security advisors (PSAs) and cyber security advisors (CSAs) so that the physical impacts and cascading consequences of a cyberattack can be better understood. This work will supplement DHS efforts to secure the electric grid and other critical infrastructure types.

Overall benefits include:

- A more accurate understanding of the potential functional consequence of a cyberattack on an ICS network
- The opportunity for planners and threat analysts to perform detailed evaluation of the impact of an attack or the failure of a specific asset
- A universal model that will allow for rapid analysis of metrics and identify concrete consequences of a cyberattack
- Enhanced understanding of the potential cascading impacts of a cyberattack on a specific component or asset that will lead to more resilient designs.

## Publications

Currently working on a paper relating structural complexity to functional consequence.

## Presentations

*Resilience Week 2016* “Transforming the Resilience of Cognitive Cyber-physical Systems Lightning Round Presentation”, August 16-18, 2016 Chicago Illinois

## Interns, Postdocs, and Staff:

Intern: Gabriel Weaver.

## Collaboration

University: University of Illinois at Urbana-Champaign.

## 16-129: Application of Radioactive Isotope Dilution Technique to Measurement of Molten Salt Mass for Electrochemical Recycling Process

Shelly Li<sup>1</sup> and Jeff Sanders<sup>1</sup>

### General Project Description

Measuring the total mass of high temperature molten salt in containers is a critical step for the IAEA to implement international safeguards on electrochemical recycling plants and molten salt reactors through nuclear material accountancy. A much needed measurement technology to determine the molten salt mass in is yet to be developed. This LDRD project seeks to investigate the application of a radioactive isotopic dilution technique to determine molten salt mass in containers of irregular shapes. The technical goal is to develop a technology for near real time nuclear material accountancy with good measurement accuracy, which can be used by the IAEA to enhance the safeguards measures on electrochemical recycling plants and molten salt reactors in its member states.

### Summary

This is the second year of the LDRD project. The proposed concept was experimentally validated through using Na-22 as the radioactive in FY-16. Na-22 has been identified due to its chemical compatibility with the processing salts as well as the nature that it is not a fission product. In FY-17, the project has made significant progress through effective collaboration with Dr Lei R. Cao of The Ohio State University. The major accomplishments in FY-17 include:

- Studies by applying different radioisotopes into the molten salt to investigate possible interference, at Na-22 peak 1275 keV, from fission product Eu-154 was performed in FY-17. Molten LiCl-KCl samples spiked with Na-22 and Eu-154 activity were prepared, mixed, cooled, separated and measured in terms of their mass and radioactivity at The Ohio State University.
- The measurement results indicated that the Na-22 activity in the sampled salt can be precisely measured even with its 1274 keV peak entirely masked off by one of Eu-154 peaks. Linear relationship shown between Na-22 activity (Figure 1) and the mass of salt validated the validity of the proposed radioactive tracer determination concept, even with the interfering fission product.

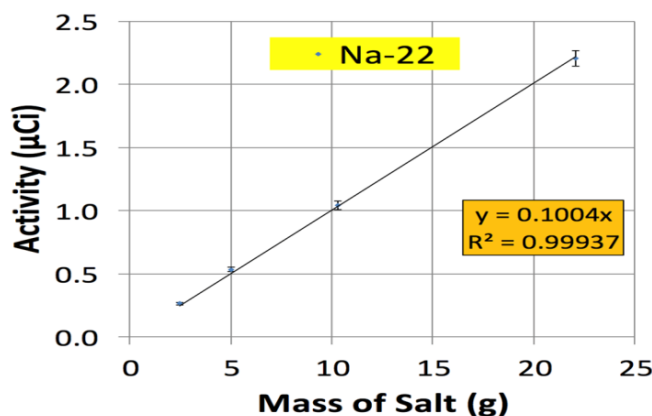


Figure 1. Na-22 activity can be determined even with its main peak 100% masked off by the

*interfering Eu-154 isotope. The deconvoluted results shown linear relationship between activity and salt mass, proving that the unknown salt mass could be determined by adding Na-22 tracer.*

## Benefits to DOE

If the proposed research is successful, it will be a breakthrough in safeguards measurements for electrochemical recycling processes and significantly improves the state of the art. The proposed technique may also be used for other safeguards purposes and applications which are of interest to DOE, such as for molten salt reactor systems.

## Publications

Cao, L., J. Jarrell, A. Kauffman, K. Herminghuysen, S. White, J. Sanders, and S. Li, 2017, “A radioactive tracer dilution method to determine the mass of molten salt,” *Journal of Radiochemistry and Nuclear Chemistry*, (2017) 314:387–393, DOI 10.1007/s10967-017-5417-5.

## Presentations

Cao, L., J. Jarrell, A. Kauffman, K. Herminghuysen, S. White, J. Sanders, and S. Li, 2017, “Measurement of molten salt mass using Na-22 nuclide as a tracer.” *9<sup>th</sup> Internal Conference on Isotopes*. November 12-16.

## Invention Disclosures

An Invention Disclosure Record BA-887 (IDR) titled “Application of Radioactive Isotope Dilution on Determination of Molten Salt Mass for Electrochemical Recycling Process” was filed in January 2016.

## Patents

A provisional patent application was filed in April 2017 by the INL Legal Department titled, “Radioactive Tracer Dilution Technique for Determining Molten Salt Mass.”

## Interns and Postdocs

Intern: Josh Jarrell

## Collaboration

University: Ohio State University

## 16-133: Secure SCADA Communications System

Briam Johnson,<sup>1</sup> Michael McCarty,<sup>1</sup> Rishi Chatterjee<sup>1</sup>

### General Project Description

The objective of this research is to significantly enhance the cyber security of industrial control systems (ICSs) by developing a network communication system that includes enhanced situational awareness and operator control of network flows and leverages unique aspects of control system networks to make them more immune to attack.

### Summary

To date, through the second year of the project, we began by integrating a simple electric-sector focused control system consisting of a single human machine interface computer and two remote terminal units (RTUs) from different manufacturers. We chose the DNP 3.0 protocol for initial implementation because it's by far the most commonly used protocol in the electric sector in the US[1].

In lieu of a traditional Ethernet switch, we implemented a software defined network (SDN) switch using open source software for basic functions. To that we added custom software to implement specific application-layer rulesets to prevent and flag control requests.

To allow for operator monitoring and control, we built a basic graphical user interface that allows the user to view real time the network flows, enable or disable control on a per-device or system level (panic button) basis and see a list of exceptions that occur. Figure 1 shows a logical block diagram of the system with a single RTU outstation.

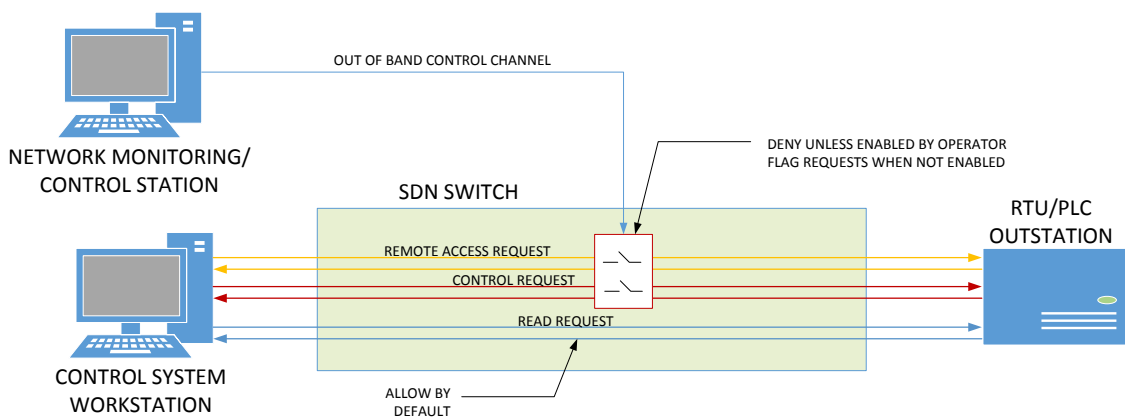


Figure 1. Block diagram of basic system with a single RTU outstation.

In the course of development, we learned several things which have made this research more challenging. One issue is that not every “DNP 3.0 compliant” device responds the same to a given message. In some cases, the slightest interruption in communications causes the device to lock up in a way that can only be fixed with a hard reboot. In general, the control equipment is very intolerant to any disruption in communications and/or any unexpected message sequences. This makes implementation of our system more difficult, but underscores just how vulnerable these devices are to cyber-attack. Nevertheless, we have found ways to work around the above issues and have met our primary objective of developing a proof of concept demonstration showing the capabilities and benefits of our system compared to typical ICS networks.

## Benefits to DOE

As the sector-specific agency responsible for the protection and reliability of the U.S. power grid, DOE has a keen interest in developing new technologies for thwarting cyberattacks against this infrastructure. There is little doubt that the threat of cyberattack is real. Seemingly every week an announcement is made of a new cyber-breach of some kind. In the case of critical infrastructure, the consequences of a successful cyberattack could be catastrophic. The recent attacks on Ukraine's infrastructure are a case in point. Although Ukraine was able to recover fairly quickly from these attacks, they show a trend toward more sophistication and potentially more damaging consequences. Better tools are needed to be able to thwart these attacks. Of the Ukraine attack, one expert had the following to say:

*You know they are opening breakers, so how do you quickly disable those features . . . No one has that capability, (Robert M. Lee, a SANS instructor and ICS/SCADA expert, says of ICS/SCADA operators).[2]*

The capability envisioned by this LDRD project, if implemented, could easily flag the initial network reconnaissance that occurs in the months leading up to an attack and allow operators a one-button solution to prevent any unauthorized controlling actions from occurring.

## References

- [1] *Newton-Evans Research Company*, "The World Market Study of SCADA, EMS, DMS, and OMS in Electrical Utilities, 2013-2015, Volume 1: North American Market".
- [2] Higgins, K. J. (2016). "Lessons from the Ukraine electric grid hack". Retrieved September 14, 2016, from <http://www.darkreading.com/vulnerabilities---threats/lessons-from-the-ukraine-electric-grid-hack/d/d-id/1324743>

## Presentations

Presented to representatives from DOE-OE and DOE-IN who were visiting INL on September 13, 2017. This research was very well received.

## Invention Disclosures, Patents, and Copyrights

IDR in progress.



## 16-152: Wireless radio Frequency signal Identification and protocol Reverse Engineering (WiFIRE)

Kurt Derr<sup>1</sup> and Samuel Ramirez<sup>1</sup>

### General Project Description

Several prominent wireless communications protocols (WiFi, Bluetooth, ZigBee, LTE) are in use today, as are proprietary protocols. Wireless technology is proliferating with the advent of low-cost computers and devices for the internet of things. The expanding role of wireless communications has created a need for rapid identification of wireless protocols in use by some black-box device (an undocumented device containing a radio that uses proprietary/ unknown protocols) or a wireless computing system (a computer system that uses a new proprietary protocol).

The objective is to build a tool—Wireless radio Frequency signal Identification and protocol Reverse Engineering (WiFIRE)—usable in an operational context for automatically analyzing the RF emanations and wireless protocols from a black-box device and performing automated wireless-protocol reverse engineering. The hypothesis is that GNU Radio, software-defined radio, computational intelligence techniques such as neural networks, and open-source protocol reverse-engineering tools may be combined to perform radio signal detection, classification, demodulation, and the reverse engineering of network protocols.

WiFIRE will scan multiple frequency ranges looking for wireless signals of interest emanating from a black box. The goal is to infer protocols from these signals and reverse engineer the protocols so that penetration testing may then generate network protocol inputs to the black-box wireless protocol, uncover and exploit potential vulnerabilities, and gain control of the device—a novel capability.

### Summary

Wireless classification of two standard protocols, WiFi and ZigBee, in *real time* was implemented this year. The wireless classification capabilities are major component of the WiFIRE tool under development and will continue to undergo further enhancement this year to include additional protocols. Demodulation of the WiFi protocol was also implemented enabling the viewing of packet data.

A working scalable prototype of WiFIRE was also developed this year. The prototype is scalable to multiple signal classification and processing nodes. WiFIRE scalability enables real-time monitoring and capturing of wireless signals in multiple frequency ranges at different locations. A graphical user interface displays the results of all of the signal classification nodes.

This important tool under development allows INL researchers to view all ongoing wireless communications activities to identify both expected and unexpected wireless communications from a device or in a geographical area. Although many other organizations have a capability view wireless signals at a specific frequency range, INL is one of few that may examine wireless signals across the spectrum, classify the signal, and reverse engineer the protocols in use. This tool could prove to be a very important milestone to further develop new tools that improve wireless security and mitigate system threats.

### Benefits to DOE

This capability will enable INL and others to determine the network protocols in use by a wireless black-box device that may pose a threat to the government or INL customers in a given area. WiFIRE will also enable the potential discovery of exploitable vulnerabilities of the black-box device that may lead to

gaining control of the device. Software-defined radio (SDR) is dramatically accelerating the pace of innovation and development of new radio technologies and enabling the development of tools that were previously impossible without unique hardware and software. Wireless communications devices are widely used in public safety, emergency response, and critical infrastructure applications. WiFIRE will enable the government to identify the wireless protocols used by a black-box device, assess the robustness of wireless implementations, analyze traffic, identify potential data leakage, and compare the implementation of a protocol with its official specifications.

The novelty of WiFIRE is that no real tool is currently available for capturing radio-frequency data, quickly (in real time) identifying the protocols in use, and performing protocol reverse engineering.

### **Publications**

Hearn, C., A. Kuznicki, C. Becker, K. Derr, and S. Ramirez, 2016, “Data Acquisition in Wireless Router Link Testbed using GNU Radio Companion”, *GNU Radio Conference (GRCON 2016)*, September 12-16, 2016, accepted.

### **Invention Disclosures, Patents, and Copyrights**

IDR BA961, Provisional Patent Application 62,472,387.

### **Interns, Postdocs, and Support Staff**

Interns: Christopher Becker and Aniqua Baset.

Staff Support: Dr. Sneha Kasera.

## 16P6-007FP: Consequence-driven Cyber-informed Engineering (CCE) Methodology Pilot

Robert Smith,<sup>1</sup> Sara Freeman,<sup>1</sup> and Curtis St Michel<sup>1</sup>

### General Project Description

The LDRD project team engaged in a high-impact effort to prioritize high-consequence cyber risk to the industrial control systems (ICSs) of the country's most critical infrastructure. This Consequence-driven Cyber-informed Engineering (CCE) Methodology Pilot Project included building a methodology to inform the conduct of an in-depth engineering evaluation of a major electric utility's operational environment in order to identify and mitigate high-consequence cyberattack scenarios. This consequence-based risk analysis methodology of the ICS environment was leveraged by the team to propose new engineering and design options, operational procedures, active defense methods, alerts, and safeguards. As part of this process, the team built a process for how to work with the intelligence community to baseline current adversarial capabilities and identify whether these skills could be applied to attack an electric utility's operational processes.

### Summary

As of 30 September 2017, the project will be effectively complete and has achieved the project team's primary goal to develop and hone the CCE process for use by key organizations to evaluate, prioritize and improve their cyber security posture. The project findings and processes have now been harvested for use in future projects sponsored by the DOE and other partner agencies, including the Department of Defense (DOD), to be leveraged to assist in analyzing cyber risk related to the nation's most critical infrastructure assets and processes. The project allowed the technical team to build out a process to work through the assessment, including phase 1 (Consequence Prioritization), phase 2 (System of Systems Breakdown), and phase 3 (Consequence Targeting).

### Benefits to DOE

Now that the CCE process has been demonstrated and validated within the electric sector, it can be applied to the oil and gas industries and military and government assets. A new project with the DoD will facilitate a cyber assessment on a key military platform. The CCE process will be used in a key project (about \$10M funding) with DOE-OE to work with four pilot electric utilities to identify and prioritize cyber risk, ultimately working towards increasing cyber-security monitoring within the operational technology/ICS environment. As a result of the LDRD project work, the US government and the INL will be able to continue their leadership roles, providing industry with practical, innovative solutions for securing the nation's critical infrastructure.

### Publications

“Consequence Prioritization Process for Potential High Consequence Events (HCE)”, *INL/EXT-16-40341*, Mission Support Center, Idaho National Laboratory, October 31, 2016, <https://www.osti.gov/scitech/biblio/1341413-consequence-prioritization-process-potential-high-consequence-events-hce>

“Consequence-driven Cyber-informed Engineering (CCE)”, *Mission Support Center, Idaho National Laboratory*, October 18, 2016, <http://www.osti.gov/scitech/servlets/purl/1341416>

## 17A1-079FP: Affixing Inert Dissimilar Materials to Structural Materials for High Performance Armor Systems

Thomas Lillo,<sup>1</sup> Joshua Kane,<sup>1</sup> and Adrian Wagner<sup>1</sup>

### General Project Description

High performance armor systems that enable future defense and increase national security will require sector-disrupting performance improvements that can resist advanced threats while maintaining a low areal density for fuel saving and vehicle agility. These requirements can be met if extremely hard ceramic materials can be metallurgically affixed to metallic structural materials, resulting in significant reductions in the weight of the armor system and increased overall structural flexural stiffness. Previously, various processes, such as encapsulation of ceramics with metal alloy and 3D front-to-back, through-thickness reinforcement have attempted to affix or bind ceramics to structures. These processes have shown improved ballistic performance, but the fabrication process is labor-intensive and neither economically viable nor conducive to integration into vehicles' structural components. This project seeks to metallurgically affix the ceramic tile to structural alloys (Fe-based, Al-based and Ti-based alloys) using solders and high-temperature brazes to simplify fabrication of economical high-performance armor systems integrated into structural components.

### Summary

Ceramics such as silicon carbide (SiC) are very hard but also relatively inert and bonding to structural metals, such as steels and titanium alloys, requires elevated temperatures to develop a chemical bond between these two material classes. Additionally, the disparity between the coefficients of the thermal expansion (CTE) between these two classes of materials, i.e. metals and ceramics, is very large and can result in residual stresses on cooling from the bonding temperature that are capable of fracturing the silicon carbide. Therefore, the approach of this work is to modify the surface of SiC to allow commercial solders and brazes to wet and bond to the SiC. The work also engineers an intermediate layer between the SiC and metal alloy substrate to alleviate CTE mismatch.

Two approaches were developed during FY-17. The first utilizes a solder with a melting point on the order of 250°C. The solder is initially applied to the SiC surface and subsequently subjected to a high temperature heat treatment to produce a metallurgical bond between the solder and the SiC, see Figure 1a. In the final step, the solder-coated SiC is bonded to the metallic substrate at 275°C, thus avoiding significant thermal stresses on cooling. Test coupons designed to determine the shear strength of the bond have been fabricated, see Figure 1b and tested. The bond strength between SiC and Ti-6Al-4V was approximately 32 MPa while the bond strength between SiC and armor steel was approximately 23 MPa, compared to bonds made using various superglues at strengths of <16 MPa. Failure occurred at the solder/metal interface, rather than the solder/SiC interface and modifications in FY-18 will enhance the solder/metal bond strength and joint strength.

The other approach focuses on higher temperature brazes (700–900°C) which exhibit higher strength than the solder in the previously described approach. The disadvantage of this approach lies in the high temperatures that are required and the CTE mismatch between braze and SiC. To date, very good brazed bonds between SiC and metal substrates have been achieved in this approach, see Figure 2a, but CTE mismatch has resulted in fracture of the SiC, see Figure 2b. Work is now focused on controlling the CTE mismatch by incorporating low-CTE material to the joint to better match the CTE of SiC while still retaining good bonding between the SiC and the titanium and steel alloys.

During FY-18, targets will be made to evaluate the ballistic performance offered by these two approaches. A peer-reviewed publication is planned to report the shear strength of the bonds produced by both methods as well as one to report the ballistic performance.

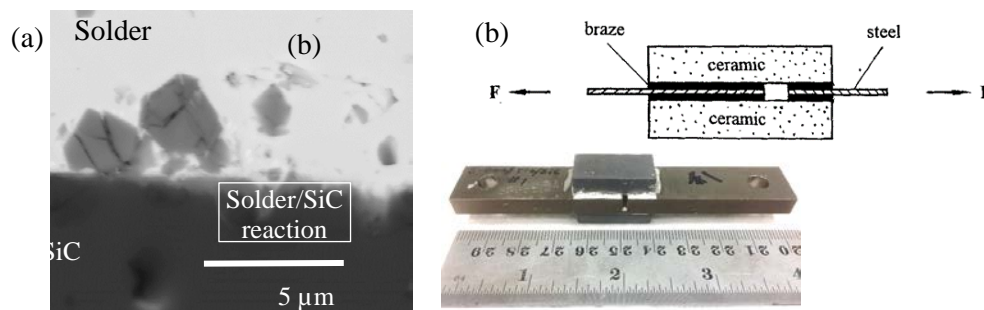


Figure 11. Interaction between the solder and SiC is shown (a) while the resulting shear strength test sample made by this approach is shown in (b).

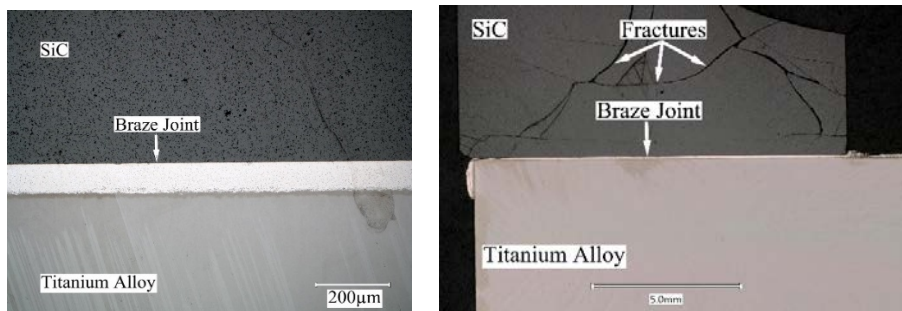


Figure 12. (a) A brazed joint between SiC and a titanium alloy, however, the SiC fractured during cooling due to CTE mismatch (b).

## Benefits to DOE

This work offers the potential for major advancements in the area of ballistic protection of national assets and protective-force personnel. Armor systems based on this work will offer increase ballistic protection at a reduced weight while retaining cost-effective manufacturability. This work also offers the potential to realize the Tactical Assault Light Operator Suit (TALOS), the so-called Iron Man suit, envisioned by United States Special Operations Command. Ongoing success in these research areas will reinforce the armor-materials development and armor-system design capabilities that INL has developed. Additionally, the brazing approach offers the potential to place SiC-based sensors to monitor operating conditions and the health of structural materials inside the harsh environment of next-generation high-temperature nuclear reactors.

## 17A1-101FP: Nuclear Instrumentation and Methods for Emergency Response

David L. Chichester,<sup>1</sup> Scott J. Thompson,<sup>1</sup> Nick R. Mann,<sup>1</sup> James T. Johnson,<sup>1</sup> and Scott M. Watson<sup>1</sup>

### General Description

New nuclear instrumentation and methods are needed to search for and characterize radiological and nuclear materials and to address emerging challenges facing personnel tasked with responding to emergencies associated with the theft, transport, and misuse of these materials. In particular, direct feedback from law enforcement and emergency responders indicates a strong desire for simpler instrumentation and systems that can be used for multiple purposes, including use in mobile platforms and unattended deployment. These systems also need more easily intuited user interfaces. This project is exploring new nuclear instrumentation and methods for emergency response applications to address these issues.

### Summary

Our work is progressing along two thrust areas. In the first area we are developing a multi-sensor detection package capable of supporting multiple search and emergency response missions. In the current year this work is studying the use of neutron sensors that have varying energy-response functions, with the goal of developing a simple approach that can differentiate man-made neutron sources from background neutrons. Prior work in this area has involved the use of sensors embedded within carrying-thickness polyethylene shields. Our approach takes a different path, informed from prior work related to active neutron interrogation, and emphasizes neutron sensors with more specific neutron energy response functions. We have assembled and performed laboratory testing of a prototype multi-energy neutron detection system that employs this alternate approach and have initiated scoping trials in the laboratory. The energy dependent neutron sensitivity of the three neutron sensors used in this system is shown in Figure 1 together with an example of the system response to fission spectrum neutrons under a variety of different neutron shielding conditions.

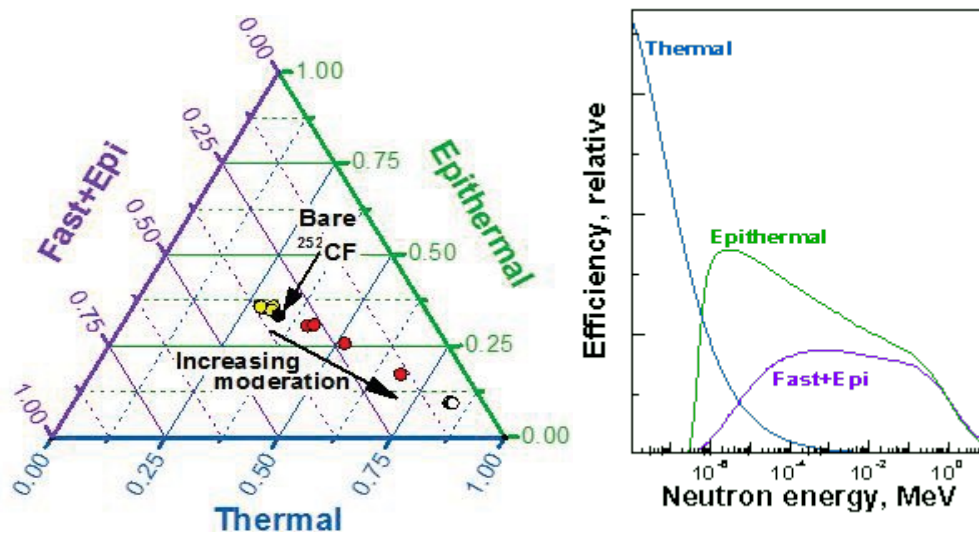
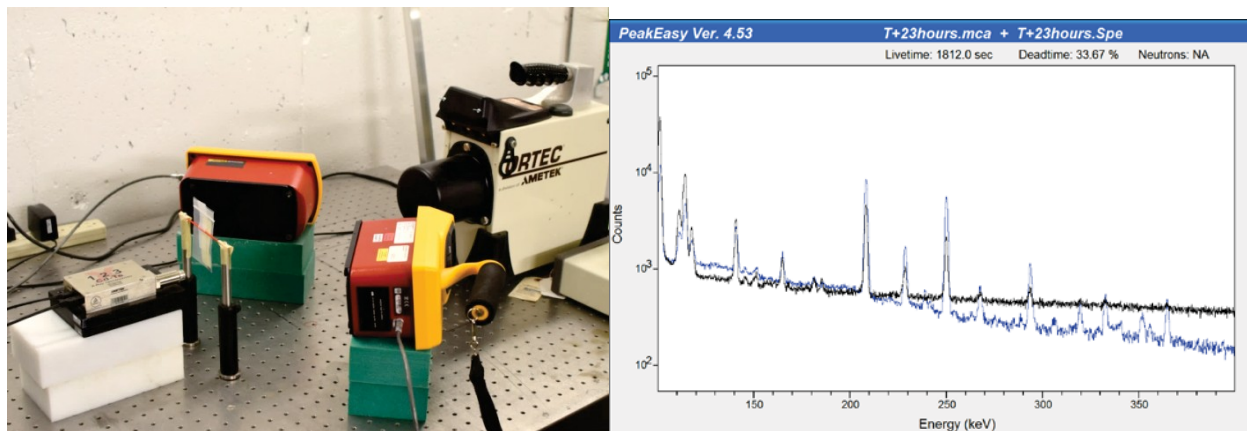


Figure 1. The plot on the left shows the spectral response of three different neutron sensors incorporated into the multi-sensor detection package. The



*plot on the right shows a tri-axis response of the sensor system to fission spectrum neutrons bare (black), shielded with tungsten (yellow), or shielded with polyethylene (red). The systems response to natural background neutron radiation is also shown (white).*

In the second area we are developing instrumentation and methodologies to perform quantitative radiation field surveys of post-detonation radiological dispersal device (RDD) and nuclear explosion environments. One example of work in this area has been scoping work performed to evaluate the feasibility of using high-resolution, room-temperature, cadmium telluride (CdTe) spectrometers for in-field, post-detonation nuclear forensic analyses. Early work (see Figure 2) has shown it is possible to determine the equivalent fission yield of short-cooled irradiated materials via analysis of the 140.5-keV line of  $^{99m}\text{Tc}$  with this type of sensor. It may also be possible to determine fractionation, via a ratio of  $^{99m}\text{Tc}$  to  $^{132}\text{Te}$  at 228.12 keV.



*Figure 2. Photograph of CdTe measurement prototype for fission gamma-ray spectrometry (left) and results (right).*

Also in this second area, are working to develop a hand-held tablet, with GPS mapping capability, to support RDD field work. This tablet includes an innovative application that allows a user to upload a computer-generated fallout ground deposition plume, and to estimate local radiological conditions to be expected at the tablet's location according to location and time after detonation. This system is intended for use as a training tool for emergency response teams, to allow realistic large-area training at their home locations.

## Benefits to DOE

This project is producing new instruments and methods with potential use in support of DOE's nuclear-nonproliferation, nuclear counterproliferation, nuclear forensics, and emergency response communities. In particular, the project aims to produce a new generation of simple field equipment and associated deployment methodologies to help improve the concept of operations of emergency response teams by reducing user error, improving response speed, and allowing the teams to focus less on their equipment and more on their missions.

## Presentations

Chichester, D. L., et al., "Post-Blast Radiological Dispersal Device Source Term Estimation", conference record and presented at, IEEE Nucl. Sci. Symp., Strasbourg, France, Oct. 29- Nov. 5 (2016).



Sosa, C. S., et al., "Improvements in Energy Resolution Using a Stilbene Crystal in Conical Geometry," INL-CON- 17-42011, submitted to IEEE Nucl. Sci. Symp., Atlanta, Georgia, Oct. 21-28 (2017).

### **Interns and Postdocs**

Interns: Jay D. Hix and Charles S. Sosa.

### **Collaboration**

Universities: Idaho State University and University of Michigan.

## 17A1-106FP: A Study of Fission Modes to Improve Nuclear Forensics

Mathew Kinlaw<sup>1</sup>

### General Project Description

This project directly addresses two areas identified as research priorities: [1] new or improved production methods for isotopes of interest to nuclear forensics, and [2] methods to provide improved nuclear data for isotopes of interest to the nuclear forensics communities. The nuclear forensics community continues to seek timely and cost-effective methods for producing low-fission yield isotopes, in particular isotopes with masses that fall within the valley of the fission fragment mass distribution. One such method that is generating interest is the use of photofission-based isotope production. In order to utilize photofission to its greatest extent, the contribution of the various fission modes and their influence on mass distributions and, consequently, their influence on valley isotope production, warrants an in-depth examination. This project leverages previous photofission-based measurements, as well as existing data from neutron analogues, to determine the energy-dependent, relative contributions of the symmetric and asymmetric fission modes. The anticipated outcomes are a relatively unique production method for fission-valley isotopes, as well as a new method to provide nuclear data, which could lead to significant advancements in the understanding of how specific mass chains can inform attribution efforts.

### Summary

FY-17 efforts also focused heavily on developing a suite of computational tools from which empirical data sets are generated. In the current context, these measured data will consist of fission fragments detected via gamma-ray and x-ray spectroscopy following irradiations with a linac-based photon beam. Despite 80+ years of fission research, the recommended fission fragment distributions suffer from large uncertainties, across the range of masses, in large part due to an inability to measure short-lived fission products preceding their longer lived daughters in the mass chains. These considerations, along with the costs associated with performing repeated experimental measurements, necessitate the development of computational tools from which experimental procedures and analysis methods can be evaluated and optimized. Hence, the team has produced custom software which interfaces with both Origen-S and MCNP to produce empirical, simulated data.

Fission fragment mass distributions are provided to the software as “ground truth” values and used to simulate production and during-irradiation decay of fission products. Output from this is processed and fed back into the software to account for decay following irradiation. An Evaluated Nuclear Structure Data File is embedded within the program; the final output is an MCNP file containing every discrete gamma-ray and x-ray, for each fission product, and for each time period selected by the user. The final result is a simulated data set upon which various analysis scheme can be evaluated for their effectiveness in returning the “ground truth” values. As an example, a simulated photofission spectrum, produced from the software and using ENDF/B-VII.1 recommended independent fission yields, is provided in Figure 13. These empirical data were analyzed to assess whether the initial “ground truth” yields could be extracted from the data. For the isotope  $^{132}\text{Sn}$  (highlighted in the inset in Figure 13) the empirical independent fission yield is  $0.0162 \pm 0.0052$ ; analysis of the simulated data resulted in an extracted independent yield of  $0.0163 \pm 0.0003$ .

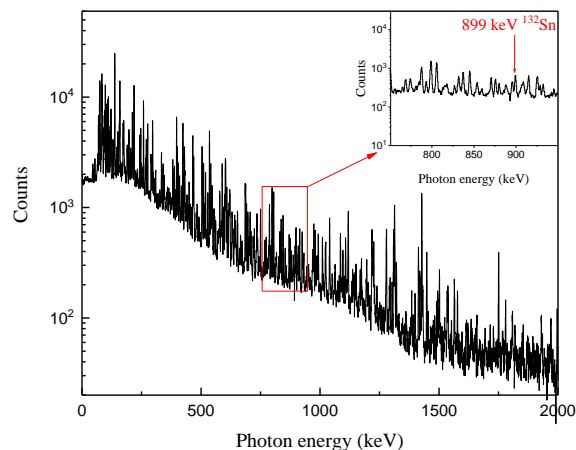


Figure 13 Gamma-ray spectrum from a simulated photofission measurement. The highlighted region shows the 899 keV gamma-ray from the isotope  $^{132}\text{Sn}$ , which was used to demonstrate the ability to extract independent fission yields.

## Benefits to DOE

The nuclear forensics community continues to seek timely and cost-effective methods for producing low-fission yield isotopes, in particular isotopes with masses that fall within the valley of the fission fragment mass distribution. Since access to high-flux, fast neutron irradiation facilities in the United States is limited, photonuclear-based production methods are proving to be more time- and cost-effective than alternative techniques that rely on reactors or other high-flux, neutron-based methods. Beyond forensics, consistent and reliable data will potentially impact several additional applications. These include, but are not limited to, the design of accelerator-driven subcritical reactors, nuclear waste transmutation and reprocessing, and design and development of electron accelerator-based, high-flux neutron sources [1–6]. From a less applied and more basic science perspective, the study of mass and charge distributions from photofission provides strong advantages over complimentary studies relying on neutron fission. The mass and charge distributions carry detailed information regarding nuclear shell structure effects and the processes that occur as the excited nucleus transitions from the initial fission stages through the scission point [7–9].

## References

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- [7] Vandenbosch, R. and J. R. Huizenga, *Nuclear Fission*, Academic, New York 1973.

[8] Wagemans, C., *The Nuclear Fission Process*, CRC Press, London 1990.

[9] Naik, H., et al., *Eur. Phys. J. A* 2013 49, 94.

### **Interns and Postdocs**

Intern: Ariana Foley

## 17A1-109FP: Scalable Binary Analysis

Jared Verba<sup>1</sup> and Jed Haile<sup>1</sup>

### General Project Description

Graph database technology is currently deployed across Google and Facebook for correlation of search and social-network relationships. Insurance and credit-card companies deploy this technology to perform risk analysis on the data collected from customers. By transforming an application or firmware image into a graph database, several new benefits to cyber focused researchers and their customers are realized:

- Researchers are able to annotate analysis work that can be shared
- CPU-intensive analysis techniques can be scaled to clusters of computers
- Collaborative research can be performed among multiple concurrent users
- Relationships between seemingly disparate information can be identified.

This project develops methods of importing software and firmware images into a distributed graph database and enables collaborative querying of that database. This will allow unique views into the structure and vulnerabilities of a binary. It will also allow automated processes or researchers to pull new information from binaries in a more efficient manner.

### Summary

This project has built a computer cluster running a distributed graph database to use as a platform for our research. Using this database we have designed schemas and done the initial work of deconstructing several binaries into flow graphs and data graphs which are stored into the database. We have begun research into how to leverage this database to find important qualities and relationships in binaries, and do some basic visualization.

A core effort during this fiscal year is to compare two different methods of populating the database. The first method constructs the graphs entirely in memory on a workstation, and then inserts the graphs into the database. The second method is to use the database throughout construction of the graphs; potentially eliminating single host CPU and memory limitations.

Additional work will compare the outcomes of approaches identified in the first year to determine the processing constraints for each method. We hope to understand when either method is superior for a given task. Work on the database will continue to refine and extend current schemas, and expand the scope and depth for each. Follow up research into applying known analysis techniques, expanding known techniques in novel directions, and developing new analysis techniques will become the focus in the second year of this project.

Some graph construction has been completed. It is clear that the user interface will need work to make it more understandable and usable in order to be effective. The following figures are graphs of memory access to a particular variable on the stack of a simple binary.

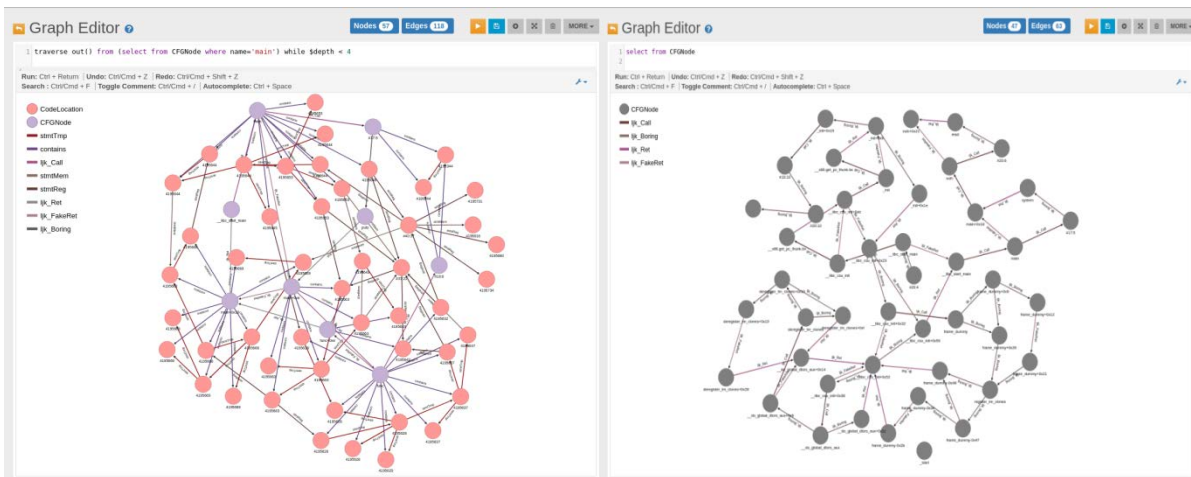


Figure 1. Example graph queries of a simple binary to show memory access of a variable

## Benefits to DOE

This is cutting-edge research into reverse-engineering techniques. This sort of research opens the door for faster and more efficient identification of cyber vulnerabilities across the DOE landscape. This research could be directly applied to improving vulnerability detection in the following:

- ICS
  - Programmable logic controller(PLC) firmware
  - Sensor firmware
  - Software and additional updates
- Nuclear-Cyber
  - Vulnerability assessments on software and firmware

## 17A1-114FP: Resilient, Scalable Cyber State Awareness of Industrial Control System Networks to Threat

Craig Rieger,<sup>1</sup> Tim McJunkin,<sup>1</sup> Michael Haney,<sup>1</sup> Brian Johnson,<sup>1</sup> and Milos Manic<sup>25</sup>

### General Project Description

A team of researchers from Idaho National Laboratory (INL), the University of Idaho (UI) and Virginia Commonwealth University (VCU) are developing an extensible, scalable cyber-threat agent or sensor for industrial control systems (ICSs). The agent design requires research of methodologies that characterize diverse performance behaviors on ICS networks and use of these methodologies to directly apply scalable methodologies to achieve a measured level of resilience. Based upon both cyber and physical characterizations of patterns of host activity and network traffic, novel proofs of concept are being developed that can conclusively recognize a cyberattack and distinguish the attack from benign, unintended actions or physical failure. The proofs of concept will be operationally tested as a prototype product to be integrated into the mature intelligent anomaly-detection platform for advanced monitoring of ICS networks.

### Summary

This project is establishing differentiating capability in cyber-physical system anomaly detection, whose grand challenges include the ability to achieve high confidence and scalable detection of ICS cyber-attack. While signature-based technologies, often focused on business enterprise systems, are still in widespread use with limited implementation of anomaly detection methods, anomaly detection systems are still dependent upon a baseline. Understanding the variations from baseline, focusing only on the communications or cyber parameters, provides only a limited view of system state. To fully characterize the problem and provide evidence for high confidence, therefore, both states must be captured and integrated. To be scalable, human interaction must be focused on the methodologies and not on the unique ICS network, allowing for the broad autonomic application to any implementation.

Microgrid are implemented on a framework that broadly comprised of a combination of renewable, energy storage resources, and managed loads, typically, on a small scale. However, ICS in Microgrids have much in common in application to our Nation's power grid, which includes many small municipalities and organizations that cannot afford a large staff to operate and maintain. Therefore, many of these systems will be highly automated, and without deep experienced staffs. The personnel will be dependent upon high confidence understanding of alerts that must be acted upon. As a result, a Microgrid was chosen as the use case in this effort. The Microgrid was emulated in a high fidelity real-time power simulator, by RTDS Technologies. The RTDS provided data to a Schweitzer Engineering Laboratories supervisory control and data acquisition (SCADA) system to provide real world responses. In and out of band networks were established to provide correlation of normal (out of band) response to the anomalous (in band) events under various concurrent and sequential cyber and physical anomalous conditions.

The first sets of experiments were focused on several types of cyber only anomalous conditions and correlated to the cyber-physical Microgrid environment. While interpreting diverse data, it is important to note that different layers contain important information about the source, destination, purpose and function of the data packet. In the initial analysis, visual inspection of a few packet header information is carried out. The following packet header information is collected: 1) Frame number, 2) time of recording; 3) time period from the previous packet, and 4) length of the packet. A number of anomalous cyber scenarios were run to correlate to data integrity and availability, which are particularly important for ICS as they impact the ability to safely perform control of the

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<sup>25</sup> Virginia Commonwealth University



Microgrid. Baselineing of the traffic was performed and is presented as examples in **Error! Reference source not found.** As an example of anomalous condition, Figure 15 provides an indication of replay—indicating an adversarial technique to mask an attack or to create an undesirable condition on the Microgrid.

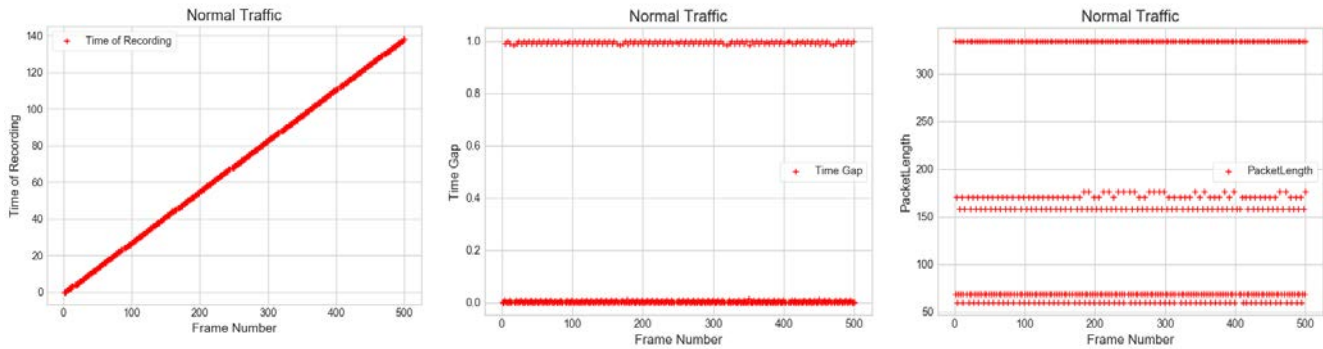


Figure 14. Normal traffic.

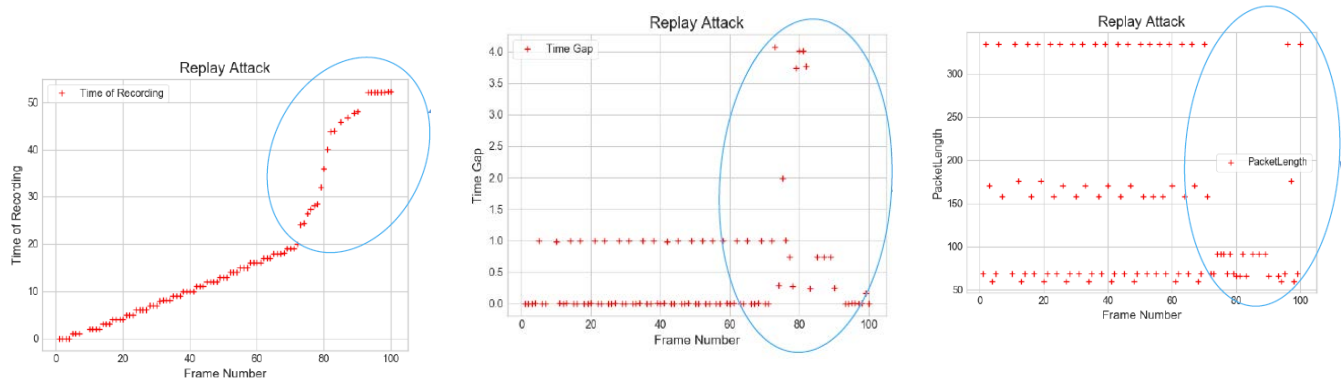


Figure 15. Replay attack.

The resulting efforts set the stage for future benchmark testing, which will script many of the cyber-attacks, to which physical scenarios will also be added to allow for full and reproducible characterization. Preliminary machine learning efforts resulted in a best paper award from the IEEE Industrial Electronics magazine (Impact Factor 10.7).

## Benefits to DOE

This effort advances the grand challenges of anomaly detection in ICS to a prototype, which will provide a basis for next-generation sensing of cyberattacks. More importantly, the ability to achieve high confidence sets the stage for stakeholder acceptance of automated response, providing mitigative actions to cyberattacks that occur in time scales of seconds and which cannot be challenged with current technologies.

## References

- C. G. Rieger, “Resilient Control Systems: Practical Metrics Basis for Defining Mission Impact,” 7th International Symposium on Resilient Control Systems, August, 2014.
- T. Vollmer and M. Manic, “Autonomic Intelligent Cyber Sensor to Support Industrial Control Network Awareness,” Transactions on Industrial Informatics, Vol. 10, No. 2, May 2014.

## Publications

Best Paper Award: Manic, M., K. Amarasinghe, J. J. Rodriguez-Andina and C. Rieger, 2016, "Intelligent Buildings of the Future: Cyberaware, Deep Learning Powered, and Human Interacting," in *IEEE Industrial Electronics Magazine*, vol. 10, no. 4, pp. 32-49, Dec. 2016.

## 17A1-142FP: Modeling and Spatial-Temporal Analysis of Cyber-Physical Impacts

Timothy Klett,<sup>1</sup> Robert Edsall,<sup>1</sup> and Michael Overton<sup>1</sup>

### General Project Description

The goal of this research is to develop a cyberattack model specific to critical infrastructure and link it to an established cyber-component model. A geospatial information system (GIS) capability will be created to allow for cyberattack setup and to visualize local effects to the target infrastructure. Expansion of the model will incorporate a knowledge framework for identifying dependent infrastructure effects. This effort will include visualization of regional impacts from a cyberattack. Scenarios will also be identified that are relevant to potential users of this technology. Finally, the technology will be refined to support real-world complex scenarios. Regional and temporal analytical capabilities will be developed to aid in supporting these advanced scenarios.

A combination of social-science methods and technical expertise will be used to characterize and categorize cyber attackers and their likely motivations and goals and then to correlate these characteristics with cyberattacks on physical critical infrastructures. Existing published research and ongoing efforts at INL are being utilized to model cyberattacks; leveraging these findings will allow the construction of cyberattack profiles that will serve as independent variables in the analysis of cyberattacks. These profiles can include the type of attacker (hactivist, hobbyist, nation state, etc.), the attack type (denial of service, vulnerability exploit, etc.), and the attacker's goals (surveillance, disruption of service, destruction, etc.). The impact of a cyberattack on physical infrastructure is (at least partially) dependent on this characterization of the attack in the profile; these categories (of attacker, type, and goal) can serve as independent variables in a functional relationship to the impact of an attack on critical infrastructure.

### Summary

To date, the team has made progress towards our goals on multiple fronts. Relative to the first year goal of developing and integrating cyber-attack profiles with cyber-component models of CI, an initial cyber risk calculation has been proposed. The experimental calculation is constructed of the following elements: asset priority, attacker weight, and the sum of the dependency strengths for the components and commodities used by the asset.

$$\text{Cyber Risk} = \text{priority} * \text{attacker weight} * \sum_{i=1}^{i<n} \text{dependency strength}[\text{commodity\&component pair}]$$

An initial question set for prioritizing regional infrastructure was developed. These questions provide a framework for quantifying the prioritization of a region's assets. The priority is calculated for each asset with a simple summation of the values from each of the 9 questions:

$$\text{priority} = \sum_{i=1}^9 \text{points}(i)$$

A matrix of attacker type, resources, time, tools, risk, access, and objectives has been formulated. An initial relative weight for each attacker type has been calculated and is denoted by attacker weight in the Cyber Risk calculation. A dependency strength calculation has been proposed. This calculation of dependency strength results in a value between 1 and 0 where 1 indicates the most reliance on a particular commodity and 0 indicates no reliance issues in a given time period. The formula is based on converting the impact with and without a backup to a fixed number of minutes in which an asset will be operational. The abbreviations below are used:

- Impact without Backup = IWOBU (in minutes)
- Degree without Backup = DWOBU (percent)
- Impact with Backup = IBU (in minutes)
- Degree with Backup = DBU (percent)
- Time the Resource was Unavailable = TRU (in minutes)

$$Strength = \begin{cases} 1 - \frac{[\min(IWOBU, TRU) * DWOBU] + [\min(DWOBU, TRU) * DBU]}{TRU}, & \text{if } TRU \leq IBU \\ 1 - \frac{[\min(IWOBU, TRU) * DWOBU] + [\min(DWOBU, TRU) * DBU]}{TRU + OPS}, & \text{otherwise} \end{cases}$$

An initial GIS component has been formulated. This “What-if” scenario allows for the selection of an area of interest on a map. All known infrastructure in the selected area are then factored into the scenario. Service providers of the known commodities for each asset can be “turned off” and the impact to downstream infrastructure can be seen on the map. A temporal option allows for the progression of the scenario through time to visualize the impacts as onsite and alternative backups are consumed.

## Benefits to DOE

The research from this initiative will address the current shortage of methods to assess the regional impacts to critical infrastructure from a cyberattack by creating attack profiles to cyber-exposed components and modeling potential physical impacts on the associated infrastructure.

## Presentations

Edsall, R., 2017, “Geographic Considerations in Cyber-Security: Modeling Physical Controls and Dependencies in Critical Infrastructure Protection”, American Association of Geographers (AAG) Annual Meeting in Boston.

## Interns, Postdocs, and Staff Support for Graduate Studies

Intern: Travis Machacek.

## Collaboration

University: University of New Mexico.

## 17A1-152FP: Building Systems: Access, Management, & Automation

Jonathan Chugg<sup>1</sup> and Kenneth Rohde<sup>1</sup>

### General Project Description

Building management systems, access control systems, and building automation systems are based on the same concepts and may contain the same exploitation opportunities as an industrial control system. Instead of pumps and valves, these systems use other embedded devices to maintain a comfortable environment for building occupants or control access to security areas. These systems need to be thoroughly evaluated for security issues in order to properly determine the risk to our critical infrastructure buildings and discover, design, and develop mitigation to potential vulnerabilities. A GAO report in December of 2014 was entitled “DHS and GSA Should Address Cyber Risk to Building and Access Control Systems.” Because these building systems are widely used in a number of different critical infrastructure sectors (e.g., nuclear, power-generation, and manufacturing facilities), they create a new and increased risk to our nation’s infrastructure.

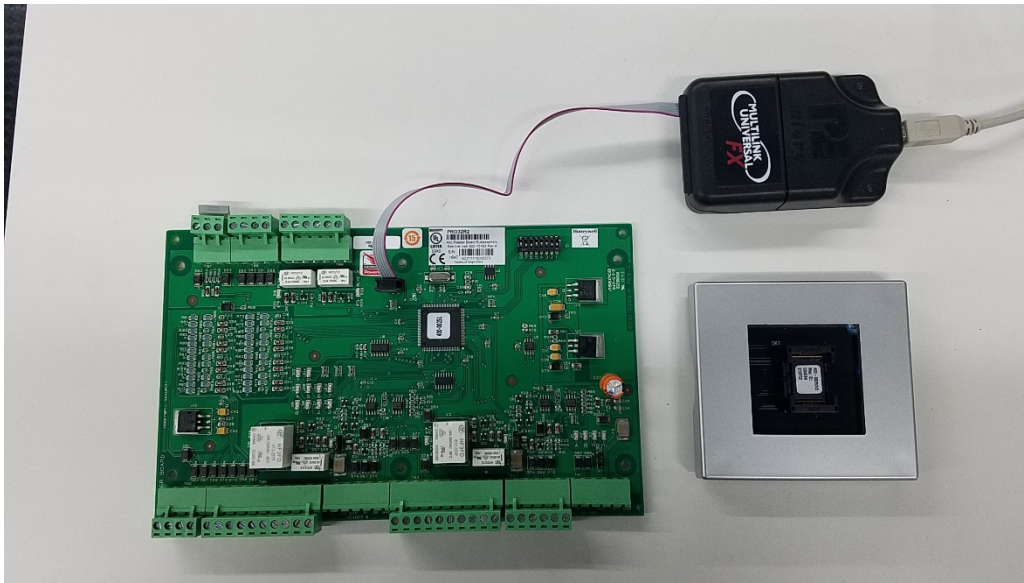
### Summary

The purpose of project is to investigate the security of building management control systems (i.e., heating, cooling, power, lighting, physical access, etc.) for the inherent cyber security strengths and vulnerabilities as weaknesses viewed from the perspectives of system defenders and adversarial hackers. Initial research focused on evaluating an integrated building access control system and its communication networks.

This research is directly applicable to characterizing the future cyber research and engineering designs that can enhance the operational security of the control systems that manage environmental and access controls of the ‘smart building’ that support our critical infrastructure.

The LDRD procured a Honeywell Access Control System (Pro 3200 series) and three cyber security researchers to assemble, analyze, and reverse engineer the various components for the access control system.

The researchers analyzed control software from a server, a control board firmware/software, and a communications board firmware/software. Firmware from the control board and from the communications board were able to be extracted from the hardware boards and were reverse engineered to understand how the software works to identify possible vulnerabilities. Debuggers were also obtained to aid in the research for reverse engineering purposes. Researchers identified some security findings and are experimented on proof of concept code. The researchers identified potential mitigations for the identified security findings and experimented on provability.



*Figure 16. Debugger and Chip Reader Attached to Control Board*

As part of the research effort, a CRADA was signed between INL and Honeywell. As part of the agreement, Honeywell will provide equipment during FY-18 and FY-19 research and experimentation.

### **Benefits to DOE**

Building systems present a huge target for cyberattack in the near future due to the heavy integration of building automation into newer smart buildings and large critical data centers that will ultimately be connected to the smart grid. DOE and INL have the opportunity to lead research into this area and push security issues and potential mitigations as it did for industrial control systems. This allows INL to gain the expertise needed to become a dominant performer within this field, recognized as the industry leader. The cyber-security research and SCADA security expertise that is already recognized by the research community can be leveraged to develop this new expertise. This project is an extension of DOE's current leadership in critical infrastructure assessment methodology as employed in DOE National SCADA Test Bed and DoE's support to National Critical Infrastructure Security Programs. This research also builds DOE's capability to improve and enhance mobile embedded systems technologies. These systems are growing rapidly in a mobile ecosystem, and enhanced capability in this area will also continue DOE's leadership across all critical infrastructure sectors. Specific applications include improvement of national, including nuclear, energy security and continued improvement for energy production and distribution security.

### **Presentations**

Chugg, J., 2017, "Strategic Advisory Committee Poster Session", EIL building at INL, June, 2017

### **Interns and Postdocs**

Interns: Oliver Reed and Jason Staggs

## 17A1-156FP: Nuclear Safety Systems Cyber Security

Jonathan Chugg<sup>1</sup> and Kenneth Rohde<sup>1</sup>

### General Project Description

Nuclear, oil- and gas-manufacturing plants, and other critical infrastructure sites use and heavily rely on safety systems. These systems are designed and tested to ensure plant safety, prevent accidents, and reduce damage and harm if an accident should occur. In the past the nuclear sector has deployed these systems in analog form, with no digital controls or devices. As these analog safety systems age, replacement parts become unavailable, and repairing components has become the only solution to the problem of keeping these systems operational. Repairing analog devices has also become difficult as components of these devices become scarce. An alternative solution has been embraced by other industries that rely on digital safety systems and triple modular redundancies (TMRs). Although programmable logic controllers, field devices, remote terminal units, and other devices and software used in SCADA and industrial control systems have faced the scrutiny of cyber security, safety systems and TMRs have not. Because these safety systems ensure critical plant safety by preventing and controlling accidents, it is imperative that they face the same cyber security scrutiny. The inherent trust the nation places on safety systems needs to be validated and corroborated. The purpose of this project is to investigate the security of the core control protocols and architectures used in the subsystems of a typical nuclear power plant's safety system. Research will be limited to a select set of critical components to evaluate the strengths and weaknesses of the control protocols and to develop concepts for strengthening the cyber security features of these components.

### Summary

This research is directly applicable to characterizing the future cyber research and engineering designs that can enhance the security of safety systems within a nuclear facility.

The LDRD has been working with Boise State University (BSU) to engage them on a digital safety system from Honeywell that they received in the middle of June. They are currently working with Honeywell to get the safety system installed, configured, and operational by the end of the year.

INL is also currently working a relationship with an energy company in the UAE that is planning for four APR-1400 reactors. The APR-1400 reactor design is an entirely digital system, including a digital safety system. With the relationship, it will allow the researchers to extrapolate the data, experimentation, and results gained from the Honeywell safety system at BSU and apply it to the nuclear digital safety system.

INL is also working a relationship with Areva with the intent of investigating the potential to work with Areva on the Teleperm XS/XP systems or simulated environments. The Teleperm XS/XP system is one of the only two digital safety systems that are approved by the Nuclear Regulatory Commission for use in domestic nuclear facilities.

### Benefits to DOE:

This project is an extension of DOE's current leadership in critical infrastructure assessment methodology as employed in DOE National SCADA Test Bed and DoE's support to National Critical Infrastructure Security Programs. This research builds DOE's capability to also improve and enhance mobile embedded systems technologies. These systems are growing rapidly in a mobile ecosystem, and enhanced capability in this area will continue DOE's leadership across all critical infrastructure sectors. Specific applications include improvement of national energy efficiency and security and continued improvement of energy production and distribution security.



## **Presentations**

Chugg, J., 2017, “Strategic Advisory Committee Poster Session,” EIL building at INL, June, 2017

## **17A1-160FP: Mass Storage Equipment Protection**

Nikki Rasmussen<sup>1</sup> and James W Schondel<sup>1</sup>

### **General Project Description**

The project goal is to enable a faster method for mass storage protection than is currently used in many overseas embassies. Protecting mass storage devices that contain sensitive materials is of utmost importance in many overseas facilities and operations. These devices may contain classified materials that must be protected from loss to intruders during an evacuation scenario such as the Benghazi compound attack or other theft scenarios. Current technology for destruction of magnetic hard drives and/or solid state hard drives involves a mechanical shredder. This shredder can effectively destroy the hard drives, but it often takes minutes to destroy a single hard drive, which can endanger personnel under attack. It also requires electrical power that may be unavailable during an attack. Thermite torch technologies could be employed to destroy multiple hard drives at once in a fraction of a second, thus protecting the sensitive material while minimizing time and power load requirements for destruction of the drives. The project will build upon previous experience with thermite torch technologies. Multiple sizes of torches and multiple torches will be tested to determine penetration power and coverage against different mass storage devices. Left over materials from the mass storage devices will be examined to determine whether data can be recovered after destruction.

### **Summary**

This research began in September 2017; at this point no reportable results have been obtained.

## 17A1-162FP: Securing Electronic Control Unit Communication

Jonathan Chugg<sup>1</sup> and Kenneth Rohde<sup>1</sup>

### General Project Description

Researchers have shown that the controller area network (CAN) bus systems in the automotive industry lack necessary security features. Public and industry research and development have only focused on CAN bus security through third-party add-ons, which only provide a quick-fix Band-Aid approach to this national grand challenge. This is a critical vulnerability area that INL's expertise with industrial control, and CAN systems can be enhanced and expanded to address the vulnerabilities of mobile embedded control systems. Electronic control units (ECUs) are designed to meet original equipment manufacturers' parameters for functionality, whereas the actual coding structure used within the ECU is a black box to the manufacturer and Tier 1 Supplier, making it very difficult to secure using traditional methods. This concept would investigate the possibility of injecting host-based security directly into the ECU firmware on a binary level. If successful, the injection process could be applied to the ECU in a transparent manner. The project would design various security payloads and inject them into an ECU, thus securing the ECU through binary code injection. This also provides an opportunity for INL to supplement current research by addressing these challenging problems, utilizing the Laboratory's unique skill sets and capabilities and addressing the most urgent challenge facing the industry. This is a quick turnover research and development opportunity that fulfills the automotive industry's need for a viable, cost effective, and broad-based solution.

### Summary

The purpose of project is to investigate developmental concepts for enhancing the security of the CAN protocol that is widely used in a number of different critical infrastructure sectors, including nearly all vehicles within the transportation sector. This research is directly applicable to characterizing the future cyber research and engineering designs that can enhance the operational security of the control systems that manage controls of gasoline vehicles, electric vehicles, electric vehicle charging stations tied to the electric grid, and many other systems that support our critical infrastructure.

Initial research focused on implementing and evaluating a secure CAN protocol injected in an Electronic Control Unit (ECU) and evaluating its cohesion within the communication networks in a vehicle, as depicted in Figure 1. The LDRD has two cyber security researchers working on the experimentation and research through firmware extraction, firmware reverse engineering, and binary code injection.

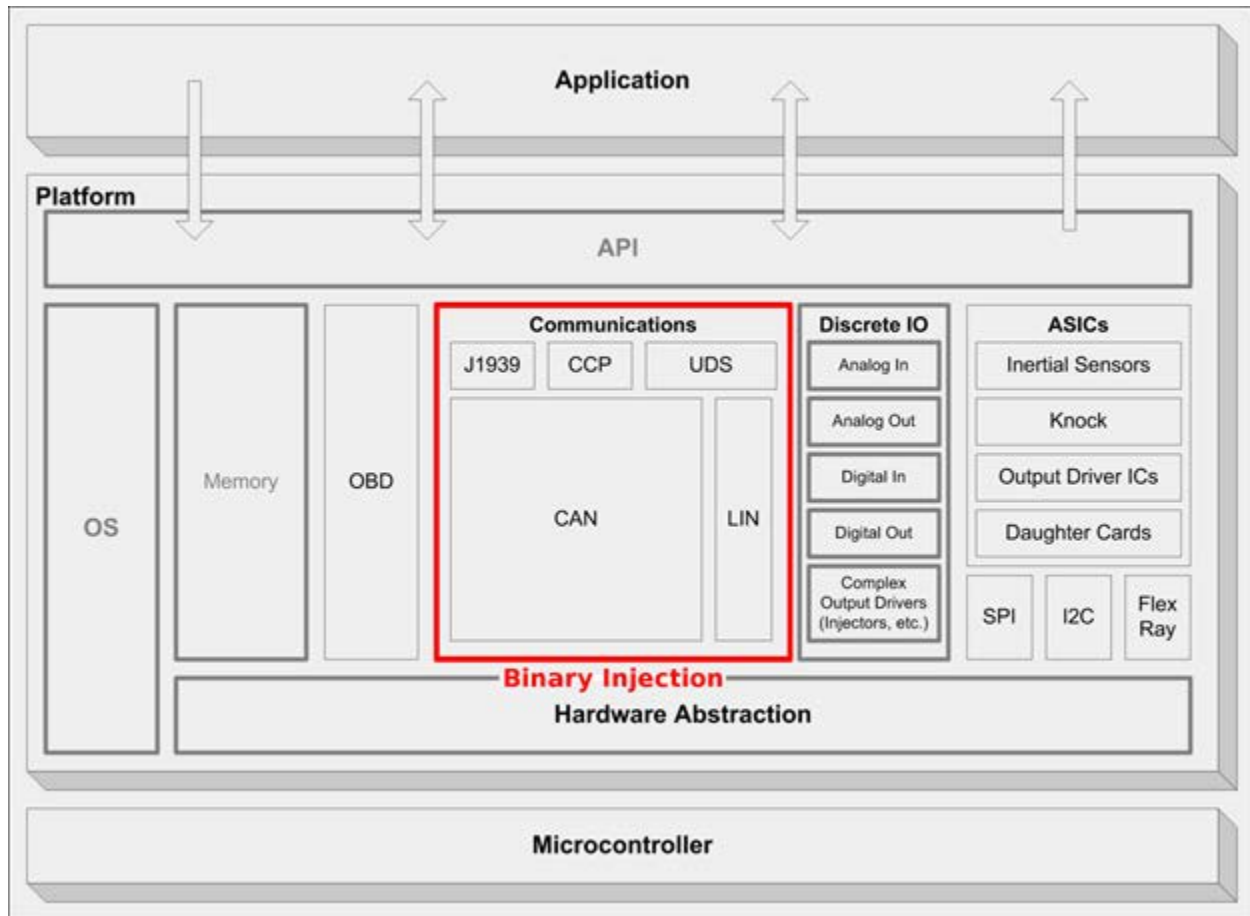


Figure 1. ECU binary injection location.

The researchers identified how to extract and update firmware on an ECU and became very familiar with the hardware. They also have identified where and how to inject the binary code to modify the CAN bus send() and receive() calls. The current research is proving to be difficult, as free space throughout the firmware image needs to be identified, mapped, and referenced correctly to achieve the desired secure injection. A debugger was procured to aid in the reverse engineering as well as the development of a novel binary code that is injected into the firmware of the ECU.

Successful results from this experimentation will be published to establish a science-based foundation for future transformational changes to how the CAN protocol is implemented - transforming from insecure CAN to secure CAN implementation. Once the binary injection is completed, thorough examination and experimentation will need to be performed to ensure that the secure implementation of the CAN protocol works consistently with the many modules and communications within the vehicle.

The VOLPE program from the Department of Transportation has expressed interest in the results from this research for future research and development of industry standards.

### **Benefits to DOE**

This project is an extension of DOE's current leadership in critical infrastructure assessment methodology as employed in DOE National SCADA Test Bed and DoE's support to National Critical Infrastructure Security Programs. This research builds DOE's capability to also improve and enhance mobile embedded systems technologies. These systems are growing rapidly in a mobile ecosystem, and enhanced capability in this area will also continue DOE's leadership across all critical infrastructure sectors. Specific applications include improvement of electric vehicle assurance, national energy efficiency and security for transportation, and continued improvement for energy production and distribution security.

### **Presentations**

Chugg, J., 2017, "Strategic Advisory Committee Poster Session," EIL building at INL, June, 2017.

### **Interns, Postdocs, and Staff support for Graduate Studies**

Intern: Braxton Cox.

## 17A1-178FP: Forensics of Embedded Devices

Jason Maughan<sup>1</sup> and Ray Fox<sup>1</sup>

### General Project Description

The advent of the network-connected industrial control systems (ICS) brought a world of efficiencies and precision that transformed U.S. critical infrastructure. As part of that transformation, control systems became increasingly vulnerable to attacks that were historically aimed at traditional personal computers (PCs) and internet protocols. Even though cyber-incident response and forensics organizations, which are tasked to provide onsite incident response for immediate investigation and resolution of cyber-attacks on traditional PCs, continue to grow, national capabilities to do the same for embedded systems within an ICS environment are woefully behind. This project aims to develop innovative forensic capabilities relevant to embedded systems (e.g., programmable logic controllers (PLCs) that manage a waste-water plants, factory assembly lines, or oil refinery process or, further, the network devices that allow for PLCs to communicate) to enable incident responders to extract firmware and analyze it to mitigate the growing cyber-threats to vital embedded systems within critical infrastructure.

### Summary

In most cases firmware controls everything an embedded device is capable of doing, is proprietary, and is designed to be inaccessible behind a variety of security barriers. Hence firmware is both an attractive target for malicious actors, and a difficult system on which to conduct forensics. In developing new capabilities for incident responders, this project hypothesizes that effective tools will need to be able to extract and analyze firmware for malware, while also assuring the forensics integrity of the discovered information. During this year's research, we completed the foundational discovery stage of our research effort. We identified and acquired four samples of different PLCs that are typical of the systems used within U.S. critical infrastructure. Our research examined different methods for extracting firmware from these four products, and in particular, we investigated different methods that were vendor-enabled through both physical and digital mechanisms. We also experimented with more invasive techniques that involved hardware-reversing based approaches available within the INL HexLab. These efforts led to three observations:

- There are few if any vendor-provided approaches for quickly and efficiently retrieving copies of firmware on devices.
- Probing of the hardware, while time-consuming and labor-intensive, does provide access to the firmware. Successful probing required overcoming the challenges of identifying the proper chips, and then finding the appropriate readers to dump the memory from those devices.
- The direct hardware-access testing proved to be a very customized expert-based process. As such, we recommended that any researchers and/or forensic examiners using direct hardware-access testing carefully record their processes and results to maintain the repeatability of the experiments and to inform future methodologies with other PLCs.

After we complete the firmware extraction experimentation, we will shift to the next phase of research by exploring software investigation capabilities. We postulate that methodologies for effective software investigation will be a significant technical challenge, since typical embedded system software contains thousands of lines of code in relationship to a small malware modification within the software. Noting this, we will explore a number of different techniques and methods to discover capabilities for finding the software equivalent of a 'micro-dot on the printer's page'. Initial experimentation will involve evaluating the effectiveness of cryptographic hashing approaches, and then comparing the results with more advanced techniques that leverage intermediate languages and code translation tactics.

### Benefits to DOE

As two of the many federal organizations charged with the protection of the nation's critical infrastructure, both the Department of Energy (DOE) and the Department of Homeland Security (DHS) will benefit by having access to the experimental results and developed capabilities. This research will lead to science-based capabilities that DOE, DHS, and other cyber defenders require to access the logic that drives embedded devices and, thereby, discover the threats that may exist and actions needed to recover from an attack. Not only will this be applicable from an incident-response perspective, but the technology and understanding that are gained from this research will enable embedded systems designers and vendors to develop improved cyber-informed firmware and software capable of preventing, deterring, or mitigating against supply-chain vulnerabilities and threats.

### Presentations

Maughan, J and A.R. Fox, 2017, *Strategic Advisory Committee Poster Session*, Idaho National Laboratory, Idaho Falls, ID, June, 2017.

Fox, A.R., 2017, "Firmware Forensics LDRD," *ICSJWG Fall 2017 Meeting*, Pittsburg, PA, September 2017.



## 17A1-183FP: V2X Communications Security

Samuel Ramirez,<sup>1</sup> Kurt Derr,<sup>1</sup> Jonathan Chugg,<sup>1</sup> Edward Springer<sup>1</sup>

### General Project Description

Vehicle communications increases as technology expands, as the market demands, and also as vehicle safety attempts to save drivers from injury and tens of thousands of deaths. With more ways to communicate—cellular, satellite, WiFi, and others—more ways are found to inform the driver of potential hazards on the road. As these technologies multiply, another potential hazard requires attention: the cyber security of the communications.

The objective of this project is to investigate the cyber security aspects of Vehicle to Vehicle (V2V), Vehicle to Infrastructure (V2I), and Vehicle to Person (V2P) communications, all known and covered by the shorter term V2X. This would leverage prior vehicle research in CAN-Bus and V2X implementations completed at INL and at other research institutions. This project will explore V2X communications disruption, take-over and/or compromise of a vehicle and/or communications infrastructure. The project will also study the possible mitigations and countermeasures of vulnerabilities and the interoperability of V2X between different manufacturers.

### Summary

The V2X Communications Security project started with a high-level overview of V2X hardware, which is composed of two main parts, the road side unit and the on board vehicle unit that resides in the vehicle connected to the Car Area Network-Bus (CAN-Bus) to obtain vehicle information and data. Effort was expended to determine all communications interfaces, which manufacturers are building into V2X systems in general. Many interfaces have been noted, which includes Dedicated Short Range Communications (DSRC), which is the basis for V2X communications, along with a plethora of other methods, such as Bluetooth, WiFi, XM-Satellite, GPS, Ethernet, Universal Serial Bus(USB), and CAN-Bus. Some hardware interfaces were also noted: Joint Test Action Group (JTAG), Serial Peripheral Interface (SPI), and Inter-Integrated Circuit(I2C). All of these methods are well known for their utility but also can be potential attack vectors into the V2X communications systems. Work has begun on exploiting Bluetooth, JTAG, and SPI to determine if there is a vector through the V2X equipment and ultimately the vehicle. Other communication methods will be investigated for the same goal, which is to traverse the V2X systems to the CAN-Bus and affect the operation of the vehicle.

More invasive methods to uncover vulnerabilities were incorporated later in the year to help to discover vulnerabilities hidden in the hardware and firmware. Also a survey of the memory, CPUs, and devices on the circuit boards was developed to help determine what, if any, vulnerabilities may exist at the lowest levels. Direct communications with the hardware architecture was established so that the underlying operation of the system could be monitored and studied at the CPU instruction level.

The V2X systems require GPS signals and data as part of the process of formulating location and basic safety messages. What are also required are messages from the vehicle itself through the vehicle's CAN-Bus network so efforts to synthetically generate those messages have begun. Once these two data sources are supplied, the V2X systems will be able to send complete messages containing the vehicle location and the vehicle operating parameters, such as speed and any currently operating tasks, such as braking to other vehicles and the road side units via DSRC.

Recent efforts have been successful in developing a basic simulated GPS signal that will feed a static location to the V2X devices. The devices have reacted to the simulated signal as if it were real, as if the signal was arriving from satellites in the GPS constellation. Efforts are currently underway to develop a dynamic GPS signal to simulate location movement. In the CAN-Bus effort, messages have been successfully transmitted and received

bidirectionally, but further tuning of the messages is required to acquire specific vehicle actions such as braking and acceleration.

### **Benefits to DOE**

This research will ultimately benefit all entities that use vehicle communications and will help to reduce the risk of cyber-security breaches within vehicle infrastructure as they become more connected to each other and the internet. If intrusions or disruptions can be reduced or eliminated, then vehicles connected to the power grid, such as electric vehicles, will remain cyber safe. This also means that the electric grid will have a reduced risk of cyber-security issues. The greatest benefit will be increased safety of our nation's drivers.

## 17A1-206FP: Large Scale Log Analysis for Control System Networks

Ryan Hruska,<sup>1</sup> Jonathan Chugg,<sup>1</sup> and Michael Haney<sup>21</sup>

### General Project Description

Modern security information and event management (SIEM) systems leverage advances in big-data storage and analytics capabilities to collect, store, and analyze system and network logs in attempt to detect intrusions and other potential threats. This project intends to advance the state-of-the-art in log, netflow, and packet analysis relevant SIEM systems for control-system networks and to support doctoral-level research for the principal investigator. Specifically, this project seeks to develop advanced database architectures and analysis methodologies to facilitate comprehensive log and netflow analysis for historical and incident investigation for control-system networks. This will include the integration of a scalable computational database with machine-learning methodologies to enable in-database analytics. This capability will eliminate the need to perform computational expensive extract, transform, load (ETL) processes required for in-depth analysis. The database will be designed to enable real-time loading of event data in both raw and aggregate form.

### Summary

The first year research focused on 2 preliminary however essential steps 1) the development of a multi-dimensional array data model such that it can be optimized for an industrial control system (ICS) environment and 2) an automated log parsing and loading capability in order to efficiently populate the previously defined data model. The benefit of this ground level development is the ability to rapidly populate new test databases from existing logs or real-time feeds in order to evaluate different intrusion and threat scenarios. This capability will significantly enhance our ability develop and test the efficacy of detection methodologies across a range of ICS systems configurations.

### Benefits to DOE

One of the primary missions of DOE is to ensure resilient, reliable, and flexible energy systems. As part of this mission, DOE-OE seeks to “mitigate the risk of energy disruption resulting from cyber incidents” through research and development of advanced cybersecurity solutions. DHS has a broader but parallel R&D mission to safeguard and secure cyberspace through DHS S&T’s goals of a trusted cyber-future and enabling the decision maker. This research will benefit DOE, DHS, and INL by advancing the state-of-the-art in security information and event management through development and application of advanced computational methodologies. If successful, this research has the capability to advance the state-of-the-art in comprehensive log and netflow analysis for incident response and forensic analysis of control systems networks by providing a valid solution to detect low-and-slow attacks as well as advanced persistent threats (APT). By developing these methodologies and demonstrating our ability to solve these complex analytic challenges, DOE’s and INL’s status as a research leader in critical infrastructure protection will be enhanced.

### Presentations

2017 N&HS Strategic Advisory Committee Poster Presentation.

## 17P11-005FP: Improved ICS Resilience through Automated Detection and Response

Craig Rieger,<sup>1</sup> Jonathan Chugg,<sup>1</sup> and Todd Vollmer<sup>1</sup>

### General Project Description

Industrial control systems (ICSs) are the nervous system for critical infrastructure yet, in many ways, the least advanced form of cyber-protection. In general for all network connected systems, but specifically for ICS cyber security, where expert cyber security resources can be limited, human response times will never be quick enough. That is, the time required for a human to recognize and mitigate a cyberattack will always be a limitation to preventing compromise from a persistent threat. As a result, the development of resilient control systems was defined by a different philosophical approach to making systems inherently resilient to attacks: autonomous response.<sup>2</sup> While such responses can be defined for different parts of an ICS architecture—such as the network, human machine interfaces, etc.—field control devices (FCDs) host the critical control logic that directly interacts with the physical systems in a power or chemical plant and, therefore, receive priority in our research. The approach to define an automated response begins with evaluating available FCD indicators of cyber-threat and identifying mitigating responses, driven by resilience measures to determine those with greatest benefit. Characterization methodologies will be based upon reverse engineering methods, including packet analysis, debug-port characterizations, pin-voltage measurements and the like to collect relevant indicators for command streams that allow for modifying control commands, memory mapping, and other characteristics of FCDs. The utility of these indicators and responses will be evaluated using a disturbance and impact resilience approach<sup>26</sup> that will yield, as a research outcome, a cyber feedback method that can be used to modify FCD behavior against cyber-attack. As a result, a means to integrate resilient anomaly detection and automated mitigation designs (not currently available in any FCD) can be advanced with ICS industries and government agencies, including the Department of Homeland Security (DHS), Department of Energy (DOE), and Department of Defense (DoD).

### Summary

Evaluations of several types of hardware to analyze for indicator and response characteristics was performed, with the observation that many of the features of information technologies (IT) have been inherited into the ICS hardware. In particular, the Siemens S7-1500 controller and Allen Bradley 1756 (**Error! Reference source not found.**) communications and controller modules are now using field programmable gate arrays (FPGA) and other programmable components that offer flexibility in programming updates, but could also be used to insert malware or other nefarious software. In the case of this LDRD, the available flexibility allows for hosting the algorithms and application programming interfaces that may be used to recognize cyber-attacks and provide a resilient response. Collection of physical device indicators from devices with existing software interfaces, as represented in Figure 18, will be aggregated into a common human interface and historian for analysis. Confidence in indicators through repeatability in experimental studies can then be assured.

Resilience metrics are a required to benchmark performance of the systems, and to ascertain the timescale that benefits can be achieved. Namely, only real anomalies should be recognized and trigger a response that occurs faster than the dynamical requirement of the controlled function. While this “left of boom” operation may not always be possible, seeking precursor detection provides temporal acuity as the team develops the algorithms in this effort. Referring to Figure 3, an active cyber feedback loop can be considered as a specific action to correct a single attack (figure left), but there are multiple points within the control loop that can be affected (right). Based upon the metrics, layered responses can be developed to protect the FDC. In line with this effort, resilience metrics and a tool are being developed that will provide a correlation of the time dynamics for the control

<sup>26</sup> C. G. Rieger, “Resilient Control Systems: Practical Metrics Basis for Defining Mission Impact,” 7<sup>th</sup> *International Symposium on Resilient Control Systems*, August, 2014.

feedback systems hosted on the FDC. The tool will provide indications as to the level of resilience that can be maintained by the individual response action, in particular, but also some indication of the effectiveness of the indicators. The resulting efforts, although started late in the year, have baselined hardware and metrics, which will be further developed in the second year.

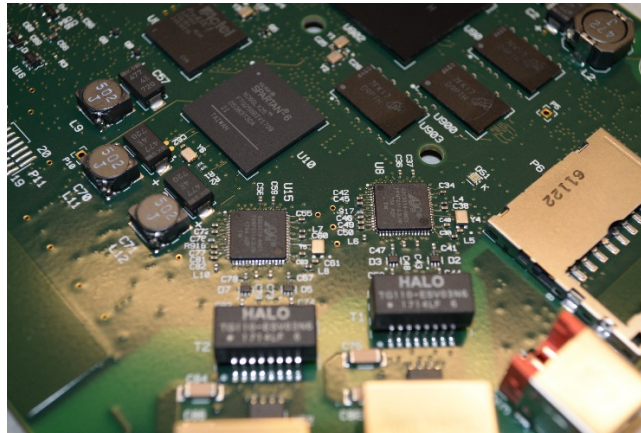


Figure 17. Allen Bradley Module

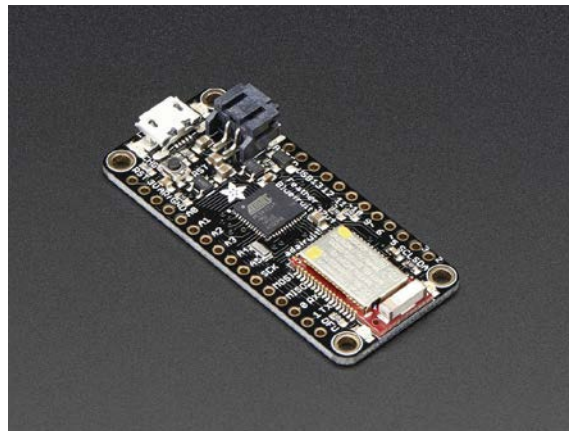


Figure 18. Arduino Physical and Environmental Measurement Interface

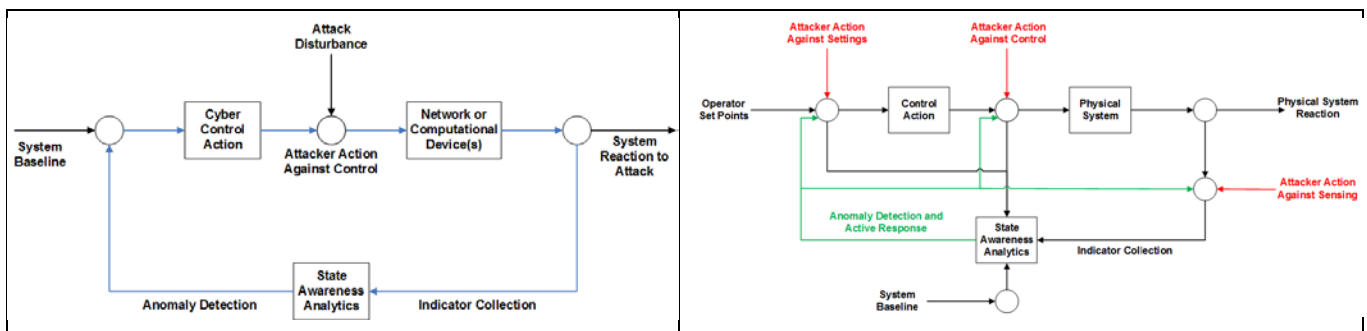


Figure 19. Cyber response to avert control action in cyber and standard control loops.

**Benefits to DOE**

The benefit of this effort is multifaceted and includes demonstration of multi-lab collaboration to more comprehensively evaluate a problem set and develop a need, building also on the diversity of the participants. The ever-increasing likelihood of cyberattack, especially in causing unsafe and damaging effects to our utilities and infrastructure, is a challenge for this nation that must be addressed. In particular, not all control systems could be replaced, even if resilient control technologies were available. Therefore, the efforts by this team to consider current hardware designs and technologies that can be scaled and applied across infrastructure is significant.





# Appendices





# **Appendix A**

## **Benefiting Agencies**



## Appendix A

### Benefiting Agencies

The following table provides a listing of individual LDRD project contributions to each benefiting agency. Green dot represents the primary beneficiary and the black dots represent secondary beneficiaries. In addition, FY 2017 total investments are provided for each benefiting agency.

- + Project total exceeds 84 projects funded in 2017 because multiple beneficiaries per project are allowed.
- \* Project total funding exceeds the approximately \$22M FY 2017 LDRD budget because multiple beneficiaries are allowed for each project.

Project	PI Name	Title	2017 Cost (\$)	Department of Homeland Security	Department of Defense	DOE Office of Energy Efficiency and Renewable Energy	DOE Office of Environmental Management	DOE Office of Environmental, Safety, and Health	DOE Office of Fossil Energy	DOE-NE	National Nuclear Security Administration	DOE Office of Naval Reactor	DOE Office of Civilian Radioactive Waste Management	DOE-Office of Electricity Delivery and Energy Reliability	DOE Office of Science
15-002	Zalupski Peter R	Experimental Scenarios of Adversity and Recovery in Aqueous Separations.	294,649			●	●			●	●				●
15-013	Smith Curtis L	Simulation Based Analysis of Procedures and Accident Management Guidelines	222,631							●					

## 2017 Project Summaries — Introduction

Project	PI Name	Title	2017 Cost (\$)	Department of Homeland Security	Department of Defense	DOE Office of Energy Efficiency and Renewable Energy	DOE Office of Environmental Management	DOE Office of Environmental, Safety, and Health	DOE Office of Fossil Energy	DOE-NE	National Nuclear Security Administration	DOE Office of Naval Reactor	DOE Office of Civilian Radioactive Waste Management	DOE-Office of Electricity Delivery and Energy Reliability	DOE Office of Science
15-023	<b>Coleman</b> Justin L	Development of Stochastic 3-Dimensional Soil Response Capability in MOOSE to Provide Design and Beyond Design Basis Seismic Motions for Nuclear Facilities	82,290				●			●	●				
15-032	<b>Gofryk</b> Krzysztof	Development of new method for high temperature thermal conductivity measurements of nuclear materials	252,191							●					●
15-039	<b>Bragg-Sitton</b> Shannon M	Transient Modeling of Integrated Nuclear Energy Systems with Thermal Energy Storage and Component Aging and Preliminary Model Validation via Experiment	426,533			●			●	●				1	

Project	PI Name	Title	2017 Cost (\$)	Department of Homeland Security	Department of Defense	DOE Office of Energy Efficiency and Renewable Energy	DOE Office of Environmental Management	DOE Office of Environmental, Safety, and Health	DOE Office of Fossil Energy	DOE-NE	National Nuclear Security Administration	DOE Office of Naval Reactor	DOE Office of Civilian Radioactive Waste Management	DOE-Office of Electricity Delivery and Energy Reliability	DOE Office of Science
15-040	Agarwal Vivek	Acoustic telemetry infrastructure for in-pile Advanced Test Reactor and Transient Test Reactor monitoring	359,247			●				●					
15-060	DeHart Mark D	Development of State-of-the-Art Capabilities to Support Transient Test Reactor Modeling and Simulation	466,466							●	●				
15-094	Sanders Jeff	Evaluation and Demonstration of the Integration of Safeguards, Safety, and Security by Design (3SBD)	76,789							●	●				
15-100	Verba Jared A	Real time Process Simulator (RTPS)	350,652	●		●								●	
15-111	Freeman Sarah G	Adversary Signature Development and Threat Analysis	178,049	●		●								●	
15-125	Dufek Eric J	Phosphoranimines for advanced battery applications	215,718			●								●	●

## 2017 Project Summaries — Introduction

Project	PI Name	Title	2017 Cost (\$)	Department of Homeland Security	Department of Defense	DOE Office of Energy Efficiency and Renewable Energy	DOE Office of Environmental Management	DOE Office of Environmental, Safety, and Health	DOE Office of Fossil Energy	DOE-NE	National Nuclear Security Administration	DOE Office of Naval Reactor	DOE Office of Civilian Radioactive Waste Management	DOE-Office of Electricity Delivery and Energy Reliability	DOE Office of Science
15-128	Huang Hai	Microstructural evolution and mesoscale coupled flow-reaction-fracturing processes in organic rich nanoporous shales	289,838			●	●		●						●
15-135	Mohanpurkar Manish U	Dynamic Simulations for Large Scale Electric Power Networks in Real Time Environment using Multiple Real Time Digital Simulator	336,189		●	●				●				●	●
15-141	Zhang Hongbin	Interfacing Multiphysics Object Oriented Simulation Environment Components to Enhance Capability	99,374							●	●				
15-142	Teyseyre Sebastien P	New in core neutron diagnostics	97,384							●	●				●
15-144	Li Shelly X	Investigation of Sonication Assisted Electrolytic Reduction of Used Oxide Fuel in Molten Salt	163,872				●			●					
15-145	Jewell James K	Advanced Neutron and X-Ray Imaging at Transient Test Reactor	181,472							●	●	●		●	●



Project	PI Name	Title	2017 Cost (\$)	Department of Homeland Security	Department of Defense	DOE Office of Energy Efficiency and Renewable Energy	DOE Office of Environmental Management	DOE Office of Environmental, Safety, and Health	DOE Office of Fossil Energy	DOE-NE	National Nuclear Security Administration	DOE Office of Naval Reactor	DOE Office of Civilian Radioactive Waste Management	DOE-Office of Electricity Delivery and Energy Reliability	DOE Office of Science
15-146	<b>Fushimi</b> Rebecca R	Tailoring the Kinetic Function of a Surface through Electronic Effects of Nanoscale Architecture	724,104			●			●						●
16-002	<b>Williams</b> Luke	Advanced Carbon Feedstock Processing Using Ionic Liquids.	392,051			●	●		●						●
16-003	<b>Tripathy</b> Prabhat K	Recycling of Tantalum-containing Waste Materials to Recover Tantalum Metal	199,991	●		●	●			●					●
16-010	<b>Schwen</b> Daniel	Development of a fully coupled radiation damage production and evolution simulation capability	497,638							●	●				
16-013	<b>Aagesen</b> Larry K Jr	Micromechanistic approach and critical experiments for quantitative predictions of delayed hydride cracking in zirconium alloys	319,871							●					●
16-026	<b>Youngblood</b> Robert W III	Computationally Efficient Prediction of Containment	147,583							●		●			

## 2017 Project Summaries — Introduction

Project	PI Name	Title	2017 Cost (\$)	Department of Homeland Security	Department of Defense	DOE Office of Energy Efficiency and Renewable Energy	DOE Office of Environmental Management	DOE Office of Environmental, Safety, and Health	DOE Office of Fossil Energy	DOE-NE	National Nuclear Security Administration	DOE Office of Naval Reactors	DOE Office of Civilian Radioactive Waste Management	DOE-Office of Electricity Delivery and Energy Reliability	DOE Office of Science
		Thermal Hydraulics Using Multi-Scale Simulation													
16-036	<b>Tolman</b> Kevin R	Neutron microscope to enable high-resolution neutron tomography at Idaho National Laboratory	379,268							●					●
16-040	<b>Agarwal</b> Vivek	Integration of Prognostic Techniques and Probabilistic Safety Assessment for Online Risk Monitoring	365,812			●			●	●				●	
16-046	<b>Adkins</b> Cynthia A	Development of a Synergistic Approach To Study Irradiated Materials Using Coupled Experiments and Simulation	279,735							●					
16-050	<b>Teyesseyre</b> Sebastien P	Stress Corrosion Cracking Testing in Supercritical Carbon Dioxide	123,746							●					●

Project	PI Name	Title	2017 Cost (\$)	Department of Homeland Security	Department of Defense	DOE Office of Energy Efficiency and Renewable Energy	DOE Office of Environmental Management	DOE Office of Environmental, Safety, and Health	DOE Office of Fossil Energy	DOE-NE	National Nuclear Security Administration	DOE Office of Naval Reactor	DOE Office of Civilian Radioactive Waste Management	DOE-Office of Electricity Delivery and Energy Reliability	DOE Office of Science
16-055	<b>Permann</b> Cody J	Capability Extension for Multiscale, Multi-Application development within the Multiphysics Object-Oriented Simulation Environment	513,152			●	●		●	●		●			●
16-058	<b>Permann</b> Cody J	Predicting Radiation-Induced Microstructural Change via Implementation and Validation of Multiscale Cluster Dynamics in Multiphysics Object Oriented Simulation Environment	84,268							●	●	●		●	●
16-070	<b>Craft</b> Aaron E	Characterization of Neutron Beamlines at Neutron Radiography reactor	207,921							●					
16-071	<b>Craft</b> Aaron E	Evaluation of Advanced Digital Neutron Imaging Systems for Post Irradiation Examination of Nuclear Fuel	267,097							●					
16-081	<b>Heaps</b> Ron	Modeling Thermite Reactions	134,806	●						●					

## 2017 Project Summaries — Introduction

Project	PI Name	Title	2017 Cost (\$)	Department of Homeland Security	Department of Defense	DOE Office of Energy Efficiency and Renewable Energy	DOE Office of Environmental Management	DOE Office of Environmental, Safety, and Health	DOE Office of Fossil Energy	DOE-NE	National Nuclear Security Administration	DOE Office of Naval Reactor	DOE Office of Civilian Radioactive Waste Management	DOE-Office of Electricity Delivery and Energy Reliability	DOE Office of Science
16-085	<b>Zarzana</b> Christopher A	Production of Fluoroanion Targets for Accelerator Mass Spectrometry	225,771							●					
16-096	<b>Le Blanc</b> Katya L	Supporting operator performance and situation awareness in highly automated nuclear power plants	148,357			●				●				●	
16-098	<b>Snow</b> Mathew S	Nuclear Nonproliferation Applications of 14C Analyses by Accelerator Mass Spectrometry	206,267	●							●				
16-106	<b>Klett</b> Mary S	Risk Analysis Method Integrating Physical, Cyber and Infrastructure Dependencies	189,113	●						●	●			●	
16-129	<b>Li</b> Shelly X	Application of Radioactive Isotope Dilution Technique to Measurement of Molten Salt Mass for Electrochemical Recycling Process	77,101							●	●				
16-133	<b>Johnson</b> Briam E	Secure Supervisory Control And Data Acquisition Communications System	194,879	●		●				●				●	

Project	PI Name	Title	2017 Cost (\$)	Department of Homeland Security	Department of Defense	DOE Office of Energy Efficiency and Renewable Energy	DOE Office of Environmental Management	DOE Office of Environmental, Safety, and Health	DOE Office of Fossil Energy	DOE-NE	National Nuclear Security Administration	DOE Office of Naval Reactor	DOE Office of Civilian Radioactive Waste Management	DOE-Office of Electricity Delivery and Energy Reliability	DOE Office of Science
16-149	<b>Daw</b> Joshua E	In-core Qualification of Developmental Instrumentation	186,984							●		●			
16-152	<b>Derr</b> Kurt W	Wireless radio frequency signal identification and protocol reverse engineering (WiFIRE)	186,984	●										●	●
16-176	<b>Ding</b> Dong	Development of Direct Carbon Fuel Cells	186,984	●					●						●
16-187	<b>Jiang</b> Chao	Micro-Scale Technique to Evaluate Grain Boundary Cohesion of Irradiated Alloys	186,984						●	●	●				●
16-215	<b>Ding</b> Dong	Electrochemical Manufacturing Processes	186,984			●			●	●					●
16P6-002FP	<b>Baroi</b> Chinmoy	Kinetic-based Scale-Up Science for an Energy Efficient Route to Ethylene	186,984			●		●	●						●
16P6-003FP	<b>Sterbentz</b> James W	Phenomena Identification and Ranking Table Technique Applied to the MegaPower Heat Pipe Reactor Concept	186,984	●						●					

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16P6-007FP	<b>Smith</b> Robert T	Consequence-driven Cyber-informed Engineering (CCE) Methodology Pilot	186,984							●	●			●	
17A1-007FP	<b>Klaehn</b> John R	High Performance Polymeric Membranes for Filtration Applications High Performance Polymeric Membranes for Nano and Ultrafiltration Applications	186,984			●	●		●						
17A1-024FP	<b>Woolstenhulme</b> Nicolas E	Design to Enable Narrow Pulse Width in Transient Tests	186,984							●					
17A1-055FP	Baek Donna L	Electro-reduction of metals in supercritical fluid-room temperature ionic liquids	186,984			●									
17A1-070FP	<b>Woolstenhulme</b> Nicolas E	Multi-Purpose Non-Destructive Examination Station in the Advanced Test Reactor Canal	162,871							●		●			
17A1-079FP	<b>Lillo</b> Thomas M	Affixing Inert Dissimilar Materials to Structural Materials for High Performance Armor Systems	7,746	●							●				1

Project	PI Name	Title	2017 Cost (\$)	Department of Homeland Security	Department of Defense	DOE Office of Energy Efficiency and Renewable Energy	DOE Office of Environmental Management	DOE Office of Environmental, Safety, and Health	DOE Office of Fossil Energy	DOE-NE	National Nuclear Security Administration	DOE Office of Naval Reactor	DOE Office of Civilian Radioactive Waste Management	DOE-Office of Electricity Delivery and Energy Reliability	DOE Office of Science
17A1-086FP	<b>Zalupski</b> Peter R	Development of a complete kinetic model for free-radical-induced degradation of formic and oxalic acids.	477,139				●			●					●
17A1-093FP	<b>Craft</b> Aaron E	Digital Neutron Imaging of Irradiated Fuel Using a Gamma-Discriminating Scintillation System	248,490							●					
17A1-101FP	<b>Chichester</b> David L	Nuclear Instrumentation and Methods for Emergency Response	191,932	●						●	●				
17A1-105FP	<b>Nielsen</b> Joseph W	Safety Margin Evaluation for Experiment Irradiation in Advanced Test Reactor	288,721							●	●	●			
17A1-106FP	<b>Kinlaw</b> T	A Study of Fission Modes to Improve Nuclear Forensics	207,979	●							●				
17A1-109FP	<b>Verba</b> Jared A	Big Data Binary Reverse Engineering	325,709	●											



## 2017 Project Summaries — Introduction

Project	PI Name	Title	2017 Cost (\$)	Department of Homeland Security	Department of Defense	DOE Office of Energy Efficiency and Renewable Energy	DOE Office of Environmental Management	DOE Office of Environmental, Safety, and Health	DOE Office of Fossil Energy	DOE-NE	National Nuclear Security Administration	DOE Office of Naval Reactor	DOE Office of Civilian Radioactive Waste Management	DOE-Office of Electricity Delivery and Energy Reliability	DOE Office of Science
17A1-111FP	<b>Woolstenhulme</b> Nicolas E	Design of Low Activation Retrievable Sample Holder for Transient Test Reactor Irradiation of Science-Based Specimens	304,728							●	●				
17A1-114FP	<b>Rieger</b> Craig G	Resilient, Scalable Cyber State Awareness of Industrial Control System Networks to Threat	209,276	●		●				●				●	
17A1-124FP	<b>Ougouag</b> Abderrafi M	Systematic Error Control in Cross Section Library Generation for Novel Reactors	379,916							●					
17A1-142FP	<b>Klett</b> Timothy R	Modeling and Spatial-Temporal Analysis of Cyber-Physical Impacts	211,418	●										●	●
17A1-150FP	<b>Sun</b> Cheng	Advanced manufacturing of metallic fuels and cladding by equal-channel angular pressing	363,178							●					●
17A1-152FP	<b>Chugg</b> Jonathan P	Building Systems: Access, Management, & Automation	150,335	●						●				●	
17A1-156FP	<b>Chugg</b> Jonathan P	Nuclear Safety Systems Cyber Security	51,471	●						●				●	

Project	PI Name	Title	2017 Cost (\$)	Department of Homeland Security	Department of Defense	DOE Office of Energy Efficiency and Renewable Energy	DOE Office of Environmental Management	DOE Office of Environmental, Safety, and Health	DOE Office of Fossil Energy	DOE-NE	National Nuclear Security Administration	DOE Office of Naval Reactor	DOE Office of Civilian Radioactive Waste Management	DOE-Office of Electricity Delivery and Energy Reliability	DOE Office of Science
17A1-160FP	<b>Rasmussen</b> Nikki	Mass Storage Equipment Protection	11,916	●											●
17A1-162FP	<b>Chugg</b> Jonathan P	Securing Electronic Control Unit Communication	149,524	●						●				●	
17A1-164FP	<b>Le Blanc</b> Katya L	Application of Traditional Risk Assessment Methods to Cyber Manipulation Scenarios	244,428							●	●				
17A1-166FP	<b>Diaz Aldana</b> Luis A	Electrochemical Reduction of Carbon Dioxide Enriched in Switchable Polarity Solvents	255,422			●			●						
17A1-173FP	<b>Fox</b> Carter	Fractionation of lignocellulosic biomass with switchable polarity solvents	149,144			●									
17A1-178FP	<b>Maughan</b> Jason C	Forensics of Embedded Devices	176,845	●											
17A1-183FP	<b>Ramirez</b> Samuel	Vehicle-to-Vehicle, -Infrastructure, and -People Communication Security	154,889	●											

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Project	PI Name	Title	2017 Cost (\$)	Department of Homeland Security	Department of Defense	DOE Office of Energy Efficiency and Renewable Energy	DOE Office of Environmental Management	DOE Office of Environmental, Safety, and Health	DOE Office of Fossil Energy	DOE-NE	National Nuclear Security Administration	DOE Office of Naval Reactor	DOE Office of Civilian Radioactive Waste Management	DOE-Office of Electricity Delivery and Energy Reliability	DOE Office of Science
17A1-201FP	<b>Boring</b> Ronald Laurids	Human Reliability Analysis for Advanced Reactor Technologies and Systems	210,909							●					●
17A1-206FP	<b>Hruska</b> Ryan C	Large Scale Log Analysis for Control System Networks	50,943	●						●				●	●
17A1-223FP	<b>Jadernas</b> Daniel G	New Approach for Post Irradiation Examination Using Modular Transportable Instrumentation	347,818							●					
17A1-227FP	<b>Jones</b> Warren F	Multi-Physics, Multi-Scale Coupled Simulation of Power Impulse Experiments	451,154							●	●	●			●
17P10-003FP	<b>Sun</b> Cheng	In-situ small-scale mechanical testing of neutron irradiated ferritic steels	171,583							●					●
17P11-001FP	<b>Hurley</b> David H	Enabling Material Discovery for Waste Heat Recovery Systems using a Multimode Optical Sensor	203,193			●			1	●					●

Project	PI Name	Title	2017 Cost (\$)	Department of Homeland Security	Department of Defense	DOE Office of Energy Efficiency and Renewable Energy	DOE Office of Environmental Management	DOE Office of Environmental, Safety, and Health	DOE Office of Fossil Energy	DOE-NE	National Nuclear Security Administration	DOE Office of Naval Reactor	DOE Office of Civilian Radioactive Waste Management	DOE-Office of Electricity Delivery and Energy Reliability	DOE Office of Science
17P11-005FP	<b>Rieger</b> Craig G	Improved Industrial Control System Resilience through Automated Detection and Response	301,062	●		●					●			●	●
17P11-007FP	<b>Sun</b> Cheng	Coupling of Modeling and Experiment to Develop Predictive Models of the Mechanical Behavior of Nuclear Fuels and Materials	289,488							●					●
17P11-014FP	<b>Jadernas</b> Daniel G	The influence of irradiation on the corrosion kinetics and hydrogen pickup of zirconium alloys	139,957							●		●			●
17P11-018FP	<b>O'Brien</b> Robert C	Advanced Manufacturing of Uranium Dioxide Fuel Pellets with radially and axially zoned burnable poisons and hour-glassing control features	65,939							●	●			●	

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Project	PI Name	Title	2017 Cost (\$)	Department of Homeland Security	Department of Defense	DOE Office of Energy Efficiency and Renewable Energy	DOE Office of Environmental Management	DOE Office of Environmental, Safety, and Health	DOE Office of Fossil Energy	DOE-NE	National Nuclear Security Administration	DOE Office of Naval Reactor	DOE Office of Civilian Radioactive Waste Management	DOE-Office of Electricity Delivery and Energy Reliability	DOE Office of Science
17P11-022FP	<b>Kong</b> Fande	Development of Nonlinear Eigenvalue Solvers in the Multiphysics Object Oriented Simulation Environment (MOOSE)	289,488							●					
17P11-030FP	<b>Hurley</b> David H	Investigation of Exciton Delocalization and Exciton Coherence in Chromophores and Acoustic Nanostructures	164,632												●
17P11-032FP	<b>Johnson</b> Stephen G	Production, Encapsulation and Process Optimization of Energy Producing Isotopes	235,383							●					●
<b>FY 2017 Projects<sup>+</sup></b>				24	0	24	9	1	13	59	23	9	0	21	35

+ Project total exceeds 84 projects funded in 2017 because multiple beneficiaries per project are allowed.

**Appendix B**  
**Publications List for 2016 and 2017**





## Appendix B

### Publications List for 2016 and 2017

#### FY 2017

Journal Citation	Impact Factor	LDRD No.	Initiative	Collaborator Affiliation State/Country
Adam, B., L. Teeter, J. Mahaffey, M. Anderson, and J. Tucker, "Effects of Corrosion in Supercritical CO <sub>2</sub> on the Microstructural Evolution in an Fe-Ni Superalloy", In progress.	N/A	16-050	ANE	None
Agarwal, V. and J.A. Smith, 2017, "Real-Time In-Pile Acoustic Measurement Infrastructure at the Advanced Test Reactor," <i>ANS Nuclear Technology Letter</i> , 197.3, pp. 329-333, 2017.	0.745	15-040	ANE	None
Agarwal, V. and J.A. Smith, 2017, "Assessing Advanced Test Reactor Process States using Acoustic Measurement Infrastructure," <i>2017 ASME Pressure Vessels and Piping Conference</i> , July 16-20, Waikoloa, HI.	N/A	15-040	ANE	None
Agarwal, V. and J.A. Smith, 2017, "Acoustic Measurement Infrastructure to Enable the Enhancement of Nuclear Reactor Efficiency and Safety," <i>173<sup>rd</sup> Acoustical Society of America</i> , June 26 - 30, Boston, MA, 2017.Smith,	N/A	15-040	ANE	None
Aydogan, E., S. A. Maloy, O. Anderoglu, C. Sun, J. G. Gigax, L. Shao, F. A. Garner, I. E. Anderson, and J. J. Lewandowski, 2017, "Effect of tube processing methods on microstructure, mechanical properties and irradiation response of 14YWT nanostructured ferritic alloy", <i>Acta Materialia</i> , 134 (2017): 116-127.	5.301	17P10-003FP	ANE	Los Almos National Laboratory, New Meixco University of New Mexico, New Mexico Texas A&M, Texas Ames Laboratory, Iowa

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Journal Citation	Impact Factor	LDRD No.	Initiative	Collaborator Affiliation State/Country
Baroi, C., A.M. Gaffney, and R. Fushimi, 2017, "Process economics and safety considerations for the oxidative dehydrogenation of ethane using the M1 catalyst", <i>Catalysis Today</i> , Accepted for publication, in press, 2017.	4.636	15-146 16P6-002FP	CED CIP	Center for Advanced Energy Studies, Idaho
Blackman, H., and R. Boring, 2017, "Assessing dependency in SPAR-H: Some practical considerations", In R. Boring (ed.), <i>Advances in Human Error, Reliability, Resilience, and Performance (Advances in Intelligent Systems and Computing)</i> . Heidelberg: Springer Verlag, pp. 13-19.	N/A	17A1-201FP	ANE	Boise State University Norwegian University of Science and Technology University of Idaho Ohio State University
Boring, R., H. Blackman, and M. Rasmussen, 2017, "Process economics and safety considerations for the oxidative dehydrogenation of ethane using the M1 catalysvalidation of new designs", <i>Proceedings of the PSAM Topical Conference on Human Reliability, Quantitative Human Factors, and Risk Management</i> .	N/A	17A1-201FP	ANE	Boise State University Norwegian University of Science and Technology University of Idaho Ohio State University
Boring, R., R. Rasmussen, T. Ulrich, S. Ewing, and D. Mandelli, (2017). "Task and procedure level primitives for modeling human error." In R. Boring (ed.), <i>Advances in Human Error, Reliability, Resilience, and Performance (Advances in Intelligent Systems and Computing)</i> , pp. 30–40. Heidelberg: Springer Verlag.	N/A	15-013	ANE	University of Idaho Norwegian University of Science and Technology
Boring, R., M. Rasmussen, C. Smith, D. Mandelli, and S. Ewing, (In press, 2017). "Dynamicizing the SPAR-H method: A simplified approach to computation-based human reliability analysis," <i>Proceedings of the 2017 Probabilistic Safety Assessment Conference</i> .	N/A	15-013	ANE	University of Idaho Norwegian University of Science and Technology
Cao, L., J. Jarrell, A. Kauffman, K. Herminghuysen, S. White, J. Sanders, and S. Li, 2017, "A radioactive tracer dilution method to determine the mass of molten salt," <i>Journal of Radiochemistry and Nuclear Chemistry</i> , (2017) 314:387–393, DOI 10.1007/s10967-017-5417-5.	1.282	16-129	ANE	Ohio State University, Ohio

Journal Citation	Impact Factor	LDRD No.	Initiative	Collaborator Affiliation State/Country
Chorney, M.P., B.P. Hurley, P. K. Tripathy, and J. P. Downey, 2017, "Effects of Oxide Precursor Preparation Parameters on the Electrochemical Reduction of Tantalum Pentoxide in Calcium Chloride Melt", <i>The Minerals, Metals and Materials Society, TMS 2017, 146th Annual Meeting &amp; Exhibition Supplemental Proceedings</i> , Springer, DOI:10.1007/978-3-319-51493-2_62, pp. 651-5.	N/A	16-003	ANE	Montana Technical University-Butte, Montana
"Consequence-driven Cyber-informed Engineering (CCE)", Mission Support Center, Idaho National Laboratory, October 18, 2016, <a href="http://www.osti.gov/scitech/servlets/purl/1341416">http://www.osti.gov/scitech/servlets/purl/1341416</a>	N/A	16P6-007FP	CIP	None
Constales, D., G. Yablonsky, L. Wang, W. Diao, V. Galvita, and R. Fushimi, 2017, "Precise non-steady-state characterization of solid active materials with no preliminary mechanistic assumptions". <i>Catalysis Today</i> , 2017.	4.636	15-146	CED	Ghent University, Department of Mathematical Analysis, Ghent, Belgium St Louis University, Missouri Center for Advanced Energy Studies, Idaho
Diaz, L. A., N. Gao, B. Adhikari, T.E. Lister, E.J. Dufek, and A. D. Wilson, "Electrochemical Production of Syngas from CO <sub>2</sub> Captured in Switchable Polarity Solvents", <i>Green Chemistry</i> , accepted manuscript; DOI: 10.1039/c7gc03069j	N/A	17A1-166FP	ANE	Oregon State University
Ding, D., Y. Zhang, W. Wu and T. He, <i>Energy Environmental Science</i> , under review.	N/A	16-215	CED	None
Dufek, E. J., J. R. Klaehn, J. S. McNally, H. W. Rollins, and D. K. Jamison, 2016, "Use of Phosphoranimines to Reduce Organic Carbonate Content in Li-ion Battery Electrolytes," <i>Electrochimica Acta</i> , 209.10, pp. 36-43.	4.798	15-125	CED	No external collaborators

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Journal Citation	Impact Factor	LDRD No.	Initiative	Collaborator Affiliation State/Country
Ellis, M., D. Gaston, B. Forget, K. Smith, 2017, "Preliminary Coupling of the Monte Carlo Code OpenMC and the Multiphysics Object-Oriented Simulation Environment for Analyzing Doppler Feedback in Monte Carlo Simulations," <i>Nuclear Science and Engineering</i> , 185 (1), pp 184-193, January 2017.	0.822	15-060	ANE	Massachusetts Institute of Technology, Massachusetts
Ewing, S.M., R. Boring, D. Mandelli, and K. Savchenko, (2017). "Determination of a generic human error probability distribution, part 2: A dynamic SPAR-H example application," <i>Transactions of the American Nuclear Society</i> , 116, pp. 295-298.		15-013	ANE	University of Idaho Norwegian University of Science and Technology
Ewing, S., R. Boring, M. Rasmussen, and T. Ulrich, (2017). "Text mining for procedure-level primitives in human reliability analysis," In R. Boring (ed.), <i>Advances in Human Error, Reliability, Resilience, and Performance (Advances in Intelligent Systems and Computing)</i> , pp. 239-249. Heidelberg: Springer Verlag.	N/A	15-013	ANE	University of Idaho Norwegian University of Science and Technology
Ewing, S.M., K. Savchenko, D. Mandelli, and R. Boring, (In press, 2017). "Determination of a generic human error probability distribution, part 1: A dynamic formulation of SPAR-H.," <i>Transactions of the American Nuclear Society</i> , 116, pp. 299-302.		15-013	ANE	University of Idaho Norwegian University of Science and Technology
Frick, K., C.T. Misenheimer, J.M. Doster, S.D. Terry, and Bragg-Sitton, 2017, "TES Configurations for Small Modular Reactor Load Shedding," <i>Nuclear Technology</i> , submitted September 2017.	N/A	15-039	CED	North Carolina State University Ohio State University Oregon State University Massachusetts Institute of Technology University of New Mexico
Gribok, A. V., V. Agarwal and V. Yadav, 2017, "Specification of Prior in Empirical Bayes Estimation through Bayesian Deconvolution for Probabilistic Risk Assessment," <i>International Topical Meeting on Probabilistic Safety Assessment and Analysis</i> , Pittsburgh, Pennsylvania, September 24-28, 2017.	N/A	16-040	ANE	None

Journal Citation	Impact Factor	LDRD No.	Initiative	Collaborator Affiliation State/Country
Gribok, A. V., V. Agarwal and V. Yadav, "Performance of Empirical Bayes Estimation Techniques Used in Probabilistic Risk Assessment," <i>Reliability Engineering &amp; System Safety</i> (under review).	N/A	16-040	ANE	None
Harter, J.R., P. A. Greaney, T. S. Palmer, "Deterministic Phonon Transport Predictions of Thermal Conductivity in Uranium Dioxide with Xenon Impurities", <i>Journal of Heat Transfer</i> , under review.	N/A	15-060	ANE	North Carolina State University Oregon State University University of New Mexico Massachusetts Institute of Technology
Hearn, C., A. Kuznicki, C. Becker, K. Derr, and S. Ramirez, 2016, "Data Acquisition in Wireless Router Link Testbed using GNU Radio Companion", <i>GNU Radio Conference (GRCON 2016)</i> , September 12-16, 2016, accepted.	N/A	16-152	CIP	None
Klaehn, J. R., H.W. Rollins, J.S. McNally, N. Arulsamy, E.J. Dufek, 2017 "Phosphoranimines containing cationic N-imidazolium moieties" <i>Inorganica Chimica Acta</i> 466, pp. 254-265.	2.002	15-125	CED	Univeristy of Wyoming, Wyoming
Kong, F., et al., 2017, "A fully coupled two-level Schwarz preconditioner based on smoothed aggregation for the transient multigroup neutron diffusion equations," INL/CON-17-40867, <i>Linear Algebra and Its Applications</i> , under review	N/A	16-055	ANE	University of Wisconsin Università della Svizzera Italiana, Lugano, Switzerland
Kong, F., Y. Wang, S. Schunert, C. J. Permann, D. Andrš, J. W. Peterson, R. C. Martineau, 2017, "A fully coupled two-level Schwarz preconditioner based on smoothed aggregation for the transient multigroup neutron diffusion equations", <i>Numerical Linear Algebra with Applications</i> , 2017 (Revision).	N/A	17P11-022FP	ANE	None
Kong, F., M. DeHart, Y. Wang, D. Andrš, J. Ortensi, C. J. Permann, J. W. Peterson, B. Alger, J. Miller, A. Slaughter, D. Gaston, R. Carlsen, and R. C. Martineau, 2017, "A parallel implementation of eigenvalue solvers for nonlinear-in-eigenvector equations in MOOSE and SLEPc", <i>ACM Transactions on Mathematical Software</i> , 2017 (In preparation).	N/A	17P11-022FP	ANE	None

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Journal Citation	Impact Factor	LDRD No.	Initiative	Collaborator Affiliation State/Country
Kundu, A., S. Instasi, I. Charit, B. Jaques, and C. Jiang, "A preliminary study on high energy ball milling of Fe-9Cr alloy", Submitted to Materials Letters.	N/A	16-187	CED	None
Le Blanc, K.L. Z. Spielman, R. Hill, R. Snuggerud, B. Pearse, J. McLerran, J., and R. Flamand, 2017, "A Human Automation Interaction Concept for a Small Modular Reactor Control Room", INL/CON-17-41509 in proceeding of <i>10th International Topical Meeting on Nuclear Plant Instrumentation, Control and Human Machine Interface Technologies</i> , San Francisco, CA, 2017.	N/A	16-096	ANE	Brigham Young University-Idaho Michigan Technological University
Lew, R., R. Boring, and T. A. Ulrich, 2017, "Ensuring operator reliability in digital control rooms", Proceedings of the 2017 American Nuclear Society Nuclear Power Instrumentation & Controls and Human-Machine Interface Technology (NPIC HMIT) Conference, pp 8-18.	N/A	17-A1-201FP	ANE	Boise State University Norwegian University of Science and Technology University of Idaho Ohio State University
Lew, R., T. A. Ulrich, R. Boring, and S. Werner, 2017 (in press), "Applications of the Rancor microworld nuclear power plant simulator", <i>IEEE Proceedings of Resilience Week 2017</i> , pp. 143-149.	N/A	17-A1-201FP	ANE	Boise State University Norwegian University of Science and Technology University of Idaho Ohio State University
Li, H., X. Diao, X. Li, B. Li, and C. Smidts, 2017, "Fault Propagation and Effects Analysis for Designing an Online Monitoring System for the Secondary Loop of a Nuclear Power Plant Part of a Hybrid Energy System," <i>selected for possible inclusion into a special issue of Nuclear Technology</i> , 2017.	N/A	15-039	CED	North Carolina State University Ohio State University Oregon State University Massachusetts Institute of Technology University of New Mexico
Liu, R., M. Mohanpurkar, M. Panwar, R. Hovsopian, A. Srivastava, and S. Suryanarayanan, 2017, "Geographically distributed real-time digital simulations using linear prediction," <i>International Journal of Electrical Power &amp; Energy Systems</i> , Volume 84, January 2017, Pages 308-317, ISSN 0142-0615	3.289	15-135	CED	Washington State University, Washington Colorado State University, Colorado

Journal Citation	Impact Factor	LDRD No.	Initiative	Collaborator Affiliation State/Country
Lu, W., T. He, B. Xu, X. He, H. Adidharma, M. Radosz and M. Fan, 2017, "Progress in Catalytic Synthesis of Advanced Carbon Nanofibers". <i>Journal of Materials Chemistry A</i> , 5 (2017) 13863-13881	8.867	16-176	CED	University of Wyoming, Wyoming Georgia Institute of Technology, Georgia
Luo, Y., M. Panwar, M. Mohanpurkar, and R. Hovsopian, 2016, "Real Time Optimal Control of Supercapacitor Operation for Frequency Response," <i>2016 IEEE Power and Energy Society General Meeting (PESGM)</i> , Boston, Massachusetts, pp. 1-5, 2016.	N/A	15-135	CED	Colorado State University, Colorado
Luo, Y., S. Srivastava, M. Mohanpurkar, S. Stevic, and R. Hovsopian, "Real Time Impact control in Pulsed Power load For Shipboard Power Systems," <i>IET Power Electronics</i> , pp. 1-12, under review.	N/A	15-135	CED	None
Lwin, S., W. Diao, C. Baroi, A. M. Gaffney, and R. R. Fushimi, 2017, "Characterization of MoVTenNbOx Catalysts during Oxidation Reactions Using In Situ/Operando Techniques: A Review". <i>Catalysts</i> 7, 109, 2017.	3.082	15-146 16P6-002FP	ANE CIP	No external collobartors
Md Hossain, R., Md. K. Hossain, Md. A.Hasan, L. Yusheng, and R. Hovsopian, 2017, "Synchronous Generator Stabilization by Thyristor Controlled Supercapacitor Energy Storage System," <i>SoutheastCon</i> , 2017, Charlotte NC, pp. 1-6.	N/A	15-135	CED	University of South Carolina, South Carolina University of Mephis, Tennessee
Misenheimer, C. and S. D. Terry, 2017, "Modeling Hybrid Nuclear Systems with Chilled-Water Storage," <i>ASME Journal of Energy Resources and Technology</i> , Vol. 139, No. 1, pp. 012002-1 - 012002-9, January 2017.	1.647	15-039	CED	North Carolina State University, North Carolina
Mohanpurkar, M., M. Panwar, S. Chanda, M. Stevic, R. Hovsopian, V. Gevorgian, S. Suryanarayanan, and A. Monti, "Distributed real-time simulations for electric power engineering," <i>Cyber-physical social systems and constructs in electric power engineering</i> , Pages 451-486, <i>The Institution of Engineering and Technology (IET)</i> , London, UK (October 2016)	N/A	15-135	CED	None



## 2017 Project Summaries — Appendices

Journal Citation	Impact Factor	LDRD No.	Initiative	Collaborator Affiliation State/Country
Morgan, K., M. Maguire, R. Fushimi, J. Gleaves, A. Goguet, M. Harold, E. Kondratenko, U. Menon, Y. Schuurman, and G. Yablonsky, 2017, "Forty Years of Temporal Analysis of Products". <i>Catalysis Science &amp; Technology</i> , 7 2416-2439, 2017.	5.773	15-146	CED	Queens University Belfast, School of Chemistry and Technology, Belfast, Ireland Washington Univesity, Washington University of Houston, Texas Univeristy of Rostock, Rostock, Germany University of Claude Bernard Lyon 1, Villeurbanne, France St Louis University, Missouri
Morrell, J.T., 2017, "Experimental evaluation of polychromatic neutron diffraction", Senior Thesis, Department of Nuclear Science and Engineering, Massachusetts Institute of Technology (2017).	N/A	16-036	ANE	Massachusetts Institute of Technology
Morris, J., J. Hendrie, S. Pelka, S. Teysseyre, J.-C. Diels, and A.A. Hecht "High precision measurements of refractive index change in CaF <sub>2</sub> crystals as a function of reactor dose."	N/A	15-142	ANE	None
Morris, J., J. Hendrie, S. Pelka, S. Teysseyre, J.-C. Diels, and A.A. Hecht, "Fabry Perot crystal rotation effects on nested cavity modes within a mode locked laser cavity."	N/A	15-142	ANE	None
Morris, J., J. Hendrie, S. Teysseyre, J.-C. Diels, and A.A. Hecht, "LAMMPS simulations and displacement energies on the CaF <sub>2</sub> crystal lattice."	N/A	15-142	ANE	None
Morris, J.P., 2017, <i>High Precision Refractive Index Measurement Techniques Applied to the Analysis of Neutron Damage and Effects in CaF<sub>2</sub> Crystals</i> , PhD Dissertation, Nuclear Engineering, University of New Mexico, 2017.	N/A	15-142	ANE	None

Journal Citation	Impact Factor	LDRD No.	Initiative	Collaborator Affiliation State/Country
Osorio, J., R. Hovsopian, and J. Ordonez, 2016, "Dynamic Analysis of Concentrated Solar Supercritical CO <sub>2</sub> -based Power Generation Closed-Loop Cycle," <i>Applied Thermal Engineering</i> , 93.C (2016): n. pag. Web. doi:10.1016/j.applthermaleng.2015.10.039.	3.444	15-135	CED	Florida State University, Florida
Panwar, M., S. Suryanarayanan, and R. Hovsopian, 2017, "A multi-criteria decision analysis-based approach for dispatch of electric microgrids," <i>International Journal of Electrical Power &amp; Energy Systems</i> 88, Pages 99-107, 2017.	3.289	15-135	CED	Colorado State University, Colorado
Pathak, M, H. Kweon, M. Deo and H. Huang, 2017, "Kergoen Swelling and Confinement: Its implication on Fluid Thermodynamic properties in Shales", <i>Nature: Scientific Reports</i> , 2017	4.259	15-128	CED	University of Utah, Department of Chemical Engineering, Utah
Pawar, G., P. Meakin, and H. Huang, 2017, "Reactive Molecular Dynamics Simulation of Kerogen Thermal Maturation and Crosslinking Pathways", <i>Energy and Fuels</i> , 2017, 31(11). Manuscripts in preparation and ready for submission during FY-17		15-128	CED	University of Utah Pioneer Natural Resources
Pawar, G., P. Meakin, and H. Huang, 2017, "Evaluation of the Adequacy of the General-Purpose DREIDING Force Field for Simulation of Kerogens", <i>Energy and Fuels</i> , 2017 (ready to submit)		15-128	CED	University of Utah Pioneer Natural Resources
Pawar, G., P. Meakin, and H. Huang, 2017, "Solvent induced swelling of kerogens: A molecular dynamics and thermodynamic integration approach", <i>Nature: Scientific reports</i> , 2017 (in preparation)		15-128	CED	University of Utah Pioneer Natural Resources
Zepper, E.T., M. L. Pantoya, S. Bhattacharya, et al. "Peering through the flames: imaging techniques for reacting aluminum powders", <i>Applied Optics</i> , Vol 56, No.9, 2017, pg 2535-2541	1.65	16-081	CIP	Texas Tech University, Texas
Pelka, S., J. Morris, S. Teyseyre, J.-C. Diels, and A.A. Hecht, "Color center formation vs. dose in CaF <sub>2</sub> crystals from reactor irradiation."	N/A	15-142	ANE	None

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Journal Citation	Impact Factor	LDRD No.	Initiative	Collaborator Affiliation State/Country
Pelka, S., 2017, <i>Examination of Color Center Formation in CaF<sub>2</sub> Crystals when Exposed to Gamma and Mixed Neutron/Gamma Fields</i> , Thesis, Nuclear Engineering, University of New Mexico, Sara Pelka, 2017.	N/A	15-142	ANE	None
Rasmussen, M. and R. Boring, (In review). "Auto-calculation of complexity in computation-based human reliability analysis," <i>EURO Journal on Decision Processes</i> .	N/A	15-013	ANE	University of Idaho Norwegian University of Science and Technology
Rasmussen, M., R. Boring, T. Ulrich, and S. Ewing, (2017). "The virtual human reliability analysis," In R. Boring (ed.), <i>Advances in Human Error, Reliability, Resilience, and Performance (Advances in Intelligent Systems and Computing)</i> , pp. 250–260. Heidelberg: Springer Verlag.	N/A	15-013	ANE	University of Idaho Norwegian University of Science and Technology
Savchenko, K., H. Medema, R. Boring, and T. Ulrich, 2017, "Comparison of mutual awareness in analog vs. digital control rooms", In R. Boring (ed.), <i>Advances in Human Error, Reliability, Resilience, and Performance (Advances in Intelligent Systems and Computing)</i> . Heidelberg: Springer Verlag, pp. 192-199.	N/A	17A1-201FP	ANE	Boise State University Norwegian University of Science and Technology University of Idaho Ohio State University
Schunert, S., D. Schwen, P. Ghassemi, et al., 2017, "Heat Source Characterization In A TREAT Fuel Particle Using Coupled Neutronics Binary Collision Monte-Carlo Calculation," <i>M&amp;C 2017 - International Conference on Mathematics &amp; Computational Methods Applied to Nuclear Science &amp; Engineering</i> , Jeju, Korea, April 16-20, 2017 (published – conference proceedings).	N/A	16-010	ANE	North Carolina State University Pennsylvania State University
Schwen, D., L. Aagesen, J. Peterson, and M. Tonks, 2017, "Rapid multiphase-field model development using a modular free energy based approach with automatic differentiation in MOOSE/MARMOT," INL/JOU-17-41181, <i>Computational Materials Science</i> , vol. 132, pg. 36-45, May 2017.	2.292	16-055	ANE	Pennsylvania State University, Pennsylvania

Journal Citation	Impact Factor	LDRD No.	Initiative	Collaborator Affiliation State/Country
Schwen, D. and S. Schunert, "Coupling binary collision Monte Carlo to finite element based microstructure evolution," <i>Computational Materials Science</i> , in preparation	N/A	16-010	ANE	North Carolina State University and Pennsylvania State University
Shi, S., X. Zhang, X. Sun, and H. Zhang, 2017, "Development of Five-equation Drift Flux Model for Thermal Non-equilibrium Phenomena in LWRs," <i>Proceedings of the 25th International Conference on Nuclear Engineering (ICONE-25)</i> , Shanghai, China, July 2017.	N/A	15-141	ANE	None
Shrestha, K., and K. Gofryk, "A new experimental setup for the thermal conductivity measurements of actinide materials based on $3\omega$ approach," under review with <i>Review of Scientific Instruments</i> .	N/A	15-032	ANE	University of Florida
Smith, J. A., S.L. Garrett, M.D. Heibel, V. Agarwal, and B.J. Heidrich, 2016, "Progress In Developing an In-Pile Acoustically Telemetered Sensor Infrastructure," <i>American Nuclear Society TOPFUEL</i> , Boise, Idaho, September 11–16, 2016.	N/A	15-040	ANE	None
Smith, J. A., S.L. Garrett, M.D. Heibel, and V. Agarwal, 2016, "Wireless In-Core Acoustic Telemetry and Self-Powered Sensing," <i>Nuclear Energy Enabling Technologies Crosscutting Technology Development Advanced Sensors and Instrumentation Newsletter</i> , Issue 3, February 2016.	N/A	15-040	ANE	None
St. Germain, S., R. Boring, G. Banaseanu, Y. Akl, and H. Chatri, 2017 (in press), "Multi-unit considerations for human reliability analysis", <i>Proceedings of the PSAM Topical Conference on Human Reliability, Quantitative Human Factors, and Risk Management</i> .	N/A	17A1-201FP	ANE	Boise State University Norwegian University of Science and Technology University of Idaho Ohio State University
Stevic, M., M. Panwar, M. Mohanpurkar, R. Hovsopian, and A. Monti, 2017, "Empirical Study of Simulation Fidelity in Geographically Distributed Real-Time Simulations," <i>North American Power Symposium 2017</i> , pp. 1-6, under print.	N/A	15-135	CED	Rhein Westfal TH Aachen, Institute for Automation of Complex Power Systems, Aachen, Germany

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Journal Citation	Impact Factor	LDRD No.	Initiative	Collaborator Affiliation State/Country
Stevic, S., V. Tuyen, M. Mohanpurkar, C. Edrington, and R. Hovsapien, "Real-time Co-simulation of Advanced Power Electronics Inverters for Studying Grid Integration of Renewable Energy Systems," <i>Applied Power Electronics Conference (APEC) 2018</i> , pp. 1-5, under review.	N/A	15-135	CED	None
Sun, C., F. A. Garner, L. Shao, X. Zhang, and S. A. Maloy, 2017, "Influence of injected interstitials on the void swelling in two structural variants of 304L stainless steel induced by self-ion irradiation at 500C", <i>Nuclear Instrumental Methods Physics Research B</i> , submitted 2017.	N/A	17P10-003FP	ANE	None
Sun, C., J. Li, and E. Fu, 2017, "Chapter 5 Radiation damage in nanoporous metals, Radiation damage of nanostructured materials", <i>Progress in Materials Science</i> , submitted 2017.	N/A	17P10-003FP	ANE	None
Sun, C., L. Malerba, M. J. Konstantinovic, F. A. Garner, and S. A. Maloy, 2017, "Microstructural characterization of high-dose ion-irradiated duplex Fe-9Cr-C model alloy", <i>18th International Conference on Environmental Degradation of Materials in Nuclear Power Systems – Water Reactors</i> , accepted 2017.	N/A	17P10-003FP	ANE	None
Tan, S., L. Wang, S. Saha, R. R. Fushimi, and D. Li, 2017, "Active Site and Electronic Structure Elucidation of Pt Nanoparticles Supported on Phase-Pure Molybdenum Carbide Nanotubes". <i>ACS Applied Materials &amp; Interfaces</i> 9, 9815-9822, 217.	7.504	15-146	CED	Center for Advanced Energy Studies, Idaho University of Wyoming, Wyoming

Journal Citation	Impact Factor	LDRD No.	Initiative	Collaborator Affiliation State/Country
Tang, Q., Z. Shen, L. Huang, T. He, H. Adidharma, A.G. Russell and M. Fan, 2017, "Synthesis of methanol by CO <sub>2</sub> hydrogenation promoted by dissociative adsorption of hydrogen on Ga <sub>3</sub> Ni <sub>5</sub> (221) surface", <i>Physical Chemistry Chemical. Physics</i> 19, (2017) 18539-18555	4.123	16-215	CED	Shanghai Jio Tong University, School of Environmental Science and Engineering, Shanghai, China University of Wyoming, Wyoming Wuhan Univeristy of Science and Technology, State Key Lab Refractories & Metallurgy, Wuhan, China Georgia Institute of Technology, Georgia
Tang, T. He, H. Adidharma, G. Tan and M. Fan. "Coal-derived carbon materials: a modern approach to unlock nature's complexity and nurture the gift from the past". <i>Progress in Materials Science</i> , submitted.	N/A	16-176	CED	None
Ulrich, T., R. Boring, S. Ewing, and M. Rasmussen, (2017). "Operator timing of task level primitives for use in computation-based human reliability analysis," In R. Boring (ed.), <i>Advances in Human Error, Reliability, Resilience, and Performance (Advances in Intelligent Systems and Computing)</i> . Heidelberg: Springer Verlag, pp. 41-49.	N/A	15-013	ANE	University of Idaho Norwegian University of Science and Technology
Veeraraghavan, S., Spears, B., Coleman, J. (2017), "High Frequency Content in Nonlinear Soil Response - A Numerical Artifact or a Reality?," <i>Soil Dynamics and Earthquake Engineering</i> , Manuscript Submitted June 2017.	N/A	15-023	ANE	University of Illinois Urbana-Champaign Purdue University Carnegie-Mellon University
Veeraraghavan, S., Bielak, J., Coleman, J. (2017), "Effect of Inclined Waves on Deeply Embedded Nuclear Facilities," <i>Structural Mechanics in Reactor Technology (SMiRT) Conference</i> , Busan, South Korea, August 2017.	N/A	15-023	ANE	University of Illinois Urbana-Champaign Purdue University Carnegie-Mellon University

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Journal Citation	Impact Factor	LDRD No.	Initiative	Collaborator Affiliation State/Country
Ward, J.W., M.S. Snow, J.E. Olson, D. Ball, D, M.L. Adamic, 2017, "Carbon-14 Content in Tree and Soil Samples at the Idaho National Laboratory Nuclear Site", <i>Nuclear Instruments and Methods in Physics Research</i> , B. 2017 (in submission)	N/A	16-098	CIP	None
Williams, C.L., C. Li, et.al. "Three Way Comparison of Hydrophilic Ionic Liquid, Hydrophobic Ionic Liquid, and Dilute Acid for the Pretreatment of Herbaceous and Woody Biomass", <i>Bioresource Technology</i> , submitted.	N/A	16-002	CED	University of Wyoming University of Idaho University of Utah
Wilson, A.D., J.R. Klaehn, C. M. Hrbac, C.J. Orme, and D. L. Daubaras , 2017, "The role of water activity (aw) in water transport through membranes," <i>Journal of Membrane Science</i> on Apr 11, 2017. INL/CON-17-41157	N/A	17A1-007FP	ANE	Benedictine College
Wu, W., D. Ding and T. He, <i>ECS Transactions</i> , 80 (2017) 167-173.	N/A	16-215	CED	None
Wu, W., Y. Zhang, D. Ding, and T. He, 2017, "A High-Performing Direct Carbon Fuel Cell with 3D Architected Anode Operated Below 600 °C", <i>Advance Materials</i> , DOI: 10.1002/adma.201704745.	19.791	16-176	CED	No external collaborators
Wu, W., D. Ding, M. Fan and T. He, 2016, "A high performance low-temperature direct carbon fuel cell", <i>ECS Transactions</i> 78 (2017) 2519-2526.	N/A	16-176	CED	None
Xia, Y., J. Goral, H. Huang, I. Miskovic, P. Meakin, and M. Deo, 2017 "Many-body dissipative particle dynamics modeling of fluid flow in fine-grained nanoporous shales". <i>Physics of Fluids</i> , 2017, 29(5).	2.232	15-128	CED	University of Utah, Utah Temple University in Philadelphia, Pennsylvania
Xiong, H., E.J. Dufek, K.L. Gering, 2017, "Batteries-Materials for Rechargeable Lithium-ion Batteries", accepted book chapter, part of <i>Comprehensive Energy Systems</i> . - Listed in <i>STIMS</i> under Title "Batteries"	N/A	15-125	CED	University of Connecticut
Xu, B., W. Lua, Z. Sun, T. He, A. Goroncy, Y. Zhang and M. Fan, 2017, "High-quality fuels/chemicals from catalytic pyrolysis of Powder River Basin coal". <i>Fuel Processing Technology</i> , 167 (2017) 334-344.	N/A	16-176	CED	None



Journal Citation	Impact Factor	LDRD No.	Initiative	Collaborator Affiliation State/Country
Xu, X., Y. Chen, P. Wan, K. Gasem, K. Wang, T. He, H. Adidharma and M. Fan, 2016, "Extraction of lithium with functionalized lithium ion-sieves". <i>Progress in Materials Science</i> 84, 276 (2016).	31.14	16-215	CED	Beijing University of Chemical Technology, Beijing, China University of Wyoming, Wyoming Georgia Institute of Technology, Georgia
Xue, S., 2017, "Modeling and experiment of fission products release and interaction with coolant for defective fuel in Light Water Reactor (LWR)", M.S. thesis, The Ohio State University, 2017.	N/A	15-141	ANE	None
Yadav, V., V. Agarwal, A. V. Gribok, and C. L. Smith, 2017, "Dynamic PRA with Component Aging and Degradation Modeled Utilizing Plant Risk Monitoring Data," <i>International Topical Meeting on Probabilistic Safety Assessment and Analysis</i> , Pittsburg, Pennsylvania, September 24-28, 2017.	N/A	16-040	ANE	None
Yadav, V., V. Agarwal A. V. Gribok and C. L. Smith, 2017, "Assessment of Dynamic PRA Techniques with Industry-Average Component Performance Data," <i>10<sup>th</sup> ANS International Topical Meeting on Nuclear Plant Instrumentation, Control and Human Machine Interface Technologies</i> , San Francisco, California, June 11-15, 2017.	N/A	16-040	ANE	None
Zabriskie, A., S. Schunert, D. Schwen, and R. Martineau, "Coupled multiscale neutronics binary collision Monte Carlo model of an LEU TREAT core," <i>Annals of Nuclear Energy, in preparation</i>	N/A	16-010	ANE	North Carolina State University and Pennsylvania State University
Zhou, J., H. Huang, J. McLennan, P. Meakin, and M. Deo, 2017, "A Dual-Lattice Discrete Element Model to Understand Hydraulic Fracturing in Naturally Fractured System". <i>Hydraulic Fracturing Journal</i> , 2017, 4(2).	N/A	15-128	CED	University of Utah Pioneer Natural Resources

CED = clean energy development

CIP = critical infrastructure

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### FY 2016

Journal Citation	Impact Factor	LDRD No.	Initiative	Collaborator Affiliation State/Country
Agarwal, V., P. Chatterjee, A. V. Gribok, and C. L. Smith, 2016, "Online Risk Monitoring of Nuclear Power Plants: System and its Components Ordering Based on Cost Importance," in Proceedings of the 13 <sup>th</sup> International Conference on Probabilistic Safety Assessment and Management, Seoul, S. Korea, October 2–7, 2016.	N/A	16-040	ANE	None
Aitkaliyeva A. and C. Papesch, 2016, "Identification of subsurface phases in ternary U-Pu-Zr fuel", <i>Journal of Nuclear Materials</i> , Vol. 473, p. 75, 2016.	N/A	16-046	ANE	None
Aitkaliyeva, A., C. A. Papesch, and S. Middlemas, 2016, "Evaluation of Microstructure and Thermal Properties of U-24Pu-15Zr Alloy", submitted to <i>Journal of Nuclear Materials</i> , November 2016, currently under revision.	N/A	16-046	ANE	None
Arthur, E., E. Blandford, J. Disser, et al., 2016, "Demonstration of the 3SBD Concept for the Pebble Bed Fluoride Salt-Cooled High Temperature Reactor (PB-FHR)," INMM Annual Meeting Proceedings, July 2016.	N/A	15-094	ANE	University of South Florida
Bao, H., N. Dinh, H. Zhao, H. Zhang, L. Zou, and R. Szilard, 2016, "A Study of BWR Mark I Station Blackout Accident: GOTHIC Modeling and Sensitivity Analysis," <i>International Congress of Advanced Nuclear Power Plants</i> , San Francisco, California, April 2016.	N/A	16-026	ANE	North Carolina State University
Botros N. Hanna, e. a., 2016, "High-fidelity simulation-driven model development for coarse-grained computational fluid dynamics". <i>International Topical Meeting on Advances in Thermal Hydraulic</i> , New Orleans, LA.	N/A	16-026	ANE	North Carolina State University

Journal Citation	Impact Factor	LDRD No.	Initiative	Collaborator Affiliation State/Country
Brown, N.R., A. J. Wysocki, K. A. Terrani, A. Ali, M. Liu, E. Blandford, 2016, "Survey of Thermal-Fluids Evaluation and Confirmatory Experimental Validation Requirements of Accident Tolerant Cladding Concepts with Focus on Boiling Heat Transfer Characteristics", June 2016.	N/A	15-060	ANE	North Carolina State University Oregon State University University of New Mexico Massachusetts Institute of Technology
Chanda, S., M. Mohanpurkar, R. Hovsopian, and A. Srivastava, 2016, "Quantifying Power Distribution System Resiliency Using Code Based Metric," <i>IEEE International Conference on Power Electronics, Drives and Energy Systems (PEDES)</i> , pp. 6, December 14-17, 2016.	N/A	15-135	CED	Washington State University, Washington
Disser, J., E. Arthur, and J. Lambert, 2016, "Preliminary Safeguards Assessment for the Pebble Bed Fluoride Salt-Cooled High Temperature Reactor (PB-FHR) Concept," <i>Advances in Nuclear Nonproliferation Technology &amp; Policy Conference Proceedings</i> , American Nuclear Society, September 2016.	N/A	15-094	CIP	University of South Florida
Hanna, B., N. Dinh, and I. Bolotnov, 2016, "A Framework for Data-Driven Model Development for Coarse-Grained Computational Fluid Dynamics," <i>International Topical Meeting on Advances in Thermal Hydraulics 2016 (ATH 16)</i> , New Orleans, Louisiana, June 12 through 16, 2016.	N/A	16-026	ANE	North Carolina State University
Heidrich, J. A., V. Agarwal, V., M. D. Heibel, S. L. Garrett, "Using the Sounds of Nuclear Power," <i>171st Meeting of the Acoustical Society of America</i> , Salt Lake UT, May 23-27, 2016. (Presented in a <b>Special Invited Session</b> on Thermal Acoustics sponsored by three ASA Technical Committees: Structural Acoustics, Vibration and Engineering Acoustics, & Physical Acoustics).	N/A	15-040	ANE	None
Le Blanc, K. and S. Freeman, 2016, "Investigating the Relationship between Need for Cognition and Skill in Ethical Hackers," publication in <i>Advances in Intelligence Systems and Computing, proceedings of the 7th International Conference on Applied Human Factors and Ergonomics</i> , Orlando, Florida, July 2016.	N/A	15-111	CIP	None

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Journal Citation	Impact Factor	LDRD No.	Initiative	Collaborator Affiliation State/Country
Lin, L., N. Dinh, R. Sampath, and N. Akinici, 2016, "A Computational Study of Thin Film Dynamics on Micro-Structured Surfaces," <i>Proceedings of the ASME 2016 Summer Heat Transfer Conference</i> , HT2016- 7382, Washington D.C., July 10 through 14, 2016.	N/A	16-026	ANE	North Carolina State University, North Carolina
Lin, L., 2016, "Assessment of the Smoothed Particle Hydrodynamics Method for Nuclear Thermal-Hydraulic Applications," Master of Science Thesis in Nuclear Engineering, North Carolina State University, 75 p, April 2016.		16-026	ANE	North Carolina State University
Madix, R., L. Wang, M. Personick, S. Karakalos, R. Fushimi, and C. Friend, 2016, "Active sites for methanol partial oxidation on nanoporous gold catalysts", <i>Journal of Catalysis</i> , 344 778-783, 2016.	N/A	15-146	CED	Cardiff University, United Kingdom University of Wyoming University of California, Berkley
Manic, M., K. Amarasinghe, J. J. Rodriguez-Andina and C. Rieger, 2016, "Intelligent Buildings of the Future: Cyberaware, Deep Learning Powered, and Human Interacting," in <i>IEEE Industrial Electronics Magazine</i> , vol. 10, no. 4, pp. 32-49, Dec. 2016.	10.1	17A1-114FP	CIP	Virginia Commonwealth University, Virginia University of Vigo, Vigo, Spain

ANE = advancing nuclear energy

CED = clean energy development

CIP = critical infrastructure

## **Appendix C**

### **List of Collaborators**



## Appendix C

### List of Collaborators

*University Collaborations (bold shows collaboration of FY-17 new starts)*

University	Projects
Boise State University	15-100: Real time Process Simulator (RTPS) 15-128: Microstructural evolution and mesoscale coupled flow-reaction-fracturing processes in organic rich nanoporous shales 16-187: Micro-Scale Technique to Evaluate Grain Boundary Cohesion of Irradiated Alloys 17A1-201FP: Human Reliability Analysis for Advanced Reactor Technologies and Systems 17P11-018FP: Advanced Manufacturing of Uranium Dioxide Fuel Pellets with radially and axially zoned burnable poisons and hour-glassing control features 17P11-030FP: Investigation of Exciton Delocalization and Exciton Coherence in Chromophores and Acoustic Nanostructures
Brigham Young University	15-032: Development of new method for high temperature thermal conductivity measurements of nuclear materials 15-111: Adversary Signature Development and Threat Analysis 16-013: Micromechanistic approach and critical experiments for quantitative predictions of delayed hydride cracking in zirconium alloys 16-096: Supporting operator performance and situation awareness in highly automated nuclear power plants
California State University Long Beach	16-106: Risk Analysis Method Integrating Physical, Cyber and Infrastructure Dependencies 17A1-086FP: Development of a complete kinetic model for free-radical-induced degradation of formic and oxalic acids.
Cardiff University	15-146: Tailoring the Kinetic Function of a Surface through Electronic Effects of Nanoscale Architecture
Carnegie Mellon	15-111: Adversary Signature Development and Threat Analysis
Colorado State University	15-135: Dynamic Simulations for Large Scale Electric Power Networks in Real Time Environment using Multiple Real Time Digital Simulator



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University	Projects
Florida State University	15-135: Dynamic Simulations for Large Scale Electric Power Networks in Real Time Environment using Multiple Real Time Digital Simulator
Harvard University	15-146: Tailoring the Kinetic Function of a Surface through Electronic Effects of Nanoscale Architecture
Idaho State University	15-100: Real time Process Simulator (RTPS) 15-145: Advanced Neutron and X-Ray Imaging at Transient Test Reactor 16-070: Characterization of Neutron Beamlines at Neutron Radiography reactor
Kyoto University	16-085: Production of Fluoroanion Targets for Accelerator Mass Spectrometry
Massachusetts Institute of Technology	15-039: Transient Modeling of Integrated Nuclear Energy Systems with Thermal Energy Storage and Component Aging and Preliminary Model Validation via Experiment 15-060: Development of State-of-the-Art Capabilities to Support Transient Test Reactor Modeling and Simulation 16-036: Neutron microscope to enable high-resolution neutron tomography at Idaho National Laboratory 16-058: Predicting Radiation-Induced Microstructural Change via Implementation and Validation of Multiscale Cluster Dynamics in Multiphysics Object Oriented Simulation Environment 17A1-105FP: Safety Margin Evaluation for Experiment Irradiation in Advanced Test Reactor
Missouri University of Science and Technology	17A1-150FP: Advanced manufacturing of metallic fuels and cladding by equal-channel angular pressing
Montana State University	15-125: Phosphoranimines for advanced battery applications
Montana Technical University	16-003: Recycling of Tantalum-containing Waste Materials to Recover Tantalum Metal
North Carolina State University	15-039: Transient Modeling of Integrated Nuclear Energy Systems with Thermal Energy Storage and Component Aging and Preliminary Model Validation via Experiment 15-040: Acoustic telemetry infrastructure for in-pile Advanced Test Reactor and Transient Test Reactor monitoring 15-060: Development of State-of-the-Art Capabilities to Support Transient Test Reactor Modeling and Simulation 16-010: Development of a fully coupled radiation damage production and evolution simulation capability 16-026: Computationally Efficient Prediction of Containment Thermal Hydraulics Using Multi-Scale Simulation

University	Projects
	16-040: Integration of Prognostic Techniques and Probabilistic Safety Assessment for Online Risk Monitoring
Ohio State University	15-039: Transient Modeling of Integrated Nuclear Energy Systems with Thermal Energy Storage and Component Aging and Preliminary Model Validation via Experiment 15-060: Development of State-of-the-Art Capabilities to Support Transient Test Reactor Modeling and Simulation 15-141: Interfacing Multiphysics Object Oriented Simulation Environment Components to Enhance Capability 16-106: Risk Analysis Method Integrating Physical, Cyber and Infrastructure Dependencies 17P11-001FP: Enabling Material Discovery for Waste Heat Recovery Systems using a Multimode Optical Sensor
Oregon State University	15-039: Transient Modeling of Integrated Nuclear Energy Systems with Thermal Energy Storage and Component Aging and Preliminary Model Validation via Experiment 15-060: Development of State-of-the-Art Capabilities to Support Transient Test Reactor Modeling and Simulation 15-141: Interfacing Multiphysics Object Oriented Simulation Environment Components to Enhance Capability 16-050: Stress Corrosion Cracking Testing in Supercritical Carbon Dioxide
Paul Scherrer Institute	17-A1-093FP: Digital Neutron Imaging of Irradiated Fuel Using a Gamma-Discriminating Scintillation System
Pennsylvania State University	15-040: Acoustic telemetry infrastructure for in-pile Advanced Test Reactor and Transient Test Reactor monitoring 16-010: Development of a fully coupled radiation damage production and evolution simulation capability 16-046: Development of a Synergistic Approach To Study Irradiated Materials Using Coupled Experiments and Simulation 17P11-014FP: The influence of irradiation on the corrosion kinetics and hydrogen pickup of zirconium alloys
Politecnico di Milano	15-023: Development of Stochastic 3-Dimensional Soil Response Capability in MOOSE to Provide Design and Beyond Design Basis Seismic Motions for Nuclear Facilities
RWTH Aachen University, Germany	15-135: Dynamic Simulations for Large Scale Electric Power Networks in Real Time Environment using Multiple Real Time Digital Simulator
Saint Louis University	15-146: Tailoring the Kinetic Function of a Surface through Electronic Effects of Nanoscale Architecture
Texas Technical University	16-081: Modeling Thermite Reactions

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University	Projects
The Ohio State University	15-039: Transient Modeling of Integrated Nuclear Energy Systems with Thermal Energy Storage and Component Aging and Preliminary Model Validation via Experiment 15-141: Interfacing Multiphysics Object Oriented Simulation Environment Components to Enhance Capability 16-129: Application of Radioactive Isotope Dilution Technique to Measurement of Molten Salt Mass for Electrochemical Recycling Process
University of California, Berkley	15-146: Tailoring the Kinetic Function of a Surface through Electronic Effects of Nanoscale Architecture 16-071: Evaluation of Advanced Digital Neutron Imaging Systems for Post Irradiation Examination of Nuclear Fuel 17P11-018FP: Advanced Manufacturing of Uranium Dioxide Fuel Pellets with radially and axially zoned burnable poisons and hour-glassing control features
Ulsan National Institute of Sci. & Tech, Korea	15-144: Investigation of Sonication Assisted Electrolytic Reduction of Used Oxide Fuel in Molten Salt
University of New Mexico	15-094: Evaluation and Demonstration of the Integration of Safeguards, Safety, and Security by Design (3SBD)
University of Florida	16-046: Development of a Synergistic Approach To Study Irradiated Materials Using Coupled Experiments and Simulation 17P11-018FP: Advanced Manufacturing of Uranium Dioxide Fuel Pellets with radially and axially zoned burnable poisons and hour-glassing control features
University of Gent	15-146: Tailoring the Kinetic Function of a Surface through Electronic Effects of Nanoscale Architecture
University of Idaho	15-144: Investigation of Sonication Assisted Electrolytic Reduction of Used Oxide Fuel in Molten Salt 16-002: Advanced Carbon Feedstock Processing Using Ionic Liquids. 16-187: Micro-Scale Technique to Evaluate Grain Boundary Cohesion of Irradiated Alloys 17A1-114FP: Resilient, Scalable Cyber State Awareness of Industrial Control System Networks to Threat
University of Illinois	15-023: Development of Stochastic 3-Dimensional Soil Response Capability in MOOSE to Provide Design and Beyond Design Basis Seismic Motions for Nuclear Facilities 16-106: Risk Analysis Method Integrating Physical, Cyber and Infrastructure Dependencies
University of Iowa	16-040: Integration of Prognostic Techniques and Probabilistic Safety Assessment for Online Risk Monitoring
University of Kansas	17A1-055FP: Electro-reduction of metals in supercritical fluid-room temperature ionic liquids

University	Projects
University of New Mexico	15-039: Transient Modeling of Integrated Nuclear Energy Systems with Thermal Energy Storage and Component Aging and Preliminary Model Validation via Experiment 15-060: Development of State-of-the-Art Capabilities to Support Transient Test Reactor Modeling and Simulation 15-094: Evaluation and Demonstration of the Integration of Safeguards, Safety, and Security by Design (3SBD) 15-142: New in core neutron diagnostics 16-040: Integration of Prognostic Techniques and Probabilistic Safety Assessment for Online Risk Monitoring
University of Oslo, Norway	15-146: Tailoring the Kinetic Function of a Surface through Electronic Effects of Nanoscale Architecture
University of Pittsburgh	15-111: Adversary Signature Development and Threat Analysis
University of South Florida	15-094: Evaluation and Demonstration of the Integration of Safeguards, Safety, and Security by Design (3SBD)
University of Utah	16-152: Wireless radio frequency signal identification and protocol reverse engineering (WiFIRE)
University of Wyoming	15-146: Tailoring the Kinetic Function of a Surface through Electronic Effects of Nanoscale Architecture 16-176: Development of Direct Carbon Fuel Cells 16-187: Micro-Scale Technique to Evaluate Grain Boundary Cohesion of Irradiated Alloys
Virginia Commonwealth University	17A1-114FP: Resilient, Scalable Cyber State Awareness of Industrial Control System Networks to Threat
Virginia Tech	16-010: Development of a fully coupled radiation damage production and evolution simulation capability
Washington State University	15-002: Experimental Scenarios of Adversity and Recovery in Aqueous Separations.
Washington University	15-146: Tailoring the Kinetic Function of a Surface through Electronic Effects of Nanoscale Architecture
Weber State University	16-152: Wireless radio frequency signal identification and protocol reverse engineering (WiFIRE)

### **Industry Collaborations**

Industry	Project
CEA	16-149: In-core Qualification of Developmental Instrumentation
General Electric	17P11-018FP: Advanced Manufacturing of Uranium Dioxide Fuel Pellets with radially and axially zoned burnable poisons and hour-glassing control features
Pioneer Natural Resources	15-128: Microstructural evolution and mesoscale coupled flow-reaction-fracturing processes in organic rich nanoporous shales

### **National Lab Collaborations**

National Laboratory	Projects
FELIX Laboratory	16-085: Production of Fluoroanion Targets for Accelerator Mass Spectrometry
Los Alamos National Laboratory	16-010: Development of a fully coupled radiation damage production and evolution simulation capability

## **Appendix D**

### **List of Interns and Postdocs**





## Appendix D

### List of Interns and Postdocs

#### *2017 LDRD Interns*

##### **Undergraduate:**

<b>Name</b>	<b>University</b>	<b>Project Number</b>
Jordan Argyle	Brigham Young University, Idaho	16-013
Allison Burns	Oregon State University	16-050
Maureen Chorney	Montana Technical University	16-003
Michael Goldstein	University of Pittsburgh	15-111
Jason Green	Texas Technical University	16-081
Rachel Hill	Brigham Young University, Idaho	15-111, 16-096
Bridger Hurley	Montana Technical University	16-003
Patrick Jarrold	Oregon State University	16-050
Ken Lim	University of California - Berkeley	15-146
Alex Lin	Carnegie Mellon	15-111
Jonathan Morrell	Massachusetts Institute of Technology	16-036
Alexander Pharr	North Carolina State University	15-040
Bobak Rashidnia	Ohio State University	15-039, 15-141
Alexander Schoonen	Montana State University	15-125
Marco Teeter	Oregon State University	15-039
Brittany Umbrage	University of New Mexico	16-040
Bjorn Westmen	Oregon State University	15-039
Muzhi Zhu	Ohio State University	15-039
Andrew Kuznicki	Weber State University	16-152

##### **Graduate:**

<b>Name</b>	<b>University</b>	<b>Project Number</b>
Ben Adams	Oregon State University	15-039, 16-050
Rachit Aggarwal	Ohio State University	15-039, 15-141
Anthony Alberti	Ohio State University	15-060
Omar Baltaji	University of Illinois	15-023
Han Bao	North Carolina State University	16-026
Chinmoy Baroi	Idaho National Laboratory	15-146
Aniqua Baset	University of Utah	16-152
Christopher Becker	University of Utah	16-152
John M. Biersdorf	Idaho National Laboratory	16P6-003FP
Ryan Bratton	Texas Technical University	16-081
Andrea Castellano	Politecnico di Milano	15-023
Payel Chattterjee	North Carolina State University	16-040

Cynthia Chavez	University of Pittsburgh	15-111
Denis Constales	University of Gent	15-146
M. Tucker Daniels	North Carolina State University	15-039
Brandon C. Day	Idaho National Laboratory	17A1-055FP
Weijian Diao	Idaho National Laboratory	15-146
Keith Drew	Idaho State University	15-100
Jeremiah Dustin	University of Idaho	15-144
Matt Ellis	Massachusetts Institute of Technology	15-060
Nima Fathi	University of New Mexico	15-039
Marina Ferreira Fonseca Sessim	Pennsylvania State University	16-010
Konor Frick	North Carolina State University	15-039
Sam H. Giegel	Idaho State University	16-070
Pedram Ghassemi	North Carolina State University	16-010
Michael V. Glazoff	Idaho National Laboratory	15-146
John Gleaves	Washington University in Saint Louis - Staff	15-146
Qingti Guo	Ohio State University	15-039
Carl Haugen	Massachusetts Institute of Technology	15-060
Naomi Hazelip	Boise State University	15-100
Christian Hearn	Weber State University	16-152
Cassara J. Higgins	Idaho National Laboratory	17A1-055FP
Kyle Hoover	Oregon State University	15-039
Joshua Hrisko	Pennsylvania State University	15-040
Hongqiang Hu	Idaho National Laboratory	16-002
Andrew J. Hummel	Idaho National Laboratory	16P6-003FP
Miaomiao Jin	Massachusetts Institute of Technology	16-058
John C. Kennedy	Idaho National Laboratory	16P6-003FP
Timothy R. Klett	Idaho National Laboratory	16-106
Karen Kursteiner	California State University Long Beach	16-106
Janine Lambert	University of South Florida	15-094
Jieun Lee	University of Idaho	15-144
Chenlin Li	Idaho National Laboratory	16-002
Dongmei (Katie) Li	University of Wyoming	15-146
Huijuan Li	Ohio State University	15-039, 15-141
Linyu Lin	North Carolina State University	16-026
Cheng Liu	Ohio State University	15-039
Soe Lwin	Idaho National Laboratory	15-146
Brendan Lyle	University of Pittsburgh	15-111
Robert Madix	Harvard University	15-146
Andrew McClusky	University of Pittsburgh	15-111
Joshua S. McNally	Idaho National Laboratory	15-146
Bobbi Merryman	University of New Mexico	15-094
Daniel Mikkelson	North Carolina State University	15-039

Corey Misenheimer	North Carolina State University	15-039
Jason M. Mitchell	Idaho National Laboratory	17A1-055FP
Joe Morris	University of New Mexico	15-142
John Nickels	North Carolina State University	15-039
Ozgun Numanoglu	University of Illinois	15-023
Adefolaoluwami Odeniyi	North Carolina State University	15-039
Seungje Oh	Ulsan National Institute of Sci. & Tech, Korea	15-144
Unni Olsbye	University of Oslo, Norway	15-146
Julian D. Osorio Ramirez	Florida State University	15-135
Nicholas Osterhouse	University of New Mexico	15-094
Mayank Panwar	Idaho National Laboratory	15-135
Gorakh M. Pawar	Idaho National Laboratory	15-146
Sara Pelka	University of New Mexico	15-142
Michael Pietrykowski	Ohio State University	15-039, 15-141
Mitchell A. Plummer	Idaho National Laboratory	15-146
Kevin Pollock	University of Pittsburgh	15-111
Christian Reece	Cardiff University	15-146
Reyixiati Repukaiti	Oregon State University	16-050
Matthew Ryals	University of New Mexico	15-060
Richard S. Skifton	Idaho National Laboratory	16-149
Eric Song	Ulsan National Institute of Sci. & Tech, Korea	15-144
Nina Colby Sorrell	North Carolina State University	15-060
Daniel Stack	Massachusetts Institute of Technology	15-039
Marija Stevic	RWTH Aachen University, Germany	15-135
Shuai Tan	University of Wyoming	15-146
Lucas Teeter	Oregon State University	15-039, 16-050
Abby Waliga	University of Pittsburgh	15-111
Lucun Wang	Idaho National Laboratory	15-146
Haoyang Wei	Idaho National Laboratory	17A1-227FP
David Weitzel	University of New Mexico	15-039
David Willock	Cardiff University	15-146
Jonathan Wormald	North Carolina State University	15-060
Richard N. Wright	Idaho National Laboratory	16P6-003FP
Huarui Wu	Massachusetts Institute of Technology	16-036
Sha Xue	Ohio State University	15-141
Yidong Xia	Idaho National Laboratory	16-055
Gregory Yablonsky	Saint Louis University	15-146
Yangmo Zhu	North Carolina State University	16-026

**2017 LDRD Postdocs**

<b>Name</b>	<b>Affiliation</b>	<b>Project Number</b>
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Muhammad Abir	Idaho National Laboratory	16-036
Birendra Adhikari	Idaho National Laboratory	17A1-166FP
Daniel J. Antonio	Idaho National Laboratory	15-032
Patrick Calderoni	Idaho National Laboratory	16-149
Chinmoy Baroi	Idaho National Laboratory	16P6-002FP
Hailong Chen	Idaho National Laboratory	17A1-227FP
Weijian Diao	Idaho National Laboratory	16P6-002FP
Colt R. Heathman	Washington State University	15-002
Wen Jiang	Idaho National Laboratory	16-187
Daniel LaBrier	University of New Mexico	15-060
Maolong Liu	University of New Mexico	15-060
Yusheng Luo	Florida State University	15-135
Soe Lwin	Idaho National Laboratory	16P6-002FP
Gorakh M. Pawar	Idaho National Laboratory	15-128
Patrick Price	Boise State University	15-128
Durgesh Rai	Massachusetts Institute of Technology	16-036
Evgeniy Redekop	University of Oslo, Norway	15-146
Shanbin Shi	Ohio State University	15-141
Michael Short	Massachusetts Institute of Technology	16-058
Keshav Shrestha	Idaho National Laboratory	15-032
Swetha Veeraraghavan	Idaho National Laboratory	15-023
Gabreil Weaver	University of Illinois	16-106
Wei Wu	Idaho National Laboratory	16-176, 16-215
Vaibhav Yadav	University of Iowa	16-040
Yunya Zhang	Idaho National Laboratory	16-215
Jing Zhou	Idaho National Laboratory	15-128, 16-081

## **Appendix E**

### **Patents**



## Appendix E

### Patents

#### Patents LDRD Program 2016-2017

Project No.	Patent No.	Title	Inventors	Date Granted	CC	Description
99-292	9,428,401	Dry Recycle of Spent Nuclear Fuel – Separation of the Rare-Earth Fission Project Poisons	James W. Sterbentz and Jerry D. Christian	8/30/16	Nuclear and Radio Chemistry	Various methods are available for recycling used nuclear fuel in order to recover more of the energy potential of a given quantity of fuel. Aqueous and electrometallurgical methods are well known, but a dry recycling method exists that does not extract plutonium, use toxic chemicals, or produce large volumes of waste. This patent describes a method for improving dry recycling further by providing a way to separate neutron-absorbing fission product poisons – primarily rare-earths – from the used nuclear fuel. Removal of the rare-earth neutron poisons reduces the amount of enriched uranium oxide feed material needed to re-use the fuel, thus improving the efficiency of this used fuel recycling method.
GB103	9,234,228	Alteration of Enzyme Stability and Activity via Covalent Modification	David N. Thompson, William A. Apel, Vicki S. Thompson, David William Reed, and Jeffrey A. Lacey	1/12/16	Biological and Bioprocess Engineering Chemical and Molecular Science	It is recognized that bacteria glycosylate (attach a carbohydrate) their proteins. Glycosylation of a protein has been shown to assist in the protein's stability and activity, modulate physical properties (such as solubility), and protect against its destruction. The glycosylated enzymes from <i>Alicyclobacillus acidocaldarius</i> have enhanced activities under industrially relevant conditions such as with acid and at very high temperatures. This patent describes some of the genes responsible for glycosylation of enzymes in the thermoacidophilic microorganism <i>Alicyclobacillus acidocaldarius</i> .
10-075	9,369,866	TT: Filter Bank Implementation of Multicarrier Spread Spectrum Systems	Hussein Moradi, Behrouz Farhang, Carl A Kutsche	6/14/2016	Cyber and Information Sciences	Methods and apparatuses using filter banks for multi-carrier spread spectrum signals: Wireless services in harsh and hostile environments must overcome challenges such as intentional jamming (for example, brought about by an enemy during wartime) and unintentional interference (for example, waveform collision in the presence of other



## 2017 Project Summaries — Appendices

Project No.	Patent No.	Title	Inventors	Date Granted	CC	Description
13-093	9,215,587	TT: Self-Generating Fault Tolerant Encryption Key	Hussein Moradi, Behrouz Farhang, and Rangam Subramanian	12/15/15	Advanced Computer Science, Visualization, and Data	<p>devices due to limited spectral resources). Known for their robustness, spread spectrum systems extend information across more bandwidth than is required by the data rate. Multicarrier spread spectrum is a particular form of spread-spectrum designed to be resistant to narrow or partial band interference. This invention uses filter-bank techniques to generate and detect multi-carrier spread-spectrum signals that can carry information at a very low power level distributed over the frequency spectrum. The signal transmission is kept at or below the noise level of other signals leading to a low probability of detection and interception.</p> <p>In wireless radio communication, spread-spectrum techniques involve increasing a signal's bandwidth for a variety of reasons, including to avoid jamming and reducing the probability of detection or interception. However, secure communication may be compromised if an eavesdropper has already obtained the spreading code being used for transmission of a spread-spectrum signal. This invention advances deployment of spread-spectrum systems by dynamically selecting the spreading code used by a pair of communicating devices in such a way that it will be inaccessible to an eavesdropper. The channel reciprocity between the communicating parties is taken advantage of to set up a common secret key (a spreading gain) among them. The self-generated key remains unknown to an eavesdropper whose different physical location, with respect to the legitimate parties, leads to a different set of channel parameters.</p>
14-079	9,399,194	TT: Thermolytic Draw Solute for Osmotically Driven Membrane Processes	Aaron D. Wilson and Christopher J. Orme	7/26/16	Chemical and Molecular Science	<p>Decreasing water supplies throughout much of the industrialized world have necessitated new methods and systems for utilizing water that contains contaminants or impurities. Additionally, certain industries have a need for safer, more energy-efficient methods and systems for removing water from a target material or solute. Traditional purification methods include thermal flash evaporation and reverse osmosis (a process where water is separated from solutes through a membrane by application of pressure). Forward osmosis circumvents several of the deficiencies of reverse osmosis by using a draw solution with a greater osmotic pressure than the feed liquid. The concentrated solution pulls the water through the membrane, leaving</p>

Project No.	Patent No.	Title	Inventors	Date Granted	CC	Description
NS153	9,641,216	Passive Bluetooth Detection and Monitoring Device (BDD)	Kurt W Derr, John G Richardson	5/2/2017	Cyber and Information Sciences	<p>the contaminants behind, and the water can be extracted from the solution with low-grade heat. This patent relates to methods and draw solutions for treating a liquid using an N-cyclicalkyl-cycloalkylamine as a switchable polarity solvent.</p> <p>Monitoring devices and systems for monitoring frequency hopping wireless communications, and related methods: Wireless technologies employing frequency, such as BLUETOOTH.RTM, are becoming more pervasive in industry and government environments. In undiscoverable mode, a device may communicate but will not be detectable to conventional monitoring devices, which may allow communications to occur in areas not necessarily desired. Various embodiments of this invention comprise monitoring devices and systems configured to monitor frequency hopping wireless communications without transmission by the device or system.</p>
10-075	9,369,866	Methods and Apparatuses Using Filter Banks for Multi-Carrier Spread Spectrum Signals	Hussein Moradi, Behrouz Farhang, and Carl A. Kutsche	6/14/16	Advanced Computer Science, Visualization, and Data	<p>Wireless services in harsh and hostile environments must overcome challenges such as intentional jamming (e.g., brought about by an enemy during wartime) and unintentional interference (e.g., collision with the presence of other devices due to limited spectral resources). Known for their robustness, spread spectrum systems extend information across more bandwidth than is required by the data rate. Multi-carrier spread spectrum is a particular form of spread-spectrum designed to be resistant to narrow or partial band interference. This invention uses filter-bank techniques to generate and detect multi-carrier spread-spectrum signals that can carry information at a very low power level distributed over the frequency spectrum. The signal transmission is kept at or below the noise level of other signals, leading to a low probability of detection and interception.</p>
10-075	9,559,748	TT: Filter Bank Implementation of Multicarrier Spread Spectrum Systems	Hussein Moradi, Behrouz Farhang, Carl A Kutsche	1/31/2017	Cyber and Information Sciences	<p>Methods and apparatuses using filter banks for multi-carrier spread-spectrum signals: As the demand for personalized applications continues to grow in mobile communications, there is an increasing need for seamless connectivity between different multi-carrier modes. Multi-Carrier Spread Spectrum (MC-SS) is a particular form of spread-spectrum technique that is designed to be resistant to narrow and/or partial band interference. There is a need for apparatuses and methods such as this Filter-Bank MC-SS that generate and detect MC-</p>

## 2017 Project Summaries — Appendices

<b>Project No.</b>	<b>Patent No.</b>	<b>Title</b>	<b>Inventors</b>	<b>Date Granted</b>	<b>CC</b>	<b>Description</b>
12-066	9,481,614	TT: ESD Resistant Energetic Materials	Michael Alan Daniels, Ronald J Heaps, Ronald S Wallace, Michelle Pantoya, Eric Collins	11/1/2016	Applied Materials Science & Engineering, Chemical Engineering, Mechanical Design and Engineering	<p>SS that can carry information at a very low power level distributed over the frequency spectrum.</p> <p>Energetic materials and methods of tailoring electrostatic discharge sensitivity of energetic materials: Energetic materials, especially those used as first-fire mixes, are susceptible to unintentional electrostatic discharge (ESD) initiation, which presents risks and is difficult to eliminate in real-world situations. Carbon nanofibers filled with a manganese oxide composition exhibited reduced friction sensitivity and decreased ESD sensitivity when compared to a composition lacking the carbon nanofibers.</p>

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