# Nuclear Safety Research and Development Annual Report



December 2014

Office of Nuclear Safety U.S. Department of Energy

#### **Executive Summary**

This is the first annual report of Nuclear Safety Research and Development (NSR&D) compiled by the Department of Energy's (DOE's) NSR&D Program. The purpose of the report is to:

- Describe how DOE and the National Nuclear Security Administration (NNSA) identify and prioritize NSR&D needs;
- Discuss how NSR&D projects are evaluated and funded; and
- Provide brief descriptions of a broad cross-section of NSR&D projects being conducted across the DOE complex.

DOE's corporate NSR&D Program was established to provide an enduring Departmental capability to perform research to strengthen the technical bases of DOE's regulatory infrastructure, enhance technical knowledge and understanding with regard to nuclear facility safety and nuclear explosives safety, and support continuous improvement in the safety of DOE and NNSA nuclear operations by contributing to the resolution of nuclear safety issues. The NSR&D Program is managed by the Office Nuclear Safety, but involves and is supported by DOE and NNSA program offices.

NSR&D projects can be managed and funded via the corporate NSR&D Program or by DOE and NNSA program offices, depending upon whether they are focused on addressing site-specific, program office-specific, or corporate issues. Regardless of sponsorship, the NSR&D Program serves to share the NSR&D results DOE-wide to facilitate gaining corporate benefit from the research effort. Consequently, although this report has been developed by the Office of Nuclear Safety as part of DOE's corporate program, its scope includes NSR&D activities and projects funded by DOE and NNSA program offices as part of their own research initiatives, as well as NSR&D undertaken by DOE contractors as part of Plant-Directed R&D or Laboratory-Directed R&D programs. Summaries of NSR&D projects from these various programs are included in the appendixes of this report.

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# **1.0 INTRODUCTION**

This is the first annual report of Nuclear Safety Research and Development (NSR&D) compiled by the Department of Energy's (DOE's) NSR&D Program. The purpose of the report is to:

- Describe how DOE and the National Nuclear Security Administration (NNSA) identify and prioritize NSR&D needs;
- Discuss how NSR&D projects are evaluated and funded; and
- Provide brief descriptions of a broad cross-section of NSR&D projects being conducted across the DOE complex.

The NSR&D Program is managed by the Office Nuclear Safety (AU-30) in the Office of Environment, Health, Safety and Security (EHSS), but involves and is supported by DOE and NNSA program offices.

Because this is the first annual report, an overview of the NSR&D program (which, in essence, comes from the NSR&D Operating Plan [reference 1]) is included.

# 2.0 DOE NSR&D PROGRAM

# 2.1 Overview and Mission

DOE's NSR&D Program provides a corporate-wide structure and process to coordinate and integrate the Department's NSR&D activities among DOE and NNSA program offices. In the context of this report, NSR&D involves a systematic search for knowledge to advance the fundamental understanding of nuclear safety science and technology through scientific study, analysis, modeling, and experiments.

The overall purpose of NSR&D is to support DOE and NNSA in standards development, validation of analytical models and methods, development of improved or enhanced technology, and improvements in operating practices. NSR&D also supports DOE and NNSA in making technically justified and well-informed nuclear safety decisions, and helps to develop and maintain the technical expertise and the analytical tools and techniques necessary to sustain a qualified and experienced workforce and a robust nuclear safety infrastructure.

The NSR&D Program's mission is to:

- Establish an enduring Departmental commitment and capability to utilize NSR&D in preventing and/or reducing high hazards and risks posed by DOE and NNSA civilian and defense nuclear facilities, operations, nuclear explosives, and environmental restoration activities;
- Foster a Departmental culture that embraces NSR&D as a standard business practice for effecting continuous improvement in nuclear facility safety, consistent with integrated safety management principles; and

• Optimize NSR&D resources to resolve existing and emerging nuclear facility safety concerns.

The NSR&D Program provides a mechanism to effectively share information addressing NSR&D activities and results, and to seek cost-effective means to conduct NSR&D that may have DOE-wide benefit. The NSR&D Program also solicits input from the Department's Nuclear Safety Council, whose membership consists of senior managers representing each of the program offices that operate and manage nuclear facilities.

The NSR&D Program is implemented under a NSR&D Program Operating Plan, which is periodically reviewed and updated as needed. Major elements of the plan include:

- NSR&D Committee
- Program Office and EHSS Roles and Responsibilities
- NSR&D Needs Identification and Proposal Evaluation Processes
- Sharing of NSR&D Results
- Integration of NSR&D efforts into DOE and NNSA Budgeting Processes

These elements are discussed further below.

#### 2.2 NSR&D Committee

The objectives of the NSR&D Committee are to: (1) promote communication and coordination among DOE and NNSA program offices to enhance synergy on NSR&D efforts that can benefit the Department; (2) identify nuclear safety research needs and opportunities within the DOE and NNSA and their program offices; (3) coordinate the review and prioritization of NSR&D Program needs and proposals in order to identify overlaps, gaps, and opportunities where joint funding may mutually benefit multiple DOE and NNSA program offices; and (4) foster and facilitate networking and information exchange on NSR&D needs and activities across DOE and NNSA programs and with external national and international organizations.

The NSR&D Program solicits proposals for projects that have corporate application (i.e., across multiple DOE and NNSA program offices). The NSR&D Committee reviews and prioritizes those proposals for support by available corporate funding, via EHSS, or, if appropriate, by joint funding. The Committee also supports development of an NSR&D Annual Report, and dissemination of the report to the Committee members' respective Program Secretarial Officer.

The NSR&D Committee established, implemented, and operates under the NSR&D Committee Charter and NSR&D Program Operating Plan. The Committee consists of the following program and staff offices:

- NNSA
- The Office of Environmental Management (EM)
- The Office of Science (SC)

- The Office of Nuclear Energy (NE)
- The Chief of Defense Nuclear Safety
- The Chiefs of Nuclear Safety for EM, NE, and SC
- The Office of Nuclear Safety, Chair

# 2.3 NSR&D Program Roles and Responsibilities

# 2.3.1 DOE and NNSA Program Office Roles and Responsibilities

DOE and NNSA program offices are responsible for the safety, design and operation of its nuclear facilities and activities. The DOE complex is engaged in a wide variety of nuclear operations, including nuclear explosives operations conducted at NNSA facilities, and nuclear waste operations conducted under the responsibility of the Office of Environmental Management. DOE also sponsors fundamental scientific research at some of its nuclear facilities operated by the Office of Science and the Office of Nuclear Energy. Many of these operations and facilities have unique designs/processes and pose different engineering and technological challenges. Thus, NSR&D needs may be specific to the individual nuclear operations and facilities and the specific program offices that manage them.

It is appropriate that DOE and NNSA program offices manage their respective NSR&D efforts to support safe nuclear operations and facility safety. Nonetheless, there are cross-cutting and synergistic elements of nuclear facility and process design and operational safety that may affect virtually all nuclear facilities. Consequently, DOE and NNSA recognize the benefit of communicating and coordinating their NSR&D activities to avoid potential gaps or duplication of effort, to identify cross-cutting NSR&D needs, and to build on each other's NSR&D efforts to the extent practicable. Thus, in addition to the program office NSR&D efforts, the Office of Nuclear Safety, within EHSS, provides a DOE-wide coordinating and information sharing function as well as limited funding for cross-cutting NSR&D projects. Appendix A provides an overview of the DOE and NNSA program office efforts related to NSR&D.

#### 2.3.2 Office of Nuclear Safety Roles and Responsibilities

The Office of Nuclear Safety has responsibility for:

- Developing and maintaining the Department-wide NSR&D process;
- Sharing of NSR&D results;
- Providing funding for NSR&D proposals selected under the NSR&D proposal review process;
- Chairing the NSR&D Committee; and
- Sponsoring and managing a range of NSR&D projects addressing cross-cutting nuclear safety issues across the DOE complex. This includes, but is not limited to, NSR&D in support of AU-30's role in ensuring that DOE's nuclear safety regulatory infrastructure is technically sound and reflects best practices.

AU-30 also evaluates the results of NSR&D projects for insights relevant to the technical bases supporting DOE nuclear safety policy, requirements, and guidance.

# 2.4 NSR&D Needs Identification and Proposal Process

Identification of specific NSR&D needs is accomplished using a variety of approaches, including: (1) workshops of subject matter experts; (2) call for proposals; (3) analysis of operational events; (4) review of emerging problems; and (5) review by the NSR&D Committee to validate and prioritize Department NSR&D needs.

Research needs can be met either by individual program offices (for those specific to a facility or project) or by selection for corporate (AU-30) funding via the NSR&D Program proposal solicitation and selection process. The identification of NSR&D needs by the individual program offices by means of the processes listed above is taken into consideration in selecting projects for corporate funding. Section 3.7 discusses the projects selected in the first annual proposal solicitation process, in Fiscal Year (FY) 2013, and the second, in FY 2014.

The NSR&D Committee has developed a process that identifies, prioritizes, and funds NSR&D proposals based on Departmental needs, which includes initial screening, review, and ranking, as well as input from the Nuclear Safety Council. To initiate the proposal solicitation process, the NSR&D Committee has developed instructions outlining the key information required for proposal submission. Selection and funding of NSR&D proposals considers the expected Department-wide benefits and costs.

# 2.5 Methods for Sharing of NSR&D Results

The NSR&D Program and NSR&D Committee have been working with the Office of Scientific and Technical Information (OSTI), within SC, to evaluate and use an existing Departmental database that collects research and development from across the DOE complex. OSTI and its predecessors have collected research and development results that date back to the Manhattan Project, and the database also includes information on projects conducted internationally. Discussions with OSTI focused on using the OSTI database to serve NSR&D needs. The interface would include a single-point-of-access portal to provide access to NSR&D results once access is granted. The NSR&D Program utilizes the OSTI database to search and collect information on previous research and to verify that research proposals are unique. Furthermore, NSR&D Program funded research will be submitted to OSTI to capture and share the results complex-wide.

# 2.6 Integration of NSR&D efforts into DOE and NNSA Budgeting Processes

NSR&D activities are integrated into DOE and NNSA planning, programming, budgeting, and execution processes through a variety of methods. For the past three years, the EHSS<sup>1</sup> budget, submitted to the Office of Management and Budget, has included an item to "*maintain a DOE-wide nuclear safety research and development program to provide corporate-level leadership supporting the coordination and integration of nuclear safety science and technology...and coordinate the conduct of nuclear safety research and development activities*". The AU-30 budget includes funding for two types of NSR&D projects: (1) projects selected via the NSR&D

<sup>&</sup>lt;sup>1</sup> Prior to FY 2015, the name of EHSS was the Office of Health, Safety and Security (HSS).

proposal process and (2) projects supporting Office of Nuclear Safety specific activities. The NNSA-wide "special funding" for NSR&D activities is supported through (1) Readiness in Technical Base and Facilities and (2) Directed Stockpile Work. NNSA, EM, NE, and SC also integrate NSR&D related activities into their annual facility and project budgets. Additionally, self-directed NSR&D activities may be funded by DOE contractors as part of Plant-Directed R&D (PDRD) or Laboratory-Directed R&D (LDRD) programs.

# 2.7 Current Corporate NSR&D Projects

The initial NSR&D proposal solicitation process was initiated in January 2013 and proposal selection concluded in May 2013. A total of 23 NSR&D proposals were submitted and reviewed. The following three proposals were selected for funding:

- Development and Manufacture of an Ergonomically Sound Glovebox Glove (Project NSRD-01)
- In-Place Filter Testing Instrument for Nuclear Material Containers (Project NSRD-02)
- Ceramic HEPA Filters (Project NSRD-03)

The second proposal solicitation was distributed in January 2014, and the selection process concluded in June 2014. Thirty-two NSR&D proposal were submitted, an increase of nearly 40% over the 2013 response. Four proposals were selected for funding:

- Study of HEPA Filter Degradation Due to Aging (Project NSRD-04)
- Development and Validation of Methodology to Model Flow in Ventilation Systems Commonly Found in Nuclear Facilities (Project NSRD-05)
- Computational Capability to Substantiate DOE-HBDK-3010 Data (Project NSRD-06)
- Stochastic Modeling of Radioactive Material Releases (Project NSRD-07)

Summaries of these seven projects are provided in Appendix B.

Other NSR&D projects initiated and managed by AU-30 are described in Appendix C.

# 2.8 DOE and NNSA Program Office NSR&D

As noted above, in addition to participating in the selection of projects to be funded by the corporate NSR&D program, DOE and NNSA program offices also support NSR&D projects from their own budgets. These projects are not part of the corporate program, and are selected based on the funding office's priorities and criteria. However, in some cases, they may be related to projects supported by AU-30. Information on these projects, as provided by the sponsoring organization, is provided in this report.

- NNSA "special funded" projects are described in Appendix D.
- Projects supported by NE are discussed in Appendix E.

• Examples of EM NSR&D related projects are provided in Appendix F.

# 2.9 Laboratory Directed and Plant Directed R&D Projects

In 1991, DOE formally established the Laboratory Directed Research and Development (LDRD) program. The program was subsequently expanded to non-laboratory DOE facilities, where it is referred to as Plant Directed Research and Development (PDRD). Funding for this program is provided as part of the overall facility budget. The objective of the program is to provide the capability for management at these facilities to initiate innovative scientific and technical research that can contribute to DOE's national mission. An annual report on the LDRD program is submitted to Congress.

There is no requirement for some fraction of a facility's LDRD or PDRD program to address nuclear safety. However, there have been cases where an LDRD or PDRD project is related to, or can be applied to, DOE nuclear safety issues. Examples of nuclear-safety-related LDRD and/or PDRD projects are provided in Appendix G.

# 3.0 FUTURE PLANS

As experience is gained with the various elements of the NSR&D Program, DOE and the NNSA, through the NSR&D Committee, will continue to work to improve and strengthen the means by which nuclear safety issues are identified and NSR&D activities are developed to address those issues. One particular area of emphasis will be on cross-cutting issues that could affect and/or benefit multiple program offices and their defense and/or civilian nuclear facilities. In this regard, AU-30 is developing a process for identifying such generic safety issues on an ongoing basis, prioritizing them using a risk-informed methodology, and, as appropriate, addressing high-priority issues through NSR&D projects. To assist in developing this process, AU-30 has consulted with the U.S. Nuclear Regulatory Commission, which has operated a program to identify and address unresolved generic safety issues since 1977.

# Appendix A

# **Overview of DOE and NNSA Program Offices NSR&D Efforts**

#### 1. National Nuclear Security Administration

The NNSA has safety basis approval authority for 70 nuclear facilities at eight sites. The NNSA is an active participant on the NSR&D Committee and also has a well-developed process for identifying NSR&D projects for its own support. That process was initiated in 2002 for R&D in support of operations at the Pantex Plant, and has been expanded to include other NNSA sites. Following the issuance of DNFSB Recommendation 2004-1, NNSA established the NNSA NSR&D Working Group (WG) to better manage the development of the annual NSR&D programs at NNSA's design and production agencies.

WG membership includes representatives from NNSA Headquarters, Los Alamos National Laboratory, Lawrence Livermore National Laboratory, Sandia National Laboratories, Pantex Plant, Savannah River National Laboratory, the Nevada National Security Site, and the Y-12 National Security Site. The NNSA design and production agencies submit to the WG prioritized lists of NSR&D projects for which special funding is requested. The WG meets periodically to review and coordinate NSR&D work, identify NSR&D needs, prioritize and integrate NSR&D projects, and develop the WG's annual report. AU-30 also attends the WG meetings for awareness and to discuss areas where NNSA proposals may have DOE-wide benefit. One of the WG Chairs is a member of and participates on the DOE NSR&D Committee.

The NSR&D WG develops an annual report that lists and briefly discusses the program-funded NSR&D projects for each NNSA design and production agency. The report also provides an NNSA-wide integrated and prioritized list of NSR&D projects for which special funding is requested. The report is forwarded by the WG Chair to the NSR&D Committee. The WG report also includes a reference to and a summary of planned criticality safety related NSR&D projects, which are separately developed and funded by the Nuclear Criticality Safety Program.

# 2. Office of Environmental Management

EM has safety basis approval authority for more than 80 nuclear facilities at 10 different sites. EM supports the operation of the NSR&D Committee; it has also supported a robust technology development and demonstration (TDD) effort for many years. EM's overarching strategy for TDD was described in its 2008 Engineering & Technology Roadmap, which received approval from the National Research Council.

EM's TDD mission focuses on environmental remediation, modeling, and risk assessment; deactivation and decommissioning (D&D); and the safe characterization, retrieval, treatment, monitoring, and disposition of wastes and nuclear materials associated with EM operations across the country.

# 3. Office of Science

SC has safety basis approval authority for 16 nuclear facilities at four laboratories. At this time, relatively little of SC's work is related to NSR&D. However, SC representatives serve as members of the NSR&D Committee, and SC has committed to support the NSR&D Program and the Committee from the perspective of overall programmatic integration and awareness. In this way, SC may bring potentially significant NSR&D issues to the attention of the NSR&D Committee, and be prepared to deal with nuclear safety issues that arise at its facilities.

# 4. Office of Nuclear Energy

NE has safety basis approval authority for 17 nuclear facilities/activities, all of which are located at the Idaho National Laboratory. NE actively supports the NSR&D Committee's efforts in assessing cross-cutting research needs, and is also responsible for its own nuclear safety research portfolio, which is developed by assessing the capabilities and technical needs required to support current and future NE and national needs. NE research program management engages key staff, including strategic planners, subject matter experts, and program managers, as needed to establish the areas or topics where new research and development is needed.

# Appendix B

#### Description of Corporate NSR&D Projects Selected Through the Annual Call for Proposals and Supported by the Office of Nuclear Safety

**Project Title:** Develop and Manufacture an Ergonomically Sound Glovebox Glove (NSRD-01)

Principal Investigator/Site(s) Involved: Cindy Lawton, LANL (with U. of New Mexico)

**Project Description and Technical Objective:** Design and develop a safer and more ergonomic glovebox glove. Partner with a manufacturer for large-scale production of the glove that can be integrated into gloveboxes throughout the DOE complex.

The approach to develop a new glovebox glove began with an extensive understanding of hand anatomy and anthropometrics, as well as an in-depth literature review of glove development for other industries, such as the National Aeronautics and Space Administration. Utilizing this data, along with collaboration with an orthopedic hand surgeon, the new glovebox glove dimensions were determined. Next, the ability to input the glove/hand dimension information into a 3D engineering program was developed. Last, workers tested the new glove dimensions for validity. The new ergonomic glove design has received a patent. The final two stages of this project are to bring this new technology to a glove manufacturer for production and, once made, testing the new glove for improved dexterity and comfort at two different DOE sites.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** This new design will be of great benefit since there are no suitable commercially available options to replace the current Los Alamos National Laboratory (LANL) glovebox glove, whose mold dates back to the 1960s. An improved glovebox glove will have three significant benefits: 1) it will reduce the risk of injury, 2) it will improve comfort and productivity for the workers, and 3) it will reduce the risk of glovebox breaches. The estimated savings from combination of these three benefits are several million dollars.

**Highlights/Status:** As a result of funding from the fiscal year 2013 NSR&D Program, the new ergonomic glove dimensions have been established and input into a 3D model. The dimensions have been verified with the glovebox workers. The LANL technical transfer organization is in the final stages of negotiating a contract agreement with Honeywell, Inc., which produces most glovebox gloves for the DOE complex. LANL purchases approximately \$500,000 in glovebox gloves yearly from Honeywell. The development phase of the project is complete and the manufacturing phase is in process. Ultimately, the project will lead to improved safety and efficiency, a decrease in injuries and glove breaches, and a significant cost savings throughout the DOE complex.

Project Title: In-Place Filter Testing Instrument for Nuclear Material Containers (NSRD-02)

#### Principal Investigator/Site(s) Involved: Murray E. Moore, LANL

**Project Description and Technical Objective:** The objective of this project is to develop a small (portable) desktop instrument to assess operational conditions of nuclear material storage containers without disassembling the containers. The instrument would determine if the high-performance filter on the storage container is clogged. Additionally, the instrument would determine if the container O-ring seal is air-tight, or if the O-ring seal has failed.

The project is developing a methodology to simulate failure conditions, procure a set of standard test filters and canisters, and define test criteria that are appropriate to storage canister operations. The testing is being conducted on two types of nuclear material storage containers. The first is the commonly used Hagan canister with three different sizes tested (5, 8 and 12 quart), and the second is the new SAVY canister being designed for use throughout the DOE complex (only the 5-quart size canister).

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** The DOE complex will benefit in regard to personnel safety and facility operations if an in-place filter test (IPFT) capability is implemented. Filter integrity assessment would indicate whether the filter was plugged or operating within an acceptable performance range. A canister could be verified for leak-tightness, either after canister packaging, or by testing the as-found condition. Additionally, a set of standard filters and a method to define and maintain them would be valuable for filter integrity assessment.

**Highlights/Status:** The Los Alamos Aerosol Engineering Facility developed a prototype IPFT device. The prototype is a microprocessor-controlled system that applies a slight vacuum to an assembled nuclear material storage canister (e.g., 0.2 psi of vacuum compared to 14.7 psi atmospheric pressure). The prototype system was used to identify flow and pressure parameters for testing actual canisters. Stainless steel fittings were custom-designed and built for a direct leak-test interface for the nuclear storage canisters, and a set of tests performed with actual canisters. The prototype work defined a set of parameters which were used specify the performance variables for a customized leak test system (the Isaac<sup>™</sup> from Zaxis). Testing with the Isaac system has been completed and the draft final report has been provided to DOE. The report is currently being reviewed.

Project Title: Ceramic High Efficiency Particulate Air (HEPA) Filters (NSRD-03)

**Principal Investigator/Site(s) Involved:** Mark Mitchell, LLNL (with California Polytechnic University)

**Project Description and Technical Objective:** The technical objective of this project is to develop and deploy advances in HEPA filter technology (e.g., related to ceramic HEPA filters) to benefit DOE nuclear facilities by providing lower life-cycle costs associated with safety class and safety significant HEPA filter systems in nuclear facilities. This project is broken into two main tasks. First, perform high temperature testing on HEPA filter materials and components at Cal Poly's High Temperature Testing Unit (HTTU). Second, develop qualification testing standards for ceramic HEPA filters at Mississippi State's Institute for Clean Energy Technology (ICET). Lawrence Livermore National Laboratory (LLNL) is the lead for the activity and collaborates with both universities.

The goal of this project is to support development and deployment of advanced HEPA filter technology by enabling testing to support the understanding, selection, and optimization of materials under key conditions (e.g., fires in a nuclear facility) and to support the development of test setups and specifications for industry codes and standards (e.g., ASME AG-1 Subsection FO Ceramic Filters). The first effort utilizes the unique capabilities of the HTTU to test new and innovative materials for HEPA filter components (e.g., media, sealants, gaskets). The second effort will use the DOE-sponsored ICET and HTTU as they relate to the development of test setups and specifications for industry codes and standards.

**Benefits or Applications of the Results to DOE/NNSA Nuclear Facilities:** This research has the potential to benefit the nuclear facilities of DOE, including the NNSA, by significantly lowering life-cycle costs, including decreasing design and operational costs associated with safety class or safety significant ventilation systems and components. Qualifying the performance of ceramic filters in a fire could also significantly reduce or eliminate costs of support systems associated with mitigating a release. This could save DOE \$1M to \$10M annually, and potentially much more. It is advantageous to DOE to focus fundamental research and development on engineering safety solutions (hardware) rather than additional analysis. Through longer filter life, DOE could save more than \$11M annually related to reductions in waste disposal costs alone. The lifecycle cost of a HEPA filter in a DOE nuclear facility is driven mostly by the cost of disposing of radioactively contaminated HEPA filters, not the price of the filter itself.

**Highlights/Status:** The ceramic test stand Technical Working Group (TWG) was established, with members from ICET, LLNL, the NSR&D Program, and the ASME AG-1 Subsection FO writing team. ICET gave a presentation on the ceramic test stand and its capabilities to the TWG. Preliminary tests will be conducted to down-select the seals, gaskets, media, and materials; and the most promising will be tested at full-scale conditions in the HTTU. The first Cal Poly student team completed its rapid prototype testing system (Mini-HTTU) for preliminary tests on a large number of material samples. The second Cal Poly student team presented its final design for the rapid change out sample chamber and preliminary material selection.

Project Title: Study of HEPA Filter Degradation Due to Aging (NSRD-04)

**Principal Investigator/Site(s) Involved:** Elaine Diaz, RL; Charles Waggoner (Mississippi State University)

**Project Description and Technical Objective:** High Efficiency Particulate Air (HEPA) filters are credited as the final barrier against release of radioactive contamination in nearly every operating DOE and NNSA nuclear facility. Approximately 6000 HEPA filters are purchased each year within the DOE/NNSA complex. Each of these filters is tested, inspected, stored in special environmental conditions until needed. When needed, they are installed, tested post-installation, in-place leak tested annually, removed, and disposed of through a rigorous procedure designed to ensure integrity of these crucial, yet fragile, components. Filter aging leads to degradation of tensile strength across the face of filter media pleats. The key mechanisms suspected in filter aging are environmental conditions in storage or in use, such as humidity, temperature, oxidation, and pleat flutter. These issues have been discussed at length without sufficient data to provide definitive conclusions.

Concerns and uncertainty associated with degradation of HEPA filter performance over time led DOE sites to limit HEPA filter service life to 10 years from date of manufacture. This policy causes hundreds of otherwise unnecessary filter changes, putting employees at risk of exposure, causing facility operational disruptions, causing otherwise compliant filters to be disposed without being used due to expiring service life, and costing DOE millions of dollars annually. Conclusive data are needed to resolve uncertainty associated with the damaging effects of aging on durability of HEPA filters.

Testing will compare performance and durability under upset or design basis conditions of new filters, as well as filters retained in storage for ten to twenty years (past current service life). Testing will evaluate the effects of flutter/vibration, which may cause fatigue failure of filter pleats, and is suspected to be a leading cause of filter "aging" when installed in operating plants. These data are necessary to determine the envelope within which nuclear safety experts can credit HEPA filter performance as an accident control, leading to establishment of a risk-informed DOE service life.

The Mississippi State University (MSU) Institute for Clean Energy Technology (ICET) is a center of excellence for HEPA filter testing. The MSU ICET full-scale HEPA test stand has been used in past testing to challenge filters under simulated accident conditions. The technical approach for this research involves bench scale and full-scale tests of aged and new HEPA media and filters for comparison. A technical working group composed of industry and DOE complex subject matter experts will guide detailed test planning and oversee progress.

**Benefits or Application of Results to DOE/NNSA Nuclear Facilities:** A deeper understanding of the effects of aging and fatigue on HEPA filter performance will help DOE define a service life for these fragile components that minimizes risk, while possibly reducing costs and work necessary to maintain these systems. There is potential cost savings to the government, as well as avoidance of operational impact and reduction of radiation exposure for DOE's facility workers, if data supports extending HEPA shelf life and change-out intervals.

Status/Highlights: None. This is a new project.

**Project Title:** Development and validation of methodology to model flow in ventilation systems commonly found in nuclear facilities (NSRD-05)

#### Principal Investigator/Site(s) Involved: James Bailey, ANL

**Project Description and Technical Objective:** Multiple sites across the DOE complex utilize hot cells, gloveboxes, and hoods to provide confinement of radioactive materials, and thereby to reduce direct doses to facility workers and mitigate the consequences to the environment due to an uncontrolled release. Each of these features has access points that interface with the personnel space. Understanding how air flow behaves at these access points is of great interest to those performing hazard analyses.

Argonne National Laboratory has recently started applying Computational Fluid Dynamics (CFD) to analyze and model the flows in hot cells and glove boxes as a way to confirm ventilation system operation. While CFD capability continues to advance, there are still important modeling assumptions that are left to the analyst's discretion. These are most notably the choice of the turbulence models, mesh structure, and wall boundary condition assumptions used in the model. The modeling assumptions have a profound impact on the analysis result and it is the purpose of this proposal to determine and validate proper choices through an iterative analysis/validation process.

In this work, the project will apply the CFD experience gained in modeling airflow in these areas to the problem of modeling air flow and particulate transport. These studies will include a specifically selected set of standard geometries commonly found in glovebox and hot cell facilities. This modeling will be supported by field measurement studies which will both inform and validate the modeling assumptions. Based on the results of field tests, the project will refine the modeling assumptions and boundary conditions and repeat the process until the results are found to be reliable with a high level of confidence.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** The main outcome of this project is the development of a methodology for using CFD to analyze the glovebox and hot cell installations. This methodology will include the modeling assumptions for a variety of typical configurations that were arrived at through the iterative modeling and validation procedure described above. Having such a methodology will provide guidance to analysts to ensure appropriate analysis of hot cells, glove boxes, and hoods. This methodology will also be beneficial to designers of hot cells, gloveboxes and hoods.

Status/Highlights: None. This is a new project.

#### Project Title: Computational Capability to Substantiate DOE-HDBK-3010 Data (NSRD-06)

#### Principal Investigator/Site(s) Involved: David L.Y. Louie, SNL

**Project Description and Technical Objective:** Safety basis analysts throughout the DOE complex rely heavily on the information provided in DOE Handbook (HDBK) 3010, *Airborne Release Fractions/Rates and Respirable Fractions for Nonreactor Nuclear Facilities* to determine source terms. Most often, the analysts simply take the bounding values because time constraints and to avoid regulatory critique. Although the Handbook is comprehensive in terms of data to derive airborne release fractions and respirable fractions to bound the main types of accidents that could be encountered in the complex, the derivation of the data often depended on table-top and bench/laboratory experiments, as well as engineering judgment which may not be substantiated and may not be representative to the actual situation. The goal of this research is to provide a more accurate method to identify bounding values for the Handbook. The advancement in computing capabilities at national laboratories allows the use of code simulation methods to provide more representative values for the source term.

This research should provide insights about the fundamental physics and phenomena associated with the types of accidents, based on the maturity of the simulation tools developed for the weapons complex. Although these tools require intense computational power, the availability of these tools and computing power allows safety analysts to utilize them for non-weapons related safety activities. These simulation tools will be used to assess whether the data used to derive the airborne release fractions and respirable fractions in the Handbook are reasonably accurate and bounding.

**Benefits or Application of Results to DOE/NNSA Nuclear Facilities:** If the reduced-scale data are conservative, the source term used for the documented safety analyses may over-specify the need for design controls. This over-specification could substantially be a cost to DOE and NNSA. If the data are non-conservative, the documented safety analysis may underestimate the source term, which could translate to a concern with respect to the adequacy of hazard controls put in place for the workers and public. In either case, the results of the research may improve how the safety basis analysts across the complex approach the selection of bounding airborne release fractions and respirable fractions, which can result in improving the defensibility of the safety analyses.

Status/Highlights: None. This is a new project.

Project Title: Stochastic Modeling of Radioactive Material Releases (NSRD-07)

**Principal Investigator/Site(s) Involved:** Jason Andrus, INL; Chad Pope, Idaho State University

Project Description and Technical Objective: Traditional radioactive material release modeling codes generally provide a bounding single point estimate of receptor dose using point value input parameters and a straight-line Gaussian plume dispersion model. However, this approach can fall short since it tends to provide bounding dose estimates rather than a dose distribution with quantification of the dose uncertainty. This is particularly problematic when one considers the impact of governing distributions for input variables such as material-at-risk, damage ratio, airborne release fraction, respirable fraction, leak path factor, breathing rate, and even dose conversion factors. Additionally, although the atmospheric dispersion model is based on a Gaussian distribution, stochastic sampling of the distribution is typically not used to reach the dose estimate. Thus, decisions regarding potential doses to members of the public are frequently overstated, leading to excessively conservative material-at-risk limits and potential over selection of safety systems structures, or components. To address this issue, a Monte Carlobased code system is proposed to stochastically analyze radiological material release scenarios and provide dose distribution estimates. This approach will support improved risk understanding, leading to better-informed decision making associated with establishing materialat-risk limits and safety system, structure or component selection. It is important to note that this project is not intended to replace or compete with codes such as MACCS or RSAC; rather it is viewed as an easy to use supplemental tool to help improve risk understanding and support better-informed decisions.

The code system will be developed using MATLAB, and will incorporate widespread use of Monte Carlo methods, as well as a graphical user interface for ease of operation. Monte Carlo techniques will include user selection of the governing distribution for such input parameters as the material-at-risk, damage ratio, airborne release fraction, respirable fraction, leak path factor, breathing rate, and dose conversion factors. Once the code system is developed, bounding value dose results will be benchmarked using traditional radioactive material release modeling codes such as MACCS or RSAC. Systematic investigation of each parameter contributing to the dose result will be pursued to quantify the parameter's contribution to the overall dose estimate and uncertainty. The process will be carried out for a suite of disruptive scenarios. Systematic study of each contributing parameter will lead to identification of the parameters that have the largest impact on the resulting dose estimate uncertainty. Once identified, investigation into reducing uncertainty in the key parameters can be accomplished. The project will initially be dedicated to distribution research, code construction, and testing of the code system. The code system will be distributed to select organizations for beta-testing and feedback.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** The most important benefit associated with this project will be improved risk understanding. Contractors and approval authority personnel will be able to make better-informed decisions by being able to compare dose estimate results that include a more systematic quantification of the impact of contributors to the dose estimate with the currently used highly conservative methods. This will allow for risk-informed decisions related to areas where use of alternative methods may justify significant cost savings without reduction in safety.

Status/Highlights: None. This is a new project.

# Appendix C

#### Nuclear Safety Research Projects Underway in EHSS's Office of Nuclear Safety

EHSS's NSR&D Program is currently funding one project initiated by the Office of Nuclear Safety. Two other projects have been completed in 2014, with the reports in management review. The three projects are as follows.

Project Title: Review of DOE Methodologies for Spray Release

**Project Description and Technical Objective:** The purpose of this project is to conduct a review of the current practices and completed research in the area of spray release.

In 2009, in response to comments from Defense Nuclear Facilities Safety Board (DNFSB) staff, the Office of River Protection (ORP) sponsored a review of the technical basis of the guidance in DOE-HDBK-3010, Airborne Release Fractions/Rates and Respirable Fractions for Nonreactor Nuclear Facilities. This review (Mishima and Foppe, 2010) indicated a concern that the Airborne Release Fraction (ARF)\*Respirable Fraction (RF) value in the current DOE guidance could be non-conservative by about a factor of 20. The issues raised were in the context of accident analysis for the Waste Treatment and Immobilization Plant (WTP) being constructed in Hanford, WA. To expand the data set upon which the WTP accident and safety analyses were based, an aerosol spray leak testing program was conducted by Pacific Northwest National Laboratory (PNNL). PNNL's test program addressed two key technical areas: (1) to quantify the role of slurry particles in small breaches where slurry particles may plug the hole and prevent high-pressure sprays, and (2) to determine aerosol droplet size distribution and total droplet volume from prototypic breaches and fluids, including sprays from larger breaches and sprays of slurries for which literature data are largely absent. In early 2013, PNNL completed and issued the research results regarding spray release accidents, where the large-scale test results were used to develop a correlation to estimate aerosol generation rate. However, a July 2013 workshop on spray release analysis indicated that PNNL's research may be applicable more broadly across the DOE complex (e.g., at the Hanford, Oak Ridge, and Savannah River Sites), particularly with regard to the methods used to calculate ARF and RF values.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** The results may be used to support decisions about a potential revision to DOE-HDBK-3010 and future guidance for conducting spray release analysis.

Status/Highlights: The project plan is expected to start early in fiscal year 2015.

**Project Title:** Calculations of Atmospheric Dispersion at Onsite Locations for DOE Nuclear Facilities

**Project Description and Technical Objective:** The Office of Nuclear Safety, within the Office of Environment, Health, Safety and Security, performed an evaluation of the technical bases for the default value of the atmospheric dispersion ( $\chi/Q$ ) parameter, which is used at DOE, including the NNSA, in the calculation of a radiological dose at the onsite receptor location (i.e., co-located worker at 100 meters) in safety analyses of DOE nuclear facilities. The evaluation included an assessment of the potential use of the default  $\chi/Q$  value to determine exposure at the co-located worker location resulting from chemical releases.

Appendix A and B of DOE-STD-1189-2008, *Integration of Safety into the Design Process* (Ref. 1), provide criteria and guidance for the calculation of the radiological dose and chemical exposure to the co-located worker from potential accidents at DOE's nuclear facilities. This calculated radiological dose and/or chemical exposure is used to determine whether safety-significant controls, to prevent or mitigate the potential accidents, are warranted for the protection of co-located workers.

The scope of the research included a review of the existing regulatory basis for the default value for radiological dispersion analysis, comparison of the value to results from a current DOE toolbox model and an approved U.S. Nuclear Regulatory Commission (NRC) model for radiological dispersion, and evaluation of the value to two DOE toolbox models for chemical dispersion.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** The benefit of the project includes a stronger technical basis for the co-located worker value which supports the Departments regulatory framework and revision of DOE Technical Standards.

Status/Highlights: The report is in management review.

**Completion Date:** January 2015

Project Title: Relationship Between DOE Nuclear Safety Goals and Evaluation Guideline

**Project Description and Technical Objective:** This project is exploratory research which evaluated the relationship between the dose to the hypothetical maximally exposed off-site individual (MOI) as calculated in the documented safety analyses (DSAs) (per DOE-STD-3009, *Preparation Guide for U.S. Department of Energy Nonreactor Nuclear Facility Safety Documented Analyses*) and DOE's quantitative safety objectives (per DOE Policy 420.1, *Nuclear Safety Policy*) for the increase in the risk of prompt fatalities and cancer fatalities for representative spill and fire accidents at three different DOE sites. Facilities evaluated include the Plutonium Facility (PF4) at Los Alamos National Laboratory (LANL), the Tritium Extraction Facility (TEF) and the F-Area Tank Farm at the Savannah River Site (SRS), and the Annular Core Research Reactor (ACRR) located at Technical Area V (TAV) at Sandia National Laboratories (SNL).

DOE's quantitative safety objectives are intended as aiming points to support the DOE Safety Goals and guide requirements and standards development. A better understanding of the relationship of the MOI dose to the quantitative safety objectives provides insights on how well DOE's set of requirements and standards are supporting meeting the Safety Goal.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** The results of this exploratory research provide a better understand the linkage of the quantitative safety objectives and the evaluation guideline and safety margins that exist at DOE facilities relative to DOE Safety Goals.

Status/Highlights: The report is in management review.

Completion Date: April 2015

# Appendix D

#### National Nuclear Security Administration's 2013 NSR&D Working Group Special Funds Projects

In fiscal year 2013, there were a total of 42 proposals submitted to NNSA's NSR&D Working Group. The following are the 18 projects selected for special funding.

#### 1. A Common Approach to QMU Explosive Safety Analysis

This project focuses on establishing the logical relationships between factors important to explosive safety analysis. A Quantification of Margins and Uncertainties (QMU)-based approach is typically used to estimate the "risk" associated with operating and fielding complex technical systems. Estimations of risk in the QMU framework are defined by certain parameters. The most significant parameters of importance include: (a) Uncertainty; (b) Upper and Lower Operating Boundaries (Thresholds); and (c) Designed Operating Margin. Values for these parameters are determined from different factors of empirical knowledge or subjective belief about the characteristics of the risk distribution. The newly-devised factorial structure will be validated for fit and suitability to electrostatic discharge (ESD) threats that would typically be encountered in the production environment.

#### 2. Current Flow Across Broken Bridge Wire in Detonators

This project investigates the initiability of detonators with broken or gapped bridge wires. This is an area that needs additional research and testing. Damaged detonator scenarios include a mechanically broken or gapped bridge wire. Understanding the bounding conditions for energy, power and voltage is important for assessing the probability of initiation and output energy for damaged detonators in a variety of weapon configurations. Previous work scoped the problem to better understand and focus on gap sizes that pose a safety threat and to identify threshold sized gaps. This effort is focused on more testing in the range of the threshold gap size. This allows a better understanding of the statistical nature of threshold breakdown due to gap widths. Two different scenarios are being addressed: (1) discharge due to increasing voltage across a given gap width, and (2) sudden application and discharge of a charged object in excess of the normal gap breakdown voltage. These different scenarios may turn out to have the same or different reaction thresholds.

#### 3. Effect of Adhesive – High Explosive (HE) Incompatibility of Thermal Initiation

The goal of this project is to evaluate the safety envelope of PBX 9501 when Barco Bond or Wilethane adhesives are cured in contact with the explosive. Recent differential scanning calorimetry (DSC) data shows that both of these adhesives are incompatible with PBX 9501 – resulting in a decrease in the temperature of peak exothermic decomposition of the explosive. The decomposition peak rise of these mixtures is also more rapid than that of the explosive alone, indicating that significant energy is generated. The implication is that the mixture is less thermally stable, is possibly more energetic, and may be more susceptible to heating induced by mechanical insult. This work will evaluate the significance of these implications.

# 4. Ceramic Filters for Nuclear Facility Ventilation

This project supports development of a ceramic HEPA filter technology to benefit DOE nuclear facilities by providing lower life-cycle costs associated with safety class and safety significant systems in nuclear facilities. The satisfactory performance of ceramic filters in a fire could significantly reduce safety basis costs of support systems associated with mitigating a release, such as fire suppression, fire detection and alarm, and internal building structure. Advanced ceramic HEPA-filters provide an excellent barrier between radioactive material in a nuclear facility and everything downwind. The technical objective is to develop improved filtration materials for ceramic filters using LLNL and DOE developed innovations. This continuing task will build on the ceramic filter medium fabrication techniques developed previously. A commercial filter membrane approach has been developed along with an advanced nanofiber filtration medium in development.

#### 5. Flash X-ray and Streak Imaging of Deflagration-to-Detonation Transition (DDT) Phenomena in HMX-based Explosives

This project uses flash x-ray radiography to perform the first direct measurements of density in an HMX-based deflagration-to detonation transition (DDT) experiment, time-resolved and coordinated with simultaneous spatially-resolved measurements of luminosity. DDT presents a clear danger for many weapons systems because it can develop under a broad range of conditions and have potentially severe consequences, but key phenomena, such as convective burning and plug formation processes, are difficult to model and predict. New quantitative measurements of these processes, which will be performed as part of this project, will enable a greatly-improved predictive capability for violence in HMX explosives.

#### 6. Development of Cookoff-Induced DDT Modeling Capabilities

The objective of this project is to develop a model for cookoff-induced deflagration-todetonation-transition (DDT) in conventional high explosives (CHEs). DDT models integrated into Advanced Simulation and Computing (ASC) codes can be used to assess the probability and outcome of thermal hazard scenarios. Predictive DDT models guide the development of preventative and mitigative measures to avoid and reduce collateral damage. DDT development will be accomplished using the convective-burn model in conjunction with the ignition and growth model. While modeling capabilities for DDT in porous bed HMX, and separately for cookoff violence, have been successfully demonstrated, modeling of cookoff-induced DDT in CHEs has not yet been developed. The project will develop and benchmark the model with recent and newly proposed DDT experiments. Special attention will be given to quantifying model parameter uncertainties and their influence on overall DDT response in order to better understand margins.

#### 7. Triboelectric Charging of Foams

This project will characterize triboelectric processes occurring in nuclear weapons foams, including the charge bound in nuclear weapons foams and the resultant energy deposition for those foams. The triboelectric effect occurs when materials become electrically charged after

they come into contact with a different material and are then separated. This occurs during the assembly/disassembly process of nuclear weapons, when pockets of charge can be generated and trapped in foams. Triboelectric processes are dependent on materials used, surface finishes, and perhaps even temperature and are not well characterized. The foam characterization study will help support weapon hazard analyses and development of mitigation techniques for assembly/disassembly processes, along with the development of foams with reduced triboelectric properties.

# 8. Visual Inspection Reliability

The goals of this project are to increase performance effectiveness, efficiency, and safety by identifying potential methods for optimizing visual inspection performance in nuclear safety operations. Visual inspection is commonly used throughout industry to identify defects in manufactured materials and components. However, humans are imperfect inspectors who sometimes miss flaws, potentially jeopardizing safety if the defective part becomes part of the inventory. At other times, inspectors label a part defective when it actually does not have any flaws. This can result in increased costs and inefficiencies in the process. Potential benefits of this project include reduced errors during visual inspection, a more efficient process, and enhanced safety in the long term if defective parts are more reliably identified.

# 9. LMA Lightning Detection Investigation

This project will investigate the effectiveness of a Lightning Mapping Array (LMA), which can detect the electrical activity in an area surrounding the plant. This array would use the high frequency characteristics of cloud-to-ground, cloud-to-cloud and inter-cloud lightning discharges. It is known that, in the majority of cases, cloud-to-cloud and inter-cloud electrical activity *precedes* cloud-to-ground lightning by up to an hour depending on atmospheric conditions. The current Lightning Location and Protection System (LLPS) only detects cloud-to-ground strikes. This newer technology may provide more advanced warnings of lightning strikes to the plant by sensing precursor events. Analysis of the data from the LMA sensors may demonstrate that LMA can be effective as an early warning system, as well as serving as a redundant system to reinforce the current LLPS.

#### 10. Experimental Measurement of Brush Discharge Characteristics

The purpose of this project is to characterize the maximum potential current pulse capable of flowing from a dielectric material to a conductive material, with emphasis on materials present in Pantex bays and cells. Based on preliminary results from the LLNL brush discharge model, a selection of dielectric materials with model-specified geometries will be uniformly charged to a high charge density. Preference will be given to materials that are readily available in Pantex bays and cells. A conductive material will then be brought into close proximity with the dielectric to determine how easily a conductor can pull charge from the dielectric and the characteristics of that current pulse, including amplitude and temporal characteristics, and deposited energy. Variables such as geometry, humidity (0-15%), temperature, material cleanliness, and porosity are also considered. A better understanding of dielectric discharge parameters for Pantex-specific materials would aid with electrostatic discharge (ESD)

calculation/modeling protocols, improve weapons response assumptions and eliminate unnecessarily conservative controls.

# 11. Continuous Wave Electromagnetic Field Effects on EED's

This project is a continuation of earlier NSR&D special-funded work to determine the effects of continuous wave electromagnetic sources (transmitters) on electrically-initiated electroexplosive devices (EEDs). The objective is to complete the computer modeling and physical validation of the models in order to relax standoff requirements between transmitters and EEDs. At issue are the actual effects to electrically initiated EED from the electromagnetic fields associated with radio frequency transmitters. The current approach to determining separation distances between EED's and transmitters uses highly conservative assumptions about the initiation energy of the device and the antenna configuration of the cabling attached to the device. This results in onerous controls that are purely administrative. It is possible that controls only need to be implemented for a limited number of components in a limited number of configurations, and may not be necessary at all.

# 12. Ceramic Ventilation Filters Deployed at Device Assembly Facility

This project supports deployment of a ceramic HEPA filter technology to benefit DOE nuclear facilities by reducing or eliminating certain safety basis costs associated with safety class and safety significant systems in nuclear facilities. This project involves field testing in a DOE nuclear facility and development of ventilation system designs and technologies that take advantage of the benefits offered by ceramic filters (e.g., a variety of on-line and off-line filter cleaning technologies). The technical objective of this project is to develop a template for deployment of ceramic HEPA filters in the DOE complex, to modify the design of an existing nuclear facility safety-significant HEPA-filtered ventilation system, then deploy, and in-situ test ceramic HEPA filters in a DOE/NNSA nuclear facility.

#### 13. Determination of ARF/RF for Use in Safety Basis Documents

The objective of this project is to determine the bounding (i.e., 95th percentile cumulative distribution) Airborne Release Fractions (ARF)/Respirable Fractions (RF) for thermal oxidation of uranium metal and uranium metal alloys resulting from a two-hour design basis facility fire event where bare uranium metal is subject to direct flame impingement. The project supports Y-12 Safety Basis Documents by repeating portions of experiments in DOE-HDBK-3010 simulating uranium metal response under catastrophic fire scenarios that led to the bounding values presented in the Handbook. The uranium samples used in testing exhibit characteristics representative of the bulk of the Y-12 inventory on a mass basis that could potentially be involved in the event (e.g., metallurgical phase, surface area to mass ratio, composition of alloys, etc.); the primary focus is on materials anticipated for use in meeting the Uranium Processing Facility design basis mission requirements. Long-term benefit to DOE includes facilitating revision of the uranium section of DOE-HDBK-3010 for use in developing safety bases complex wide.

# 14. Development of New Holdup Measurement System with Medium Resolution Detectors

This project supports development of a new Holdup Measurement System, using medium resolution gamma-ray detectors. The current Holdup Measurement System is based on sodium iodide detectors, which are low-resolution gamma detectors that only analyze the U-235 region in the gamma spectrum. Because of its low resolution, this system cannot distinguish the multiple gamma rays emitted by U-235. This forces the analyst to treat the entire U-235 region as a single peak. Moreover, the presence of U-238 and other isotopes is ignored, which means that the current system cannot measure the enrichment of in-situ material, nor provide a limited capability to identify other isotopes. The new system will be able to confirm the enrichment of *in situ* material and provide an enhanced capability to identify isotopes other than uranium. Consequently, it will improve the ability of nondestructive assay personnel to quantify, in the field, deposits of uranium and other radioactive materials, including those deposits that are dense or inhomogeneous.

# 15. In Situ NCS Holdup Monitoring System Upgrade

The objective of this project is to develop a modern, long-term sustainable Holdup Measurement System (HMS) for supporting *in situ* nondestructive assay (NDA) measurements of fissionable materials for nuclear criticality safety. HMS Version 4 (HMS-4) is the current "state-of-the-art" NDA system deployed in the field. Further, HMS-4 is a portable measurement system that has been used for years in DOE facilities to conduct passive NDA measurements for quantifying nuclear material residues held up, *in situ* in processes and equipment; however, HMS-4 is plagued with software/hardware compatibility issues that are not tenable for long-term NDA measurement system sustainability. The proposed work will result in the development of the next generation NDA measurement system (i.e., HMS-5).

#### 16. Validation of Hydrogen Exchange Methodology on Molecular Sieves for Tritium Removal from Contaminated Water

The technical objective of this R&D effort is to evaluate various platinum (Pt)-catalyzed molecular sieve materials to determine their hydrogen isotope exchange efficiency, with the eventual goal of using these materials to effectively remove tritium from contaminated water in various facilities in the DOE complex and commercial entities. In addition, this technology could be used to successfully remove tritium from contaminated groundwater. The Pt-catalyzed molecular sieve material will be evaluated using protium (H<sub>2</sub>), deuterium (D<sub>2</sub>), and tritium. In addition, the project will determine the optimum catalyst level needed to maximize the hydrogen exchange efficiency with a minimal amount of Pt. Previous studies were only able to detect about 1% D<sub>2</sub> in the effluent. In order for this process to be applicable for the removal of tritium from contaminated water, it is necessary to determine the amount of exchange gas needed to reduce the amount of heavy isotope to parts per million levels on the molecular sieve bed. The successful demonstration of this technology could eliminate the use of magnesium beds in facilities that process tritiated water (especially the Savannah River Site (SRS) Tritium Facilities). This would result in a significant reduction in the amount of radioactive waste generated.

#### 17. Development of a Safe Disposition Path for Tritiated Hydride Storage Material

The technical objective of this NSR&D effort is to develop an experimentally based oxidation strategy for end-of-life hydrogen storage bed material. This technology will be used to provide a safe disposal path for hydride beds retired from service at the SRS Tritium Plant. The activity consists of performing recovery of a tritium aged sample and thermogravimetric analysis (TGA) with mass spectrometry (MS). Recovery of a tritium aged sample will be accomplished by performing a series of isotopic dilutions with deuterium to reduce the tritium concentration in the sample to acceptable levels. Tritium concentration will be tracked via high resolution mass spectrometry. Oxidation testing will consist of heating the sample at a prescribed temperature ramp in the presence of an oxygen containing gas. Changes in mass will be detected by the TGA while the composition of the TGA effluent will be monitored by the MS. The successful demonstration of this technology will allow the SRS Tritium Plant to simultaneously eliminate concerns related to pressure buildup and potentially pyrophoric materials to support safe disposal of the beds in a timely manner.

#### 18. Non-Linear Seismic Soil Structure Interaction Analysis of Nuclear Facilities

The focus of this research is to develop and document a method for performing time domain, non-linear seismic soil structure interaction (SSI) analysis. Non-linear SSI analysis will provide a more accurate representation of the seismic demands on nuclear facilities and their systems and components, and, for intense ground motions, lower in-structure response spectral ordinates. This method will accommodate both geometric non-linearity (e.g., separation of structure and soil) and material non-linearity in the soil and structure. Developing a robust non-linear method for SSI analysis of DOE-regulated nuclear facilities should typically lower the in-structure response of facilities during design basis shaking and improve the safety basis by providing a better understanding of its response during earthquake shaking.

# Appendix E

# **Office of Nuclear Energy Projects**

Project Title: Advanced Test Reactor Core Modeling Update Project

Headquarters Element(s): NE

#### Site(s) Involved: INL

**Project Description and Technical Objective:** This research is modernizing the computational reactor physics tools and validation protocols needed for support of ongoing Advanced Test Reactor (ATR) operations as well as for new applications. The new computational methods and verify and validate (V&V) protocols will be broadly applicable across all programs that use the ATR and ATR Criticality Facility (ATRC). Accomplishments have encompassed computational as well as experimental work. A new suite of stochastic and deterministic transport theory based reactor physics codes and their supporting nuclear data libraries have been installed at the INL. Models of the ATR and ATRC are now operational with all seven codes, demonstrating the basic feasibility of the new code packages for their intended purpose. Acquisition of Monte Carlo stochastic neutronics simulation codes has also been completed and some basic analysis for validation purposes has been demonstrated. These offer significant additional capability, including the possibility of fully integrated 3D Monte Carlo core fuel management and experiment management support capabilities for the ATR at an appropriate point in the future

A complete statistical analysis of the first ATRC physics code validation measurements was completed in 2012 in accordance with applicable national and international standards. Validation will continue with another experiment in 2014, which will include the introduction of additional new experimental hardware to broaden the scope of the validation protocols. An additional experimental validation campaign involves the possible construction of a system for non-invasive measurement of the burnup of ATR fuel elements *in-situ* in the ATR canal. Post-irradiation non-invasive ATR fuel burnup measurements will serve as a key fuel depletion model validation tool and also as an aid in improved fuel management.

**Drivers:** Legacy computational reactor physics software tools and protocols currently used for support of ATR core fuel management and safety assurance, and to some extent, experiment management, are inconsistent with the state of modern nuclear engineering practice, and are difficult, if not impossible, to V&V according to modern standards.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** Key enhanced capabilities include: Implementation of complementary, self-consistent multidimensional stochastic and deterministic neutron transport models of the ATR and ATRC; development of standardized computational procedures and training, more easily transferred to new staff members; additional ATR core physics V&V for detailed neutron flux distribution and spectrum validation measurements in the core; and selected flux traps that can be adapted as needed for changing experimental conditions and repeated on a regular basis.

**Highlights of the Research:** The ATR Core Modeling Update Project, targeted for full implementation in the 2015-2016 time frame, began during the last quarter of Fiscal Year 2009, and is now in its fifth full year. Key accomplishments have encompassed both computational as

well as experimental work. A new suite of stochastic and deterministic transport theory based reactor physics codes and their supporting nuclear data libraries has been installed at the INL under various licensing arrangements. Corresponding models of the ATR and ATRC are now operational. An updated set of as-run core depletion calculations for all ATR cycles since August 2009, through the current cycle has been successfully completed, with excellent statistical consistency between calculation and measurement. There is now a formal phased incorporation of this methodology into the ATR Core Safety Analysis Package (CSAP) preparation process.

On the experimental side of the project, a complete statistical analysis of the first four of six planned application-specific ATRC physics code validation measurements based on neutron activation spectrometry was completed in 2012.

**Completion Date:** Establishment of all basic new technical capabilities and protocols is expected to be completed by the end of FY 2014. This will enable a phased incorporation of the new methodology into production use during FY 2015.

Project Title: Analysis of Methods for Assessing Storage Containers at the TREAT Warehouse

#### Headquarters Element(s): NE

#### Site(s) Involved: INL

**Project Description and Technical Objective:** The purpose of this research was to assess different technical approaches for determining the location and spacing of low-enriched uranium (LEU) ingots stored within Outer Waste Canisters (OWCs) (also called spent fuel treatment product (SFTP) storage containers) at the INL's Transient Reactor Experiment and Test (TREAT) Facility warehouse. These LEU ingots are recovered from irradiated, sodium-bonded fuel during treatment operations conducted at INL's Fuel Conditioning Facility (FCF). A one-dimensional (1-D) scanning technique was demonstrated to meet the measurement requirements; this technique was able to confirm that the minimum spacing between ingots is greater than 20 cm. As demonstrated during these tests, the 1-D scanner was able to locate the edge of each ingot with a precision defined as one-half of the full-width half maximum (FWHM) of the system, 2.75 cm. This precision, when doubled to account for the measurement of the adjacent edges of two ingots, is 5.5 cm, well less than the engineered excess separation of 5.375 in (13.6 cm) of the as-designed uranium product storage (UPS).

**Drivers:** A recently completed Criticality Safety Evaluation for storage of LEU ingots in the TREAT warehouse established that the ingots within the OWCs should be separated by a minimum distance of 7.875 in (20 cm) when in UPS containers and 14 in (35.6 cm) when in high-throughput uranium product (HUP) storage containers. These containers are stacked within the cylindrical OWCs and are designed to maintain a criticality-safe spacing between ingots.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** This scanning technique has the following advantages for configuring LEU storage containers for interim storage: ability to meet the technical measurement requirements; reduced ALARA, i.e., how much personnel radiation exposure will be expected; reduced labor costs for preparation, better material and equipment costs; reduced labor requirements for execution.

**Highlights of the Research:** As demonstrated during these tests, the 1-D scanning technique was able to locate the edge of each ingot with a precision defined as one-half of the full-width half maximum (FWHM) of the system, 2.75 cm. This precision, when doubled to account for the measurement of the adjacent edges of two ingots, is 5.5 cm, well less than the engineered excess separation of 5.375 in (13.6 cm) of the as-designed UPS.

**Project Title:** Neutron Irradiation of Luna Innovations Incorporated (Luna) Innovations Optical Fibers

#### Headquarters Element(s): NE/ (SBIR)

#### Site(s) Involved: INL

**Project Description and Technical Objective:** The goal of the Luna experiment is to irradiate optical fibers at a fluence of at least 6.0E+20 n/cm2 (>0.1 MeV) and temperatures of 800 °C and 1000 °C. This irradiation is to characterize performance and limitations of the optical fibers at temperatures and neutron fluence levels typical of future high temperature gas reactors. Extra optical fibers may be included in additional capsules placed above and below the five prime capsules, and these additional capsules may achieve fast neutron fluences below the minimum requested by Luna due to the axial flux profile of the ATR core. The Luna specimens (sensor packages) consist of a quartz rod approximately 0.070-inch diameter x 3.5-inch long housed inside a vanadium protective sleeve. The sensor packages will be provided whole by Luna. INL is recording all specimen serial numbers versus capsule assignment. To achieve the appropriate fluence levels, the Luna experiment is being irradiated for one standard ATR reactor cycle of 45-to-50 days' duration, with a northwest lobe power of 20-to-23 MW nominal.

**Drivers:** Luna, a research and development corporation headquartered in Roanoke, Virginia, has developed thermal sensors based on fiber optic technologies. Testing conducted to date at Ohio State University indicates that these sensors are promising candidates for use in high temperature Gen-IV reactor designs. Luna Innovations has received Small Business Innovation Research (SBIR) Phase III funding under the DOE's Accelerator program to bring their low drift thermal sensors to a product stage of development for use in Gen-IV reactor designs.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** Robust and reliable, low-drift thermal sensors based on fiber-optic technologies will have multiple applications inside the harsh environments of DOE nuclear facilities.

Highlights of the Research: N/A

Completion Date: July 30, 2017

**Project Title:** On-Line Monitoring (OLM) Technology for Aging Management and Life Extension of the Advanced Test Reactor (ATR) at Idaho National Laboratory

**Headquarters Element(s)**: NE/(SBIR)

Site(s) Involved: INL

**Project Description and Technical Objective:** This research and development (R&D) effort was aimed at implementing existing on-line monitoring (OLM) technology at research reactors. A few key systems were selected of OLM technologies were selected for testing. They included the primary coolant system temperature sensors, Resistance Temperature Detectors (RTDs), and transmitters (pressure, level, flow).

The OLM applications that Analysis and Measurement Systems Corporation (AMS) evaluated for use at the ATR include:

• On-line calibration monitoring of pressure transmitters using data from plant computers;

• Response time (dynamic performance) tests of pressure transmitters using noise analysis technique;

• Response time testing of Resistance Temperature Detectors (RTDs) using the Loop Current Step Response (LCSR) and self-heating tests; and

• On-line calibration monitoring of RTDs using the cross calibration technique.

**Drivers:** Over the last decade, OLM technologies have become prevalent in most industrial processes including nuclear power plants for equipment and process condition monitoring, predictive maintenance, aging management, equipment reliability assessment, and life extension. However, research reactors have not yet received the full benefit from all that OLM can offer. This R&D is adapting an existing array of OLM technologies to the needs of research reactors with specific emphasis on performance monitoring of Instrumentation and Control (I&C) systems, with ATR serving as the primary test bed.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** Better monitoring for the ATR and for DOE-sponsored research reactors will result in improved safety at these facilities. Also, an ongoing adaptation of these types of monitors could also result on monitors for use in other DOE nuclear facilities.

**Highlights of the Research:** All of the OLM applications were found acceptable and recommended for use at ATR. There is some ongoing work to improve the equipment reliability of these components. Steps are being taken to implement these OLM applications for use at ATR.

Project Title: Risk Informed Safety Margins Characterization (RISMC) Pathway

Headquarters Element(s): NE

Site(s) Involved: INL

**OSTI Identifier:** # 1115616

Project Description and Technical Objective: Central to nuclear reactor safety is the concept of a safety margin. In general terms, a "margin" is usually characterized in one of two ways: A deterministic margin, defined by the ratio (or, alternatively, the difference) of an applied capacity (i.e., strength) to the load. For example, we test a pressure tank to failure where the tank design is rated for a pressure C, it is known to fail at pressure L, thus the margin is (L - C) (safety margin) or L/C (safety factor). A probabilistic margin is defined by the probability that the load exceeds the capacity. For example, we model failure of a pressure tank where the tank design capacity is a distribution f(C), its loading condition is a second distribution f(L), the probabilistic margin would be represented by the expression Pr[f(L) > f(C)]. In practice, actual loads (L) and capacities (C) are uncertain and, as a consequence, most engineering margin evaluations are of the probabilistic type (in cases where deterministic margins are evaluated, the analysis is typically very conservative in order to account for uncertainties). The RISMC Pathway uses the probability margin approach to quantify impacts to economics, reliability, and safety in order to avoid conservatisms (where possible) and treat uncertainties directly. Further, we use this approach in risk informed margins management to present results to decision makers as it relates to margin evaluation, management, and recovery strategies.

**Drivers:** Safety is central to the design, licensing, operation, and economics of nuclear power plants and other nuclear reactors. As many reactors age beyond 60 years, there are possibilities for increased frequency of systems, structures, and components (SSC) degradations or failures that initiate safety significant events, reduce existing accident mitigation capabilities, or create new failure modes. Plant designers commonly "over-design" portions of reactors and provide robustness in the form of redundant and diverse engineered safety features to ensure that, even in the case of well-beyond design basis scenarios, public health and safety will be protected with a very high degree of assurance. This form of defense-in depth is a reasoned response to uncertainties and is often referred to generically as "safety margin." Historically, specific safety margin provisions have been formulated primarily based on "engineering judgment." Further, these historical safety margins have been set conservatively (for example in design and operational limits) in order to compensate for uncertainties. Since safety is important to successful operation of nuclear reactor, there are strong motivations to better characterize and manage safety and its associated "margin."

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** The ability to better characterize and quantify safety margin is important to improved decision making about nuclear reactor design, operation, and plant life extension. A systematic approach to characterizing safety margins and the subsequent margins management options represents a vital input to the regulatory analysis and decision making that will be involved.

**Highlights of the Research:** The RISMC tool has been used to assess leading accident resistant fuel technologies to understand potential changes in safety; INL has completed the software structure of the coupled RAVEN/RELAP-7 portion of the RISMC Toolkit and demonstrated RISMC approach using LWR Case Study for Enhanced Accident Tolerance design changes using Risk-Informed Margins Management approaches.

Project Title: Transuranic Surveillance Glovebox Project

## Headquarters Element(s): NE

## Site(s) Involved: INL

**Project Description and Technical Objective:** The Transuranic Surveillance Glovebox (TSG) will be a system of interconnected equipment components that will establish a very specific work platform that provides radiological containment and an inert atmosphere for transuranic material surveillance and repackaging. This equipment will complement existing hood capabilities that do not provide adequate protection when opening secondary containment of transuranic material to inspect primary packaging that may be suspect. The TSG will provide defense-in-depth as an additional confinement barrier in those situations.

**Drivers:** This project is needed to develop better radiological containment and an inert atmosphere for transuranic material surveillance and repackaging. These needs include: routine surveillance such as opening overpacked primary containers and packages containing clad radioactive materials, performing contamination swipes, verifying integrity of the cladding, and closing packages; characterization and repackaging of transuranic material when the condition of the primary confinement (cladding or primary canister) is intact; providing a defense-in-depth confinement barrier for radioactive or hazardous materials used in the hood and surveillance glovebox; allowance of ingress and egress of materials, small equipment, and waste between the surveillance glovebox and the facility; providing atmospheric pressure control, purification, recirculation, and associated monitoring systems for the glovebox; and providing heat (fire) detection, atmosphere sampling, and data acquisition signals to support glovebox and hood activities.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** This new glovebox capability will provide a platform to enable enhanced surveillance and repackaging of transuranic material in the INL's Zero Power Physics Reactor (ZPPR). It also will provide a platform for repackaging of programmatic transuranic material for offsite shipments to meet mission critical commitments of special nuclear material to the Department of Energy (DOE).

# Appendix F

#### Nuclear Safety Related Laboratory and Plant Directed Research and Development Projects

Project Title: Advanced 3D Characterization and Reconstruction of Reactor Materials

Headquarters Element(s): NE/ INL LDRD

Site(s) Involved: INL (and Washington State University)

**Project Description and Technical Objective:** This research is developing a critical line of inquiry that integrates advanced materials characterization techniques developed for reactor materials with state-of-the-art mesoscale modeling and simulation tools. This project proposes steps to address current characterization limitations and to enhance characterization and reconstruction capabilities, in order to allow for efficient characterization of reactor microstructures and their reconstruction using INL's MARMOT modeling and simulation software. This three-year project consists of three key objectives that will push the limits of present technology, including:

1) Explore new sample preparation techniques for reactor materials using broad beam ionetching methods to decrease sample preparation time, improve scan quality, increase scan size, and reduce radiation exposure/waste;

2) Implement an advanced characterization technique known as High-Resolution Electron Backscattered Diffraction (HR-EBSD) to enable estimation of critical material properties like dislocation density and residual strain from reactor materials; and

3) Develop necessary post-processing tools and procedures to utilize the HR-EBSD data obtained in Objective 2 for microstructure reconstruction into MARMOT and perform model validation based on the HR-EBSD data.

**Drivers:** This research is important because the development of advanced characterization and reconstruction techniques is essential to understanding and predicting the behavior of reactor materials operating in severe conditions.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** Enhancing modeling and experimental capabilities is critical to understanding material behavior at extreme conditions, thus improving the safety of new materials and reducing costs of materials used in energy applications. The research is applicable to a wide range of material problems, including: new fuel development, spent fuel analysis, and fuel storage assessment. Improved materials may add value for maintenance and upgrade of the INL Advanced Test Reactor (ATR)

**Highlights of the Research**: None to date, as this is a new project. However, it will provide training for the next generation of nuclear scientists through university collaboration with Washington State University.

Project Title: Advanced Fracture Modeling for Nuclear Fuel

Headquarters Element(s): NE/ INL LDRD

## Site(s) Involved: INL

**Project Description and Technical Objective**: Fracture in nuclear fuel plays an important role in its thermo-mechanical response at multiple time scales. The techniques currently employed for modeling fuel fracture use empirical equations that are inherently applicable only for a limited range of conditions. This research will apply predictive fuel modeling capability and physics-based techniques for modeling fracture and relocation that are less sensitive to the specific computational framework being used.

This work will apply advanced fracture modeling techniques in the BISON fuel performance code to model fuel fracture in a physically-based manner in ways that are less sensitive to the computational mesh. This improved fracture modeling capability will provide a stronger physical basis for fuel modeling in both normal and accident conditions. It will allow for modeling of fuel having geometries and computational meshes that differ from those for which relocation models were developed. Most importantly, this work will also improve predictivity of fuel behavior during postulated accident scenarios, which will facilitate the development of more accident-tolerant fuel designs.

**Drivers:** The performance of nuclear reactor fuel is heavily influenced by fracture of the ceramic fuel pellets, both at the engineering scale and at the mesoscale. In addition to affecting the thermal conductivity of the material and the expansion of the fuel pellets, fuel cracking plays an important role in cladding failures induced due to pellet-clad mechanical interaction. The combined effects of thermal expansion in the pellet, frictional contact between the pellet and clad, and the presence of the crack in the pellet cause a stress concentration in the cladding immediately adjacent to the location of the crack in the pellet. This stress concentration, potentially in combination with chemistry favorable to stress corrosion cracking, can lead to the formation of a through-crack in the cladding and subsequent leakage. Cracking is also a significant factor in fuel behavior during a reactivity insertion accident (RIA) or a loss of coolant accident (LOCA). Both of these can lead to cladding ballooning accompanied by extensive fuel relocation, which is highly effected by fuel fracture. If a cladding actually ruptures, the dispersal of the fuel fragments is also highly influenced by the fracture pattern in the fuel.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** The ability to model the behavior of nuclear fuels in accident conditions. Fuel fracture plays a fundamental role in the behavior of nuclear fuel under both normal operation and under accident conditions. Improvements in our ability to model fuel fracture will provide a stronger basis for predictive simulations of fuel designs and accident scenarios. Improved fuel modeling will help improve the efficiency and safety of nuclear reactor operation. Also, improved understanding of fuel behavior will lead to designs that use fuel more efficiently, which will help minimize nuclear waste.

**Highlights of the Research:** To date, researchers have developed the extended finite element method (XFEM) to rigorously treat the effects of cracking as a strong discontinuity within the elements traversed by a crack. This method overcomes the mathematical dependencies inherent in earlier smeared crack modeling approaches. It permits cracks to be modeled discretely, but allows them to propagate arbitrarily through the mesh without regard to the locations of finite element boundaries; i.e., cracks are modeled in a physically realistic way.

Project Title: Advanced In-Situ Measurement Techniques in TREAT

Headquarters Element(s): NE/ INL LDRD

## Site(s) Involved: INL

Project Description and Technical Objective: This project focuses on Transient Reactor Experiment and Test (TREAT) core configurations that can facilitate high-resolution, in-situ measurements on smaller, specially prepared samples, and on the feasibility of mating current micro-structure measurements technologies and techniques to the new experimental environment. The results will be made available as an engineering report on a science-based irradiation facility in the TREAT reactor and a scientific report on the feasibility of current micro-structure measurement technologies and techniques and their integration into the proposed irradiation environment in TREAT. This research will provide a proof of concept for delivering advanced science-based information on in-situ fuel performance and underlying phenomena. An analysis including neutronics modeling and simulation will be performed to determine the spatial and temporal resolution requirements for high-fidelity imaging and microstructure characterization of fuel samples within the modified TREAT configuration and line-of sight access to the pile. The analysis will produce a framework for the detection and imaging requirements that can be implemented alongside nominal TREAT operations with improved functionality for science-based in-situ studies. In this way, both the macroscopic and the microstructure behavior of the fuel can be studied simultaneously under the same power profile. Two areas of research development will be considered for eventual integration into an advanced microstructure imaging and characterization capability for the TREAT reactor facility.

**Drivers:** DOE-NE is considering the restart of transient fuels testing in order to develop more accident tolerant fuels. The proposed advanced measurement techniques would increase the scientific data available during those irradiations. Real time, microstructure characterization during irradiation would provide scientific understanding of fuel behavior for the development of predictive modeling and simulation for fuels, including performance under accident conditions.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** Better in-situ measurements and modeling will facilitate the safer and more efficient operation of DOE's transient testing program.

Highlights of the Research: None: new project.

Project Title: Advanced Seismic PRA

## Headquarters Element(s): NE/ INL LDRD

## Site(s) Involved: INL

**Project Description and Technical Objective:** This research will demonstrate the capability for performing advanced seismic probabilistic risk assessment (SPRA) using INL's Multiphysics Object Oriented Simulation Environment (MOOSE) framework. It will build on the Risk Informed Safety Margin Characterization (RISMC) toolkit under development in the Light Water Reactor Sustainability (LWRS) program. This will be accomplished by forming a team of qualified individuals at universities and INL to implement an advanced SPRA methodology. The focus of this project is producing best estimate SPRA's by developing a structural dynamics capability using the MOOSE framework coupled with ESSI (nonlinear stochastic seismic analysis code). This provides the user with the capability to provide an accurate, stochastic representation of a nuclear facility response during earthquakes.

Development of this capability will fill a current gap in available finite element codes by coupling the structural dynamics capability with stochastic elasto-plastic finite elements, and implementation of an advanced seismic PRA methodology. These capabilities will be developed and implemented using the MOOSE framework so that the structural dynamics capability can be coupled with other physics to perform additional simulations such as thermal hydraulic shock.

**Drivers:** The nuclear industry is currently addressing the Near Term Task Force (NTTF) recommendations. One specific recommendation that they are dealing with is recommendation 2.1, which states, "Order licensees to reevaluate the seismic and flooding hazards at their sites against current NRC requirements and guidance, and if necessary, update the design basis documents important to safety to protect against the updated hazards. The screening re-evaluation process includes the following steps:

- 1. Develop new site specific hazard curves based on the Central and Eastern United States Seismic Source Characterization for Nuclear Facilities (CEUS);
- 2. Utilize screening process to eliminate certain plants from further review;
- 3. Perform SPRA or SMA; and
- 4. Submit proposed actions to evaluate seismic risk contributions (update seismic analysis where necessary).

The updated site-specific hazard curves have potential for higher magnitude, higher frequency content accelerations. This would cause site-specific seismic PRA parameters such as peak ground acceleration (PGA) to increase. The increase creates a potential for the core damage frequency numbers in these SPRA's to increase beyond what NRC sets as an acceptable limit.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** While this project was developed to address commercial nuclear power plants, it seems likely that the revised seismic risk assessment requirements could be applied to DOE nuclear facilities as well, in which case newer, more accurate modeling and simulation tools will be beneficial. For example, The Advanced Test Reactor (ATR) at INL recently had "state of the art" SPRA analysis performed. This project will develop a more advanced, higher fidelity approach to SPRA for safety systems for the ATR and other DOE nuclear facilities.

Highlights of the Research: None: new project

Project Title: Alert/Alarm Dashboard

# Headquarters Element(s): NE/ INL LDRD

# Site(s) Involved: INL

**Project Description and Technical Objective:** The focus of the research is to develop first principles of alarm management that will help establish the technical basis for the design of new alarm systems at nuclear facilities. The short-term and longer-term objectives are:

• Evaluation of alarm management system technologies. INL and the University of Idaho (UI) are evaluating various alarm management system principles and technologies, deploying them on the simulator, developing a test plan for testing operator performance with these systems, and disseminating the findings to the plant.

• Deployment of a microworld simulator model for nuclear power plant process control A microworld simulator represents a simplified form of the process control system that may be tailored to less skilled operators. Because full-scope simulator testing requires extensive setup and is prohibitively expensive, there is a great opportunity to develop a simplified model that may be used for first principles research and generalized to nuclear operations.

A full-scope plant simulator comprises several layers of systems. At the heart are system models that interact to create a realistic model of plant behavior, including thermal-hydraulic software modeling using RELAP thermal-hydraulic modeling software, a simulator and a plant- specific model executed on the simulator platform. These models combine to form the back end called the engineering simulator. The engineering simulator interfaces with the front-end simulator, which consists of the control room human-system interface (HSI) that the operator uses to understand plant states and control plant functions.

**Drivers:** There are human engineering deficiencies associated with conventional alarm systems in nuclear power plants (NPPs), including analogue alarm systems that fail to enhance the operators' situation awareness and that provide no ready means of prioritization. The need to improve the human factors engineering of alarm systems has led to the development of advanced alarm systems in which alarm data are processed beyond the one sensor, one alarm framework. Alarm system effectiveness continues to be a problem in many facilities. Under typical normal operations and minor transients the alarm systems function well. However, the alarm avalanche that occurs during major transients and accidents is commonly recognized as a problem area that needs to be addressed.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** Improved alarm systems and response time to off normal or critical events.

**Highlights of the Research:** Initial phase development of a microworld simulator model for nuclear power plant process control. A microworld simulator represents a simplified form of the process control system that may be tailored to less skilled operators.

**Project Title:** Concurrent Atomistic-to-Macroscale Modeling of Materials under Irradiation Using the Phase Field Crystal Model

#### **Headquarters Element(s)**: NE/ INL LDRD

#### Site(s) Involved: INL and ANL

**Project Description and Technical Objective:** The aim of this research is to create a first-ofits kind multiscale model of irradiation damages which have a large impact on material behavior, leading to material swelling and embrittlement, as well as significant changes in material properties such as thermal conductivity. The proposed model will span the atomistic to the macroscale level. This will be accomplished by building on progress from an earlier project focused on coupling the mesoscale MARMOT code to the macroscale BISON code. The project will extend the existing multiscale framework to the atomistic-scale by implementing the recently developed phase field crystal (PFC) model. The PFC model will be directly coupled to the traditional phase field (PF) models already implemented in MARMOT, and then further coupled to the macroscale BISON code. Specifically, we will employ this proposed innovative multiscale capability to model the early stages of irradiation. By coupling the PFC model to traditional PF models to study the early stages of irradiation, we will elucidate the interaction between microstructure and void nucleation. This high-fidelity multiscale model will play a role in identifying critical phenomena that have a high impact on the continuum material response.

**Drivers:** Radiation damage has a large impact on material behavior, leading to material swelling and embrittlement, as well as significant changes in material properties such as thermal conductivity. These material changes have the potential to lead to safety problems in power reactor operations. While material changes are observed at the macroscale, they are caused by the generation and migration of point defects at the atomic scale. Thus, to capture the effects of radiation damage at the macroscale, especially during the early stages of radiation, atomistic information must be integrated into the model. This research will provide a state-of-the-art capability to predict material behavior during the early stages of radiation. This capability will be a resource in designing fuel and structural materials that are more radiation resistant, improving the inherent safety of nuclear reactors.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** Improved safety of fuels and structural materials in nuclear facilities.

**Highlights of the Research:** The phase field crystal approach is being implemented using implicit time integration. Thus, each time step will require a numerical solution of a system of tightly coupled nonlinear equations. The MOOSE model is using the PETSc linear/nonlinear solver from Argonne National Laboratory (ANL) to solve the system of nonlinear equations resulting from the discretization of the model PDEs. While PETSc provides powerful solvers for the system of PDEs, research is ongoing on developing an efficient and scalable solver for the PFC model at adequate resolution.

**Project Title:** Development and Validation of a Societal-Risk Goal for Nuclear Power Plant Safety

#### **Headquarters Element(s)**: NE/ INL LDRD

#### Site(s) Involved: INL

**Project Description and Technical Objective:** The objective of this work is to evaluate the social disruption effects from severe reactor accidents as a basis for developing a societal-risk goal for nuclear facilities. This work would consider health effects and non-health concerns like property damage and land interdiction. The research will use data on accident consequences at various reactor sites in the U.S., to assess its reasonableness, and the implications of concern about societal risk for nuclear-power regulation.

This project is analyzing the possible societal disruptions that could occur from nuclear-power accidents, both past accidents and potential future accident scenarios. It will then structure a proposed societal-risk goal for nuclear-power plants, relying on the idea of value structuring from decision analysis. The goal will be calibrated based on consequence assessments for U.S. nuclear-power plants in areas with differing land values and population densities. Finally, we will evaluate the implications of the recommended societal-risk goal for regulation.

**Drivers:** Enabling deployment of new nuclear energy sources is fundamental to the mission of DOE, to "Catalyze the timely, material, and efficient transformation of the nation's energy system and secure U.S. leadership in clean energy technologies," but has been complicated by events at Fukushima. The importance of societal risk is pronounced at present, since the Fukushima accident has reawakened public concern about the potential for beyond-design basis accidents (i.e., severe accidents). This creates changes in required safety measures and/or siting policies for next-generation nuclear plants (integral small modular LWRs, very-high-temperature gas-cooled reactors, fast reactors as well as fluoride-salt-cooled reactors) as well as for DOE facilities. Fukushima has shown that even if a severe accident does not cause early fatalities or latent health effects, its societal impact can be large due to environmental impacts. The project will assist in development of more risk-informed design specifications for next-generation technologies.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** Better understanding of risk at nuclear facilities and enhanced stakeholder outreach on nuclear safety.

**Highlights of the Research**: Progress on developing a candidate structure for a societal-risk goal for nuclear-power plants, relying on the idea of values structuring from decision analysis. This includes health and mortality objectives (such as acute and latent fatalities), land-related objectives (such as property damage and land interdiction), environmental objectives (such as ecosystem damage and cleanup), and social disruption (such as evacuation or damage to infrastructure services).

**Project Title:** Development of a Multiphysics Algorithm for Analyzing the Integrity of Nuclear Reactor Containment Vessels Subjected to Extreme Thermal and Overpressure-Loading Conditions

#### Headquarters Element(s): NE/ INL LDRD

Site(s) Involved: INL

**Project Description and Technical Objective:** The technical objective of this research is to develop a first-of-its kind multiscale, multiphysics algorithm for analyzing the integrity of nuclear reactor containment vessels subjected to extreme thermal and overpressure-loading conditions. The various specific physical phenomena to be considered in developing an algorithm for analyzing nuclear containment events are:

1. Single phase, multi-component, and multiphase flow and transport;

- 2. Chemical reactions, including combustion, and deflagration to detonation transition;
- 3. Shock wave formation and propagation;

4. Conjugate heat transfer, including solid-state and hydrodynamic heat conduction, forced and natural convection, and thermal radiation; and

5. Fluid-structure interaction (thermo-mechanical-hydrodynamic coupling).

Simulations include multi-phase fluid flow, heat transfer (heat conduction, forced and natural convection, and thermal radiation), fission product transport and deposition, hydrogen transport and detonation, chemical reactions, and thermo-mechanical responses (fluid-structure interaction). The model will encompass the millimeter scale to hundred-meter scale, including boundary layers from small scales such as condensation layer with non-condensable gas and hydrogen plumes to large-scale simulations such as the entire containment recirculation pattern. In with this new model, a true three-dimensional analysis capability will be realized

**Drivers:** There are no current simulations for analysis of nuclear reactor containment vessel for extreme thermal and overpressure effects with a strongly coupled multiphysics algorithm. Successfully developing an advanced and more realistic multiphysics thermo-mechanical and hydrodynamic algorithmic approach for containment vessel extreme thermal and overpressure-loading conditions will improve safety at DOE and NNSA nuclear reactors.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** Successfully developing more realistic modeling and simulation for containment vessel extreme thermal and overpressure-loading conditions will improve safety at DOE and NNSA nuclear reactors.

Highlights of the Research: None- newly initiated research

**Project Title:** End-to-End Radiation Detector Enhancements for Improved Safety and Security in Safeguarded Facilities

#### Headquarters Element(s): NE/ INL LDRD

#### Site(s) Involved: INL

**Project Description and Technical Objective:** The project's primary focus will be a parameterized study to optimize scintillator-based radiation detection methods. This work will begin by focusing on polyvinyl toluene based organic scintillators, allowing for prototypes to be inexpensively manufactured at INL. Modeling efforts will utilize Geometry and Tracking (GEANT) 4's ability to simulate the generation and transport of visible light. Parameter space for this study will include crystal size and shape, reflective/absorptive crystal coatings, light collection methods, and high-Z elemental doping for improved Compton edge discrimination. A substantial enhancement in detection sensitivity and operational efficacy of scintillation based sensors can be achieved through the optimization of currently available scintillating materials and detection methodologies. This research perform an end-to-end optimization study to increase the detection sensitivity and data security of scintillation detectors commonly used in nonproliferation, global, and facility security applications.

**Drivers:** Recent shortages in <sup>3</sup>He have brought about a substantial amount of research and development focused on organics and other scintillating compounds with the ability to efficiently detect neutrons, and in many cases, differentiate neutrons from photons. An increase in detection sensitivity, and potentially isotopic specificity, will allow for the detection of smaller amounts of radioactive materials, reducing the risk of material theft while also reducing false alarm rates. Improved detector performance can also lead to improved tools for radiological protection and health safety.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** An increase in detection sensitivity, and potentially isotopic specificity, will allow for the detection of smaller amounts of radioactive materials, reducing the risk of material theft while also reducing false alarm rates. Improved detector performance can also lead to improved tools for radiological protection and health safety.

Highlights of the Research: None-newly initiated research

Project Title: Epistemic Uncertainty Quantification in Dynamic Probabilistic Risk Assessment

**Headquarters Element(s)**: NE/ INL LDRD

## Site(s) Involved: INL

**Project Description and Technical Objective:** Dynamic Probabilistic Risk Assessment (DPRA) provides a more rigorous analysis of complex dynamic system as opposed to more traditional PRA methods. A major advantage of dynamic PRA is the explicit coupling required between simulation tools such as RELAP and the risk analysis code. The objective of this research is to develop a methodology and algorithm to quantify the time dependent epistemic uncertainty within a DPRA framework. The methodology can be used to support risk informed decisions with regards to plant operations, experiment design, and viability of modeling and simulation needs. Traditionally, within the PRA methodology, epistemic uncertainty is treated only in general and typically based on a Phenomena Identification and Ranking Table (PIRT), which is typically based on expert judgment. This proposed work will provide for a means to establish a Quantified PIRT (QPIRT).

The methodology developed from this research is cross-cutting across many risk-based hard and soft industries. It is of relevance and significance to reactor technologies as well as risk analysis in the air, chemical, petroleum and even financial sectors. It can directly impact the interface of nuclear, renewable and linked process plants; thus safety issues of hybrid and process energy systems. The algorithms developed can be incorporated into code development currently supporting LWRS, CASL, CAMS and the ATR LEP. The research is intended to 'bridge the gap via code development and experimental designs (and practice) to support not only the DOE, but also the commercial energy, and risk-inherent laboratories and industries such as the INL itself.

**Drivers:** Better risk assessment is needed for quantifying epistemic uncertainty will improve modeling fidelity, which then can be tested with experimental validation, and against plant operating conditions. The overall objective is to focus on areas where risk can be improved with regards to uncertainty in modeling. By quantifying uncertainty in the modeling tools with regards to risk, users can focus resources in design of experiments, improve computational models, and improve operating conditions.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** This research will be used to support risk informed decisions with regards to operation of DOE and NNSA nuclear facilities, and the viability of modeling and simulation needs.

**Highlights of the Research:** An initial methodology for performing forward sensitivity analysis in uncertainty quantification has been developed and adapted for High Performance Computing (HPC).

**Project Title:** Experimental and Computational Analysis of Hydride Microstructures in Zirconium in Dry Storage Conditions

#### Headquarters Element(s): NE/ INL LDRD

#### Site(s) Involved: INL

**Project Description and Technical Objective:** The objective of this research is to establish a state-of-the-art program to computationally and experimentally predict zirconium embrittlement and failure due to hydride re-orientation for wet and dry fuel storage conditions. Extending the dry storage period of fuel at reactor utilities presents large uncertainties with respect to the integrity of the cladding material, particularly for high burn-up fuels. In order to save cost and time, it is desirable to determine how accurately accelerated experiments, involving elevated temperatures and/or radiation fields, represent actual dry storage conditions over a 60-year time frame. During dry storage, Zr hydrides that have developed in the cladding in-reactor have been shown to re-orient from a longitudinal direction to a radial direction; this is an undesirable change that results in severe embrittlement and potentially a complete breach of the cladding. This re-orientation of the hydride is facilitated by changes in temperature and the stress state. In order to accurately predict hydride evolution, and the associated Delayed Hydride Cracking (DHC), it is necessary to develop a quantitative modeling and simulation capability that can be validated with carefully-designed experiments. This program will develop better management for used fuel disposition.

**Drivers:** Due to the cancellation of the Yucca Mountain long-term fuel storage repository, extending the wet and dry fuel storage periods is becoming critical. However, extending storage requires a more reliable understanding of the cladding performance over a 60-100 year period. Current models only consider low-to-mid-level burnup fuels. It is not clear how high-burnup fuels, which are currently in many reactors and will have higher cladding pressure and hydrogen content, will behave over this longer storage period. This project will be a technical advancement in both modeling and experiments that will position the laboratory as a leader in the science and engineering of fuel storage. As stated, this project is novel in that it will develop and validate a quantitative phase-field model of Zr hydrides, with detailed characterization of the influence of stress, temperature, grain boundary properties, and texture.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** Better understanding of the performance of zirconium clad and high burn-up used fuel for long term storage at DOE sites.

**Highlights of the Research:** The first module of an experimentally-verified microstructural simulation model, implemented in a continuum code, has been developed.

Project Title: Extended Stability Gamma-Gamma Prime Containing Nickel-Base Alloys

**Headquarters Element(s)**: NE/ INL LDRD

## Site(s) Involved: INL

**Project Description and Technical Objective**: The objective of this work is to develop a nickel-based alloy capable of operating for several decades while maintaining adequate strength at temperatures approaching or exceeding 1000 °C. The alloy will be substantially more micro structurally stable, thus providing a consistent set of mechanical properties at elevated temperatures while demonstrating superior oxidation resistance. The hypothesis for this program links a proven concept – high strength, high temperature superalloys – with the new and novel proposed idea of inverting the microstructure to create a superalloy that is stable for extended service durations. This transformational alloy will differentiate itself from the present state-or-the-art superalloys in that it is engineered specifically to be suitable for the extended service durations and extreme environment necessary for specific components in solar, fossil, and nuclear applications. It is hypothesized that it will exhibit similar mechanical properties to an advanced alloy, such as Alloy 718 and ME3, but contains higher levels of refractory elements to allow for the increased temperature creep strength.

**Drivers**: Nuclear reactor components need an alloy capable of operating for several decades while maintaining adequate strength at temperatures approaching or exceeding 1000 °C. The higher temperatures will make life extension of DOE plants more technically feasible. Hot section components require materials that exceed the capabilities of available state-of-the-art alloys, and the development of a single extended-stability alloy capable of operating at 1000 °C for 100,000 hours would be ideal for applications in DOE reactor and other nuclear facilities.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** Tailored alloys with enhanced microstructure for stability for long service durations and associated mechanical properties will provide a composition or composition range that is capable of forming an inverted microstructure (precipitates in a matrix) that will provide a balance of high temperature mechanical properties better suited for use in DOE nuclear facilities.

Highlights of the Research: None-newly initiated research

Project Title: Innovative Research for Fieldable Nuclear Measurements

# Headquarters Element(s): NE/ INL LDRD

# Site(s) Involved: INL

**Project Description and Technical Objective:** This work is intended to support exploration of new ideas for fieldable nuclear measurements in support of these missions, and will explore entirely new concepts for detecting and measuring radiation in the field. Technical objectives are: 1) to develop a long (up to 1 km), 1-dimensional (1-D) scintillating fiber bundle sensor (SFBS) to serve as a neutron/photon radiation detector for operational deployment - a radiological/nuclear (R/N) trip-wire perimeter threat sensor; 2) to develop two types of lowmass, low-power-consumption radiation detector systems, one for gross counting and one with spectroscopic capabilities which could be used to improve the detection of weak radiation signals in the field, focused towards the creation of large-terrain radiation field maps; and 3) to develop wearable radiation sensors that are capable of providing rough localization for radiation sources due to torso-caused attenuation, and couple these sensors with personal-dead-reckoning (PDR) technology.

**Drivers:** Recent developments in the field of radiation measurement instrumentation combined with advances in the development of low-power, high-performance miniature computers have the potential to lead to transformational advances for in-the-field nuclear measurements for emergency first responders and safeguards inspectors. These advances include new concepts for portable instrumentation for use in monitoring radiation fields, such as would be needed for securing a facility as part of a force-protection envelop, and new approaches for monitoring needed to search and respond to nuclear and radiological emergencies. There is also great interest in this area for emerging concepts and enabling technology related to wearable computing.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** This project will contribute to nuclear safety through the development of new diagnostic tools and capabilities a) for use in on-site protection, b) for use in monitoring radiation levels in around domestic and international nuclear facilities, c) for transformational nuclear safeguards, d) for radiological safety and dosimetry, and e) for severe-accident environmental radiation monitoring and post-accident verification. Technology explored in this project may also find use for future used-fuel transportation/storage and facilitate new concepts for safe and secure interim spent fuel storage.

Highlights of the Research: None-newly initiated research

Project Title: In-Pile Detection of Crack Growth in the ATR

Headquarters Element(s): NE/ INL LDRD

## Site(s) Involved: INL

**Project Description and Technical Objective:** In this project, Idaho National Laboratory (INL), Massachusetts Institute of Technology (MIT), and the Halden Reactor Project Institute for Energy Technology (IFE/HRP) researchers are developing and validating a technique to perform in pile crack growth rate measurement of environmentally assisted cracking (EAC) using the Direct Current Potential Drop DCPD techniques with active loading provided by a "bellows assembly" similar to what is used at the INL for in-pile creep testing. Previously, MIT completed an effort to review the state of the art for measuring in-core crack growth with the objective of recommending a conceptual design for implementation in the ATR. Laboratory testing of the proposed MIT design will be completed using MIT expertise and existing equipment at INL's High Temperature Test Laboratory (HTTL). Results from these evaluations are being used to develop and demonstrate an improved design, and if successful, would ultimately provide sufficient data to attract future customers to use this design for conducting irradiations in the ATR. The project will pursue actively loaded specimens for in-core crack growth measurements. Specimens will be machined from appropriate materials, a fatigue precrack will be initiated; instrumentation cables will be attached; and the specimen will be fixtured for exposure in a loop that contains in the MITR. Note that the use of active loading simplifies the specimen design because it is not necessary to use a geometry that attempts to compensate for changes in crack tip stress intensity as the crack grows. Rather, stress intensity can be controlled by changes in applied load. Adaptations of the compact tension specimen geometry developed and specified for fracture toughness testing are commonly used for EAC growth rate studies

**Drivers:** Until recently, it was believed that the current database on EAC, coupled with theoretical modeling, predict in-core crack growth experiments. As new materials become of interest and as service materials reach higher fluences, this conclusion no longer holds. EAC is a phenomenon that involves the synergy between dislocation movement and pile ups formation, diffusion of elements in the material (from the bulk to the surfaces), diffusion of elements (oxygen, hydrogen) though the oxide layer toward the material at a very long time scale. In addition, radiolysis of water will occur, changing the environment reacting with these materials. There remain questions about the accuracy of out of pile tests for predicting the EAC crack propagation rate in a nuclear reactor internal component.

**Benefits or Application of the Results to DOE and NNSA Nuclear Facilities**: Results from these evaluations would be used to develop and demonstrate an improved design, which would provide sufficient data for conducting novel irradiations in the ATR safely.

**Highlights of the Research:** Researchers have completed an effort to review the state of the art for measuring in-core crack growth with the objective of recommending a conceptual design for implementation in the ATR. Bench top testing (i.e. room temperature, air atmosphere) of load fixture operation has been accomplished.

Project Title: MOOSE Capability Extension In Support of Full Core Modeling

Headquarters Element(s): NE/ INL LDRD

# Site(s) Involved: INL

Project Description and Technical Objective: The objective of this research is to extend INL's Multiphysics Object Oriented Simulation Environment (MOOSE) framework in support of nuclear reactor core modeling. This project will be focused on adding capability to MOOSE to enhance those applications and provide the foundation for solving multiple coupled physical systems (such as fluid flow, neutronics and fuels performance) simultaneously in order to better simulate reactor operation and safety parameters. This will enhance reactor simulation capabilities. The current phase of the project is focused on implementation of the advanced coupling capabilities, specifically, completion of the fully coupled on disparate meshes capability. This advanced capability would enable users to target each the physics of each component with a particular geometric discretization tailored specifically to that physics. For instance, in conjugate heat transfer involving fuel cladding and coolant flow, the ideal mesh for heat conduction is quite different from the ideal mesh for fluid flow. Another example where disparate meshes are desirable is in the multigroup approximation of the neutronics equations; there it is natural for different groups to use different meshes due to varying material properties. The ability to do either full coupling or loose coupling on dissimilar meshes will be a new capability.

**Drivers:** The proposed enhancements in this project will provide a platform for understanding the complex multiphysics phenomena happening within nuclear reactors. The insight gained with this capability will allow for design optimization of existing reactors and fuels while also providing a platform for exploring future design ideas that could ultimately lead to safer and more efficient nuclear reactors.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** The benefit will be a more realistic simulation of the conditions and interactions inside nuclear reactors in general and inside the ATR in particular. More realistic simulation and modeling will lead to more informed risk based decisions.

**Highlights of the Research:** The project has been successful developing time integration enhancements and take initial steps towards loose coupling using different meshes and is implementing advanced coupling capabilities, specifically, completion of the fully coupled on disparate meshes capability. A first prototype of reactor core simulation has been published.

**Project Title**: Multidimensional Multiphysics Modeling of Fuel Behavior during Accident Conditions

**Headquarters Element(s)**: NE/ INL LDRD

Site(s) Involved: INL

**Project Description and Technical Objective:** The objective of this research is to develop and validate a fully coupled multidimensional multiphysics model of Zircaloy clad and oxide fuel under accident conditions. Specific research objectives are identified as follows:

1. Develop advanced models to describe rapid steam-cladding oxidation and the associated oxide layer growth and cladding thickness reduction during high temperature accidents.

2. Develop accurate fully-coupled multiphysics models to predict hydrogen generation and transport from the coolant boundary through the clad layer.

3. Investigate and implement cladding material models to describe phase transformations leading to embrittlement, high temperature non-linear mechanical behavior, and failure prediction during high temperature accident conditions.

4. Enhance the BISON fission gas release model to include an appropriate model for burst release, capable of describing grain boundary separation driven by the over-pressure of gas bubbles during fast temperature transients. This model will include the potential large release occurring from within the high-burnup structure (HBS) zone of the fuel.

5. Verify and validate models by comparison to analytical solutions, separate effects tests and integral rod experiments.

**Drivers:** Fuel designers and safety authorities rely heavily on fuel performance codes, since they require minimal costs in comparison with the cost of experiments or an unexpected fuel rod failure. The proposed research will provide an enhanced understanding of the complex multidimensional multiphysics behavior that occurs during an accident and result in an important advancement to the state-of-the-art in fuel performance analysis.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** Better codes and models for understanding fuel behavior inside DOE and NNSA reactors; the research will provide a basic platform which can be expanded to model used nuclear fuel.

# Highlights of the Research: None - newly initiated research

Project Title: Multi-Scale Full Core Reactor Physics Simulation of the Advanced Test Reactor

**Headquarters Element(s)**: NE/ INL LDRD

# Site(s) Involved: INL

**Project Description and Technical Objective:** The objective of this research is to develop a flexible multi-scale code for high order spatially accurate time-dependent reactor physics calculations within the ATR. This approach will yield the ability to use a multi-resolution radiation transport approach ranging in spatial scales from a full core representation down to detailed fuel meat resolution within individual fuel plates in a single element. For example, a conceptual model could simultaneously represent (1) the detailed structure of an individual fuel element using high-resolution discrete ordinates theory; (2) fuel elements within the same lobe via a medium resolution discrete ordinates/spherical harmonics hybrid; and (3) reactor lobe scale representing the balance of the fueled portion of the core with a low resolution spherical harmonics diffusion approximation. This capability would allow a transient neutron transport calculation to be strongly coupled to: the time-dependent change in isotopic composition (decay and burn-up) for cycle-length calculations; temporal variation of cross-sections due to Doppler effect (temperature dependency) for rapid transient analyses; and variations in isotopic densities and spatial redistributions (through chemical thermomechanics and conjugate heat transfer) for both short and long term transient performance evaluation. This first-of-its-kind approach has the potential of coupling high accuracy transport directly to depletion, spatial kinetics and fuels performance and taking into account the global effect of the entire core on a localized spatial region. ATR is in fact a one-off reactor that challenges classical homogenization techniques that are well established for the light water reactor (LWR) community (both pressurized water reactors (PWRs) and boiling water reactors (BWRs)) because of its irregular geometry. The current methodology for ATR is based on a very coarse level of homogenization and raw parameterization of nuclear cross-sections. The reason for those choices is essentially the very complex geometry of the ATR that makes it very difficult to perform a decomposition suitable for cross-section homogenization. The approach here proposed will allow the manufacture of a coherent software and mathematical framework to deliver a step by step improvement of the ATR simulation capability.

**Drivers**: In the real world of reactor dynamics, multiple phenomena occur simultaneously, and coupled effects drive a response that is well within the envelope of stacked conservative assumptions. The essence of multi-physics simulation is to solve a subset of coupled phenomena (e.g., coupled neutron transport and heat transfer, or even neutron transport, physics, and mechanics) simultaneously, such that a consistent solution is obtained that simulates real world behavior.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** This approach will provide a best-estimate representation of physical phenomena that can be used to reduce the compound effect of multiple conservatisms and define more credible operational limits for the ATR. Higher operating limits (if justified by this approach) will result in improved performance of the ATR by allowing higher target fluxes (when needed) or compensation for reduced thermal fluxes that may be see in an LEU core. In addition, this work will open the door for implementation of a three-dimensional reactor kinetics approach for ATR transient calculations.

**Highlights of the Research:** INL used the model developed under this program to demonstrate nuclear power simulation at the ANS Mathematics & Computation Conference. The simulation

demonstrated a first-of-its-kind multiphysics calculation incorporating neutronics, multi-scale fuels performance, thermal fluids, and "crud" formation for a realistic scale reactor simulation based on the Westinghouse AP1000.

**Project Title:** Multiscale Modeling on Delayed Hydride Cracking in Zirconium: Hydrogen Transport and Hydride Nucleation

#### Headquarters Element(s): NE/ INL LDRD

#### Site(s) Involved: INL

Project Description and Technical Objective: This project targets fundamental understanding of and a science-based modeling framework for hydride nucleation, the very first step of delayed hydride cracking (DHC) in zirconium and its alloys, using multiscale modeling tools including the first-principle density-functional-theory (DFT) calculations, molecular dynamics (MD) simulations, temperature accelerated dynamics (TAD), Metropolis-Monte-Carlo (MMC) and atomic-kinetic-Monte-Carlo (AKMC) simulations. DHC is one of the primary concerns on the dimensional and mechanical stability of Zircaloy based fuel cladding during dry storage. A quantitative description of DHC is critical for the quantitative prediction of materials degradation over long period of storage. However, as the very first step of DHC, the nucleation mechanism of hydrides has not been well understood at the necessary atomic scale. This proposal targets a fundamental understanding at the atomic scale and development of a multiscale modeling tool which can be connected to the meso- and engineering-scale modeling tools on the growth and mechanical behavior of hydrided zirconium alloys. The proposed research will establish a stateof-the-art understanding of hydride nucleation on which current understanding is limited. The unique multiscale tool coupling DFT, TAD, MD and AKMC will be the first of its kind to address hydride nucleation. It will also provide a bridging opportunity with the mesoscale modeling tools to increased total understanding of nuclear fuel behavior.

**Drivers:** The termination of the proposed geologic high-level waste repository at Yucca Mountain requires the used nuclear fuels to be stored for an extended period, primarily under a dry-storage condition. The materials degradation during the long-term aging has been a substantial concern on the integrity of nuclear fuels pins, due to the lack of knowledge on the material evolution over time. In particular, for high burn-up fuels, the production of large amount of hydrogen at high temperature during service leads to the formation of hydrides and subsequent DHC. A quantitative description of DHC, from either experimental or modeling approaches, is essential to the decision-making of possible storage period extension; however, it relies extensively on modeling and simulation due to the difficulties performing very long-time (decades) aging experiments. This research targets specifically the nucleation of hydrides - the very first step of DHC - with the necessary atomic resolution.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** The data produced will benefit safety assessments and interim disposition of Used Fuel in dry storage.

Highlights of the Research: None, research newly initiated

**Project Title:** Protectiveness and Stability of the Zirconium Oxide in Early-Phase Corrosion of Zirconium Alloys

**Headquarters Element(s)**: NE/ INL LDRD

Site(s) Involved: INL

**Project Description and Technical Objective:** This project aims at better understanding and controlling of the protectiveness and stability of zirconia surface films in Zr and Zr-alloy corrosion at the atomic level, taking an integrated surface-sensitive experimental and computational approach. The scientific objectives are to uncover the microscopic mechanisms and kinetics governing:

1) Structure, chemistry and reactivity of the thin layer of zirconium oxide at the early phases of corrosion; and

2) The relation of the zirconium oxide protective characteristics to i) its electronic and ionic conductivity, surface chemistry, reactivity and atomic structure, and ii) the metal/oxide interface stability, including the presence of mechanical deformation (dislocations) at that interface.

This new knowledge will provide the necessary foundation for designing fuel cladding surfaces and interfaces with high stability against chemical extremes. The project focuses on two main controlling parameters that govern the protectiveness and stability: the alloying elements in the zirconium matrix, and the microstructure (grain boundary density) of the zirconium surface.

**Drivers**: The oxidative corrosion of zirconium (Zr) alloys as nuclear fuel cladding in chemically harsh conditions poses a safety and operational limit on nuclear reactors. The goal of this research is to develop fundamental and predictive relations of the Zr alloy surface structure and composition to the protectiveness and stability of the early-phase zirconium oxide. The physical-chemical nature of this early-phase oxide strongly affects the long-term corrosion kinetics on zirconium alloys. A mechanistic understanding of the effects of surface texture and alloy elements on the oxidation kinetics can enable novel surface chemistry design strategies with superior corrosion resistance. However, such an understanding is still lacking.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** This work will help guide the design of corrosion-resistant Zr alloys for cladding and improve nuclear energy safety and economics.

**Highlights of the Research:** In situ high resolution and surface-sensitive structural and chemical analysis tools have been developed, and the surface oxygen and cation stoichiometry (metal/oxygen ratio), surface electronic structure and reactivity on the zirconia films in corrosion as a function of alloy/SPP composition, surface grain boundary density, and mechanical deformation have been identified. The information from experiments is providing validation input on the structure and chemistry of the oxides for modeling.

Project Title: Resilient Monitoring, Adaptation, and Control (ReMAC) System

Headquarters Element(s): NE/ INL LDRD

#### Site(s) Involved: INL

Project Description and Technical Objective: Resilient monitoring and control systems consisting of multiple sensors and actuators are being be used for management, health and controllability of monitored processes. The objective of this research is to develop and demonstrate a rigorous framework and supporting methods for the implementation of condition monitoring and control systems that are both resilient and adaptive. The proposed project is aimed to render monitoring and control systems with three key properties, namely, resiliency, adaptation, and efficiency. The resiliency property will be achieved by: i) relying on variable sets of active sensors and control strategies for assessing and controlling system conditions; ii) accommodating variability in sensors, actuators, and process perturbations via self-optimization in an autonomous manner with the feature of graceful system degradation; and iii) exhibiting stealth behavior via time varying selection of active sensors and controllers that is difficult to track and attack. Likewise, the adaptation property will be achieved by: i) conducting condition assessment and control based on varying information-quality (IQ), assessment quality (AQ), and control quality (CQ) requirements and estimations; and ii) marshalling data and reconfiguring control strategies based on the level of confidence required, the severity of anomaly assessed, and the degradation of control quality of the monitored system at hand. Finally, the efficiency property will be achieved by: i) selecting sensor and control configurations that optimize specified AQ and CQ; ii) allowing more efficient analysis of distributed information collected from systems of sensors and actuators; and iii) optimizing data collection and decision-making to reduce operational requirements.

**Drivers:** The need to be able to assess and control process conditions of critical infrastructures, such as operation of nuclear facilities is crucial for the protection of capital, the public, and the environment. The development of resilient monitoring and control systems will be important for the systematic synthesis and evaluation of efficient Instrumentation, Control, and Intelligent Systems (ICIS) solutions. This proposed resilient monitoring and control solution will enable the implementation of monitoring and control systems that not only dynamically collect information for health assessment at the given level of fidelity about the monitored system but also adaptively configure its control strategies based on assessed condition.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities**: Real time monitoring can lead to better control of key operations in DOE Nuclear Facilities.

**Highlights of the Research:** This research has developed assessment methods for evaluating plant conditions and detecting and isolating anomalies, developed assessment methods for evaluating observed performance on control strategies and developed methods for translating control performance observations into control quality (CQ).

**Project Title:** Separate Effects Fuels Development Capability

Headquarters Element(s): NE/ INL LDRD

# Site(s) Involved: INL

**Project Description and Technical Objective:** This project is developing a separate effects testing program to perform in situ irradiation studies and characterization of the nanoscale to mesoscale behavior of nuclear fuel materials under a wide variety of in-pile conditions. Separate effects testing including growth, irradiation, and monitoring of these materials encompasses the full science based approach for fuels development from the nanoscale to the mesoscale behavior of the sample material and other defects driven by the modeling and simulation efforts of INL. Analysis is being performed to determine the requirements and necessary components for a successful, game-changing program in the microstructure study of fuel materials under irradiation. Three areas of research development are being integrated into a prototype fuel/irradiation/monitoring demonstration. The three areas are:

1) Test sample fabrication including:

a. Metal organic chemical vapor deposition (MOCVD) and bulk crystal growth of engineered samples; and

b. Allowing for control of stoichiometry, grain configuration, and defect introduction.

2) Fast flux neutron irradiation with independent control of in-pile reactor conditions including:

- a. Independent gamma, temperature, hydraulic and coolant/gas environs; and
- b. Accelerator driven neutron irradiation facilities.
- 3) Advanced detection, imaging and monitoring including:
  - a. In-situ and ex-situ imaging; and
  - b. Monitoring technologies.

**Drivers:** Historically, nuclear fuel materials research has emphasized the homogeneous, integral and bulk properties of the materials. This approach, while essential for qualifying new fuel forms, is necessarily informed by data from two extremes; one at fabrication prior to irradiation, and one at post-irradiation. The "cook and look" approach has yielded almost all the current fuel performance knowledge available today. However, fuel performance models derived from this approach are limited to the exact integral conditions that produced the limited data. The kinetic, early life, time-evolution phenomena that drives the ultimate performance is not easily accessible under the current reactor irradiation paradigm.

**Benefits or Application of the Results to DOE/NNSA Nuclear Facilities:** Development of new, more robust fuels for DOE facilities