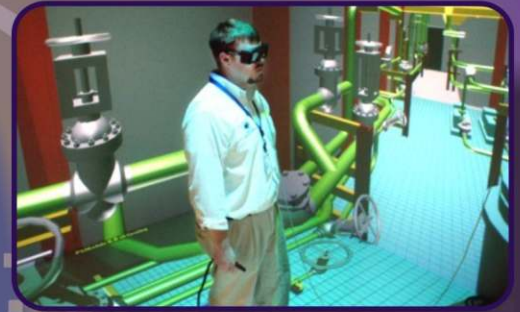


# NUCLEAR ENERGY RESEARCH INITIATIVE

2003 ANNUAL REPORT





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# Foreword

The Nuclear Energy Research Initiative (NERI) began in Fiscal Year (FY) 1999 as the core of a new, restructured Federal effort to develop advanced nuclear energy concepts and technologies. NERI was developed based on recommendations made in the November 1997 report of the President's Committee of Advisors on Science and Technology on *Federal Energy Research and Development for the Challenges of the Twenty-First Century*.

The NERI program focuses on preserving, advancing, and encouraging innovative nuclear science and technology R&D within the Nation's universities, laboratories, and industry. It supports the *National Energy Policy* by conducting research that addresses the potential, long-term barriers to both maintaining and expanding nuclear generation of electricity in this country. Working in tandem with other nuclear energy programs, such as the Generation IV Nuclear Energy Systems Initiative, the Advanced Fuel Cycle Initiative, the Nuclear Hydrogen Initiative, and the Nuclear Power 2010 program, the NERI program assists in responding to the Nation's need for economical and environmentally conscious sources of energy.

Since its inception, NERI has been realizing its goal of both developing advanced nuclear energy systems and providing state-of-the-art research concerning nuclear science and technology. The research effort conducted by the Nation's universities, laboratories, and industry partners has helped to maintain and improve the nuclear research infrastructure in this country. University involvement in NERI-funded research has been particularly important in renewing student interest in pursuing degrees in nuclear engineering and related sciences and enabling educational institutions across the country to stay at the forefront of nuclear science research.

This annual report summarizes the results of the ten NERI research projects initiated in FY 2000 and completed in FY 2003, and the research progress on the NERI projects initiated in FY 2001 and FY 2002. The final summaries for the NERI projects initiated in FY 1999 can be found in the NERI 2002 Annual Report. This report disseminates the results of NERI-sponsored research to the wide R&D community to spur yet more innovation, assuring a bright future for nuclear energy in the United States and the world.



William D. Magwood IV, Director  
Office of Nuclear Energy, Science and Technology  
U.S. Department of Energy



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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## I. Introduction

The United States Department of Energy (DOE) created the Nuclear Energy Research Initiative (NERI) in Fiscal Year (FY) 1999 in response to recommendations provided by the President's Committee of Advisors on Science and Technology. The purpose of NERI is to sponsor research and development (R&D) in the nuclear energy sciences to address the principal barriers to the future use of nuclear energy in the United States. NERI is helping to preserve the nuclear science and engineering infrastructure within the Nation's universities, laboratories, and industry, and is advancing the development of nuclear energy technology, enabling the United States to maintain a competitive position in nuclear science and technology. Research under this initiative also addresses issues associated with the maintenance of existing U.S. nuclear plants. The NERI program is managed and funded by DOE's Office of Nuclear Energy, Science and Technology (NE).

The *Nuclear Energy Research Initiative 2003 Annual Report* serves to inform interested parties of progress made in NERI on a programmatic level as well as research

progress made on individual NERI projects. Section 2 of this report provides background on the creation and implementation of NERI and on the focus areas for NERI research. Section 3 provides a discussion on the NERI mission and its goals and objectives, and on the work scope of the program. Section 4 highlights the major accomplishments of the NERI projects and provides brief summaries of the NERI research efforts that have been completed this year. Section 5 provides a discussion on the impact NERI has had on U.S. university nuclear programs.

Sections 6 through 8 provide project status reports by research area. Research objectives, progress made over the last two years, and activities planned for the next year are described for each project. Project numbers are designated by the fiscal year (FY) in which their proposal was submitted and the award was made. At the end of the document, there is an Index of NERI Projects sequentially ordered by FY and project number.

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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## 2. Background

In January 1997, the President tasked his Committee of Advisors on Science and Technology (PCAST) to review the current national energy R&D portfolio and to provide a strategy to ensure that the United States has a program to address the Nation's energy and environmental needs for the next century.

In its November 1997 Report to the President, *Federal Energy Research and Development for the Challenges of the Twenty-First Century*, the PCAST panel on Energy Research and Development determined that it was important to establish nuclear energy as a viable and expandable option and that a properly focused R&D effort to address the potential long-term barriers to the expanded use of nuclear power (e.g., nuclear waste, proliferation, safety, and economics) was appropriate. The PCAST panel further recommended that DOE reinvigorate its nuclear energy R&D activities with a new nuclear energy research initiative to address these potential barriers. DOE would fund research through this new initiative, based on a competitive selection of proposals from the national laboratories, universities, and industry.

DOE endorsed the PCAST recommendations and received Congressional appropriations in FY 1999, allowing NERI to sponsor innovative scientific and engineering R&D to address the key issues affecting the future use of nuclear energy and preserve the Nation's nuclear science and technology leadership.

In 1999, the PCAST report, *Powerful Partnerships: The Federal Role in International Cooperation on Energy Innovation*, recommended creation of an international component to NERI to promote "bilateral and multilateral research focused on advanced technologies for improving the cost, safety, waste management, and proliferation-resistance of nuclear fission energy systems." In FY 2001, the Department launched the new International Nuclear Energy Research Initiative (I-NERI) for bilateral and multilateral nuclear energy research. In 2002, appropriated funding supported bilateral, cost-shared research work under the I-NERI program with South Korea, France, and a third collaboration involving Argonne National Laboratory and a consortium of ten international participants represented by the U.S. Nuclear Regulatory Commission (NRC)

and the European Organization for Economic Co-operation and Development (OECD). Three new agreements with the European Union, Brazil, and Canada were established in 2003. Similar international agreements with Japan, the Republic of South Africa, and the United Kingdom are being considered.

I-NERI allows DOE to leverage Federal investment and international resources through cost-share arrangements with each participating country on a wide range of nuclear technology topics. I-NERI will further enhance the influence of the United States and DOE in international policy discussions on the future direction of nuclear energy. Similar to NERI, I-NERI features competitive, researcher-initiated R&D that is selected through an independent peer-review process by international experts from the United States and its partners. A separate report covering the research effort conducted in the I-NERI program is expected to be published in early 2004.

### NERI's Focus

In order to determine the initial focus of the NERI research areas, DOE convened a workshop of nuclear community stakeholders in April 1998, representing national laboratories, universities, and industry. As a result of this NERI workshop<sup>1</sup>, DOE focused its initial scientific and engineering R&D in the following areas:

- Proliferation-resistant reactors and fuel technology
- New reactor designs to achieve improved performance, higher efficiency, and reduced cost, including low-output power reactors for use where large reactors are not attractive
- Advanced nuclear fuels
- New technologies for management of nuclear waste
- Fundamental nuclear science

To encourage innovative R&D, a unique process for selecting new NERI projects has been employed since the program's inception. In response to the NERI solicitations, principal investigators (PIs) select research topics of interest and define the scope and extent of the R&D in their

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<sup>1</sup> *Summary Report of the Nuclear Energy Research Initiative Workshop—An Assessment of Research Opportunities for Nuclear Energy, Technology, and Education*, June 1998.

proposals. DOE employs an independent, expert peer review process to judge the scientific and technical merit of the R&D proposals. DOE reviews those proposals judged to have the highest scientific and technical merit to ensure their conformance with DOE policy and programmatic requirements. After the proposals are judged and the projects are reviewed by DOE, the award-selections are recommended to DOE's Source Selection Official.

Since the initiation of NERI, a number of events have influenced the focus of NERI research activities.

- In 1998, DOE established the independent Nuclear Energy Research Advisory Committee (NERAC). This committee provides advice to the Secretary and to the Director, Office of Nuclear Energy, Science and Technology (NE), on DOE's civilian nuclear technology program. In June 2000, NERAC issued the *Long-Term Nuclear Technology Research and Development Plan*. This plan identifies the research and technology development that is necessary over the next 10-20 years to help ensure the long-term viability of nuclear energy as an electricity generation option in the United States. NERAC also established a task force to identify R&D needs related to non-proliferation issues associated with nuclear power production. Their recommendations for appropriate research in this area were provided to DOE in a January 2001 report titled, *Technical Opportunities to Increase the Proliferation Resistance of Global Civilian Nuclear Power Systems (TOPS)*.
- The *National Energy Policy*, issued in May 2001 by the Vice President's National Energy Policy Development Group, supports the expansion of nuclear energy as one of its major initiatives for meeting the growing energy requirements of the United States. The *National Energy Policy* provides the core element in the planning for DOE's nuclear energy research programs addressing, among other areas, the research and development of advanced reactor and fuel cycle concepts, hydrogen production from nuclear energy, and the associated enabling sciences and technologies.
- In September 2002, NERAC issued the "Draft Technology Roadmap for Generation IV Nuclear Energy Systems." In coordination with the ten-country-member Generation IV International Forum (GIF), six reactor system concepts were selected for further development. These include the Very-High-Temperature Reactor System, the Gas-Cooled Fast Reactor System, the Supercritical Water-Cooled Reactor System, the Lead-Cooled Fast Reactor System, the Sodium-Cooled Fast Reactor System, and the Molten Salt Reactor System.
- With the initiation of new nuclear R&D programs such as the Generation IV Nuclear Energy Systems Initiative, the Advanced Fuel Cycle Initiative, the Nuclear Hydrogen Initiative, and the Nuclear Power 2010 program, NERI project selection has been more focused on providing a supportive role to these important programs and has assisted them in accomplishing their goals and objectives.

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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## 3. NERI Program Description

### NERI's Mission

The importance of nuclear power to the world's future energy supply requires that DOE apply its unique resources, specialized expertise, and national leadership to address key issues affecting the future of nuclear energy. NERI is a national, research-oriented initiative focused on innovation and competitiveness. It brings together national laboratories, universities, and industry to explore and develop new nuclear power technology. In so doing, NERI advances the state of scientific knowledge and promotes an enhanced domestic nuclear energy research and science infrastructure at universities, national laboratories, and industry that directly supports DOE's energy mission—a Secretarial priority. The program supports the *National Energy Policy* by conducting research to address the key technical issues impacting the expanded use of nuclear energy.

NERI is helping DOE foster innovative ideas in such areas as advanced nuclear energy systems, hydrogen production from nuclear power, advanced nuclear fuels and fuel cycles, and fundamental science. This research enhances the ability of nuclear energy to help meet the Nation's future energy needs and environmental goals. To achieve these long-range goals, NERI has the following objectives:

- Address and help overcome the potential technical and scientific obstacles to the long-term, future use of nuclear energy in the United States, including those involving non-proliferation, economics, and nuclear waste disposition.
- Advance the state of U.S. nuclear technology so that it can maintain a competitive position in overseas markets and a future domestic market.
- Promote and maintain a nuclear science and engineering infrastructure to meet future technical challenges.

### NERI's Work Scope

In FY 2003, NERI continued its R&D focus to address new research requirements introduced in the *National Energy Policy*. The following paragraphs define NERI's four research areas:

**Advanced Nuclear Energy Systems.** This program element includes the investigation and preliminary

development of advanced concepts for reactor and power conversion systems. These systems offer the prospect of improved performance and operation, design simplification, enhanced safety, and reduced overall cost. Projects involve innovative reactors, system and component designs, alternative power conversion cycles for terrestrial applications, new research in advanced digital instrumentation and control and automation technologies, and other important design features and characteristics.

**Hydrogen Production from Nuclear Power.** This program element includes R&D to identify and evaluate new and innovative concepts for producing hydrogen using nuclear reactors. This research includes investigating hydrogen generation processes compatible with advanced reactor systems and integrating parameters needed to develop systems that are efficient and cost effective. Projects in this area have been integrated into either the Advanced Nuclear Energy Systems area or the Fundamental Science area, depending on their technical focus.

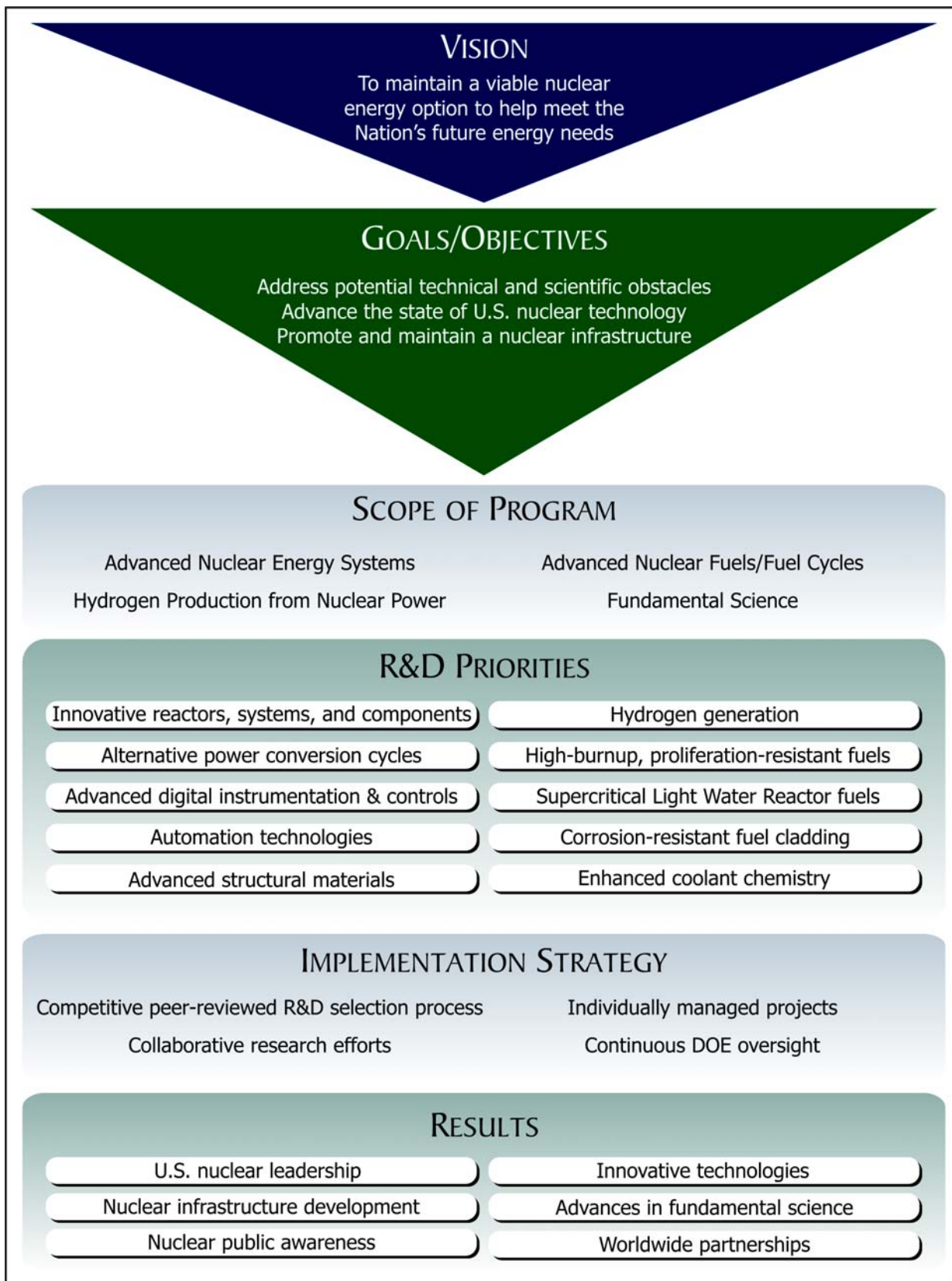
**Advanced Nuclear Fuels/Fuel Cycles.** This element includes R&D to provide measurable improvements in the understanding and performance of nuclear fuel and fuel cycles with respect to safety, waste production, proliferation resistance, and economics in order to enhance the long-term viability of nuclear energy systems. This research supports the Generation IV concepts by improving the performance of fuels, developing fuels capable of withstanding higher temperature and more highly corrosive environments, and developing advanced proliferation resistant-fuels capable of high burn-up.

**Fundamental Science.** This element includes R&D in the fields of materials science and fundamental chemistry. Fundamental science research funded by NERI applies to and supports the preceding program elements in advanced nuclear engineering technology. Material sciences applications include research and development on materials for use in advanced nuclear reactor systems, structures, and components, including fuel cladding, that may perform in high-radiation fields, high-temperatures and pressures, and/or in highly corrosive environments (i.e., lead-bismuth). Chemical science research may focus on developing and improving primary and secondary coolant chemistry in advanced reactors. Another research subject includes investigating nuclear isomers that could prove beneficial in civilian applications.

Safety, non-proliferation, and waste management are considerations intrinsic to all four research topics, especially for the advanced nuclear energy systems and advanced fuels/fuel cycles. Thus, they become selection criteria

across all four focus areas, and do not in themselves constitute focus areas.

The graphic below summarizes the key features of the NERI program.



# NUCLEAR ENERGY RESEARCH INITIATIVE

## 4. NERI's Accomplishments

This section discusses the program's progress in attracting research proposals, awarding annual R&D funding, and facilitating the successful completion of the NERI-funded projects.

### Project Awards

In FY 1999, DOE's NERI program received 308 R&D proposals from U.S. universities, national laboratories, and industry in response to its first solicitation. The initial FY 1999 procurement was completed with the awarding and issuing of grants and laboratory work authorizations for 46 R&D projects. The proposed research included participants from 45 organizations. Thirty-two of the projects involved collaborations of multiple organizations. Eleven foreign R&D organizations also participated in NERI collaborative projects. The duration of these annually funded projects was one to three years, with the majority lasting three years. The total cost of these 46 research projects for the three-year period was approximately \$52 million. A summary of these projects was included in the Nuclear Energy Research Initiative 2002 Annual Report.

In FY 2003, scientific and technical development advanced through the continuation of research efforts begun in FY 2000, FY 2001, and FY 2002. In FY 2000, 10 NERI R&D projects were awarded involving 18 U.S. and 6 foreign R&D organizations. In FY 2001, 13 NERI R&D projects were awarded involving 23 U.S. and 5 foreign R&D organizations. In FY 2002, 24 projects were awarded involving 32 U.S. and 5 foreign R&D organizations.

Funding for NERI is appropriated annually by Congress in the Energy and Water Development Appropriations Act.

- NERI funding for FY 1999 was a total of \$19 million with \$17.5 million available for new awards.
- Funding for FY 2000 was \$21.5 million, which provided for Year 2 funding of FY 1999 awards in addition to approximately \$2.7 million for 10 new FY 2000 awards.
- FY 2001 funding was \$27.1 million, which provided for Year 3 funding of FY 1999 awards, Year 2 funding for FY 2000 awards, and approximately \$5.7 million for 13 new FY 2001 awards.

- In FY 2002, NERI funding was \$22.0 million which provided for continuing ongoing research projects begun in FY 2000 and FY 2001 and approximately \$10 million for 24 new FY 2002 awards.
- In FY 2003, NERI funding was \$17.5 million, which provided \$15.8 million for continuing ongoing research projects initiated in FY 2001 and FY 2002.

Figure 1 illustrates the cumulative total of research projects awarded for FY 2000, FY 2001, and FY 2002 in the three major R&D areas. To date, over \$110 million has been awarded to fund NERI research projects, with a total of \$58 million being allocated to the recently completed FY 2000 projects and the ongoing FY 2001 and 2002 projects. Figure 2 shows the distribution of the \$58 million among the national laboratories, U.S. universities, and industry.

DOE has not funded foreign participants in existing projects as part of the NERI program. Their participation has been supported by the foreign organizations interested in the research being conducted. Although the PIs have been responsible for soliciting such support, foreign participation in NERI projects is contingent upon DOE approval.

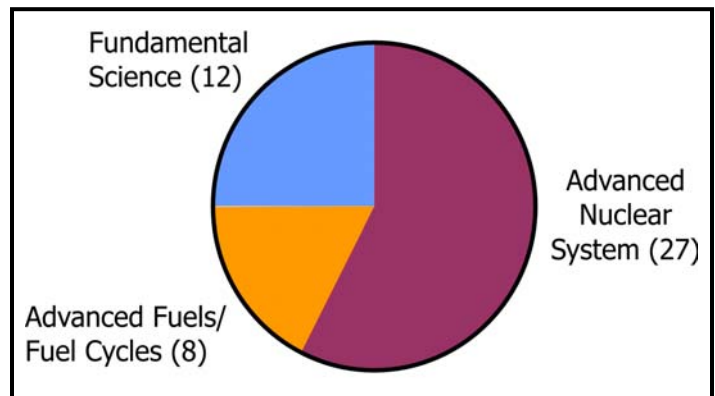


Figure 1. Division of ongoing NERI projects by R&D areas.

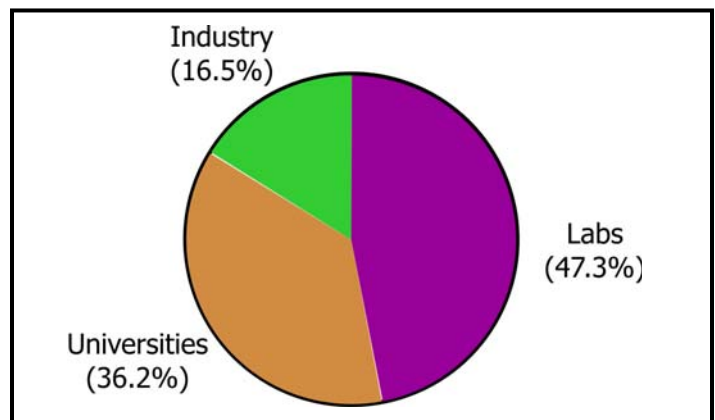


Figure 2. Distribution of NERI research funds among the national laboratories, universities, and industry.

## NERI Project Review

On May 20-22, 2003, the Office of Nuclear Energy, Science and Technology conducted an independent project review of the ongoing FY 2000, 2001, and 2002 NERI projects. Project presentations were made by each of the PIs or their designated representatives and the information presented was evaluated by other PIs in the field of research. The results of the project evaluations were documented in the NERI Project Review Meeting Report, dated May 20-22, 2003.

The meeting provided a unique opportunity for DOE to facilitate communication among the scientists and engineers engaged in NERI-sponsored research. The review allowed for the evaluation of all 47 ongoing projects in terms of each project's technical merit, its progress in accomplishing its stated objectives, and its programmatic contributions. The meeting report provides feedback to the PIs on the performance of each research project and assists in evaluating the overall NERI program for quality, relevance, and performance.

## NERI Participants

NERI research participants in FY 2003 included 20 U.S. universities, 10 national laboratories, 18 private businesses, and 7 foreign organizations. The participating organizations are provided in the following tables.

### U.S. Universities

Georgia Institute of Technology  
 Iowa State University  
 Kansas State University  
 Massachusetts Institute of Technology  
 North Carolina State University (NCSU)  
 Ohio State University  
 Oregon State University  
 Penn State University  
 Purdue University  
 Texas A&M University  
 University of Arizona  
 University of California-Berkeley  
 University of California-Los Angeles  
 University of Cincinnati  
 University of Florida  
 University of Michigan  
 University of Nevada  
 University of South Carolina  
 University of Tennessee  
 University of Wisconsin

### U.S. Department of Energy Laboratories

Ames Laboratory  
 Argonne National Laboratory  
 Brookhaven National Laboratory  
 Idaho National Engineering & Environmental Laboratory  
 Lawrence Livermore National Laboratory  
 Los Alamos National Laboratory  
 Oak Ridge National Laboratory  
 Pacific Northwest National Laboratory  
 Sandia National Laboratories  
 Westinghouse Savannah River Technology Center

### Industrial Organizations

Burns & Roe Enterprises  
 Duke Engineering  
 Entergy Nuclear, Inc.  
 Florida Power & Light  
 Framatome ANP, Inc.  
 Gamma Engineering Corporation  
 General Electric Global Research Center  
 General Atomics  
 Northern Engineering & Research  
 Northrop Grumman Newport News  
 Pacific Southern Electric & Gas  
 Panylon Technologies  
 PBMR (Pty.) Limited  
 SRI International  
 United Technology Research Center  
 Westinghouse Electric Company LLC  
 Westinghouse Science & Technology Center  
 (n,p) Energy, Inc.

### International Collaborators

Atomic Energy of Canada Limited (Canada)  
 Commissariat a l'Energie Atomique (France)  
 Forschungszentrum (Germany)  
 Japan Nuclear Cycle Development Institute (Japan)  
 University of Rome (Italy)  
 University of Tokyo (Japan)  
 VTT Manufacturing Technology (Finland)

## FY 2000 Project Completions

This year marked the scheduled completion of the FY 2000 NERI projects. Based on noted accomplishments, it is clear that NERI's stated goals and objectives are being met. These collaborative efforts between the public and private sectors have resulted in significant enhancements in the U.S. nuclear science and engineering infrastructure, especially in the areas of human and physical resources and capabilities. These efforts, coupled with those of I-NERI, the Generation IV Nuclear Systems Initiative, and the Advanced Fuel Cycle Initiative, have helped to revive the Nation's leadership role in international nuclear R&D. The technology advances will allow the United States to maintain a competitive position in overseas energy markets and a future domestic market.

By accomplishing their research objectives, these NERI projects have addressed and helped overcome a number of potential technical and scientific obstacles to the long-term, future use of nuclear energy in the United States. The accomplishments for each of the 10 completed FY 2000 projects are presented below. More detailed information on these projects is contained in the project summaries located in the following chapters.

### *Optimization of Heterogeneous Schemes for the Utilization of Thorium in PWRs to Enhance Proliferation Resistance and Reduce Waste*

Brookhaven National Laboratory (BNL) led a team that examined heterogeneous core design options and fuel management strategies that would maximize the benefits of using thorium (TH-U233) in the fuel cycle of pressurized water reactors (PWRs). Two different thorium implementation options were studied by the team: 1) the Seed-Blanket Unit (SBU) concept and 2) the Whole Assembly Seed and Blanket (WASB) concept. Researchers have developed designs for both the SBU and WASB approaches, which significantly improve the intrinsic proliferation resistance and waste characteristics of the fuel and reduce the total amount of plutonium produced. In addition, the plutonium that is produced is of inferior quality for potential utilization in weapons. Furthermore, the SBU and WASB approaches are based on an assembly design where only the fuel rods have been modified. Therefore, these approaches are retrofittable into existing PWRs with little or no modification. (Project #00-014)

### *Study of Cost-Effective, Large, Advanced Pressurized Water Reactors that Employ Passive Safety Features*

Westinghouse Electric Company LLC conducted this project to support the development and analysis of some areas of the AP1000 standard plant design that are included in the Design Certification application that was submitted to the Nuclear Regulatory Commission (NRC) on March 28, 2002. The AP1000 utilizes the passive safety systems used in the AP600, which was certified by the NRC and met NRC's deterministic safety criteria and probabilistic risk criteria with large margins. Researchers on this project provided support for several design certification activities. For example, in one activity they prepared safeguards data packages to perform the safety analyses necessary to answer Requests for Additional Information (RAIs) from the NRC. While this project focused on design certification activities unique to AP1000, these activities are representative of research that is necessary to realize successful licensing of the next generation of nuclear power plants in the United States. (Project #00-023)

### *Design and Layout Concepts for Compact, Factory-Produced, Transportable, Generation IV Reactor Systems*

The University of Tennessee (UT) and the Massachusetts Institute of Technology (MIT), along with industry and laboratory participants, developed compact Generation IV power plant designs and layout concepts to maximize the benefits of factory fabrication, optimal packaging, transportation, and siting. Plant concepts identified by the type of coolant (water, gas, or liquid metal) were developed by three engineering teams. UT led the teams for water and liquid-metal cooled reactors while MIT led the team for the gas-cooled reactor. A fourth team addressed computer simulation and optimization of the factory fabrication processes for the three reactor concepts. As a result of this project, researchers discovered the two most important aspects of successful modular construction and have provided recommendations on how to achieve these specific criteria. They concluded that further cost reductions are possible if additional steps are taken to make the modules and components more amenable to automated fabrication and if they can use manufacturing processes that result in near nominal production dimensions. (Project #00-047)



*Integrated Nuclear and Hydrogen-Based Energy Supply/Carrier System (STAR-H2)*

Since October 2000, Argonne National Laboratory, along with support from Texas A&M University, has been developing a secure, transportable autonomous reactor for hydrogen production (STAR-H2). This modular, fast reactor design is intended for the growing energy market of the twenty-first century and would provide both hydrogen and electricity. This design is based on full transuranic recycle in a passively safe, environmentally friendly, and proliferation-resistant manner suitable for widespread, worldwide deployment. STAR-H2 is a member of the Generation IV Small Pb-Alloy Reactor concept family, which is one of the six concepts selected for further R&D work under the Generation IV Nuclear Energy Systems Initiative. (Project #00-060)

*Development of Design Criteria for Fluid-Induced Structural Vibrations in Steam Generators and Heat Exchangers*

This University of California-Los Angeles project focused on developing design criteria to eliminate fluid-induced, structural vibrations in steam generators and heat exchangers. The project's deliverables included reports on experimentally based, single-phase entrance region flow; air-water stability maps and the impact of tube boiling; the comparison of predictions and experimental results; the importance of prototype design variables in conducting laboratory tests of stability; and results from the evaluation of the impact of vibration avoidance on heat transfer. (Project #00-062)

*An In-Core Power Deposition and Fuel Thermal Environmental Monitor for Long-Lived Cores*

The Ohio State University, along with Westinghouse Electric Company and the University of Akron, have worked together to develop the constant temperature power sensor (CTPS) as an in-core instrument. This sensor provides a detailed map of local nuclear power deposition and coolant thermal-hydraulic conditions during the entire life of the core. In some of the Generation IV reactor cores, this could include normal operation, post-accident operation, and monitoring after the core is placed in permanent storage. The majority of this research focused on completing four different sensor prototypes. Sensors of each type are available for performance evaluation at Ohio State University's nuclear reactor. This project provided insight into the additional R&D required to develop a viable commercial product. (Project #00-069)

*Design and Construction of a Prototype Advanced On-Line Fuel Burn-up Monitoring System for the Modular Pebble Bed Reactor*

Headed by the University of Cincinnati, this project's goal was to design, construct, and test an advanced, on-line, fuel burn-up monitoring system for the next generation Modular Pebble Bed Reactor. It involved all phases necessary to develop a burn-up monitoring system, including a review of the design requirements of the system; identification of materials and methodologies that would satisfy the design requirements; modeling and development of potential designs; and, finally, the construction and testing of an operational monitoring system. (Project #00-100)

*Balance-of-Plant System Analysis and Component Design of Turbo-Machinery for High-Temperature Gas Reactor Systems*

In this project, Massachusetts Institute of Technology, with Northern Engineering & Research, developed systems analysis tools for evaluating turbo-machinery and balance-of-plant (BOP) power conversion systems in high-temperature gas-cooled reactors (HTGRs). The three design goals of this project were to develop a "reference" plant design that could be built today with no significant advancement technology, to answer key questions related to the design of the power conversion system, and to develop an "advanced" design that allows for prudent and achievable extensions of the technology. Given the design requirements and constraints, researchers on this project designed and configured a final reference plant: a 250-MWth design with a gross power of 131.4 MWe that yielded a net efficiency of 48 percent. (Project #00-105)

*Failure Forewarning in Critical Equipment at Next-Generation Nuclear Power Plants*

Researchers at Oak Ridge National Laboratory (ORNL) applied new, non-linear methods to assess condition change and forewarn machine failures. The three main objectives of this project were to: 1) acquire test data for various equipment, 2) analyze the test data to show compelling demonstration of timely and robust forewarning failure, and 3) evaluate the effectiveness and cost of timely forewarning. Anticipation of failure in critical equipment at next-generation nuclear power plants will help in the scheduling of maintenance to minimize safety concerns, unscheduled non-productive down time, and collateral damage due to unexpected failure. Results from this research provide compelling evidence for forewarning of

failures via ORNL's nonlinear forewarning technology. This technology has substantial intellectual property protection in the form of six U.S. Patents and two patents pending. Products of this work also include software implementation of the nonlinear technology, a cost-benefit analysis of the prognostication approach, and a commercialization roadmap. (Project #00-109)

*Isomer Research: Energy Release Validation, Production, and Applications*

A collaborative team from Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), and Argonne National Laboratory (ANL) participated in an applied nuclear isomer research project for the discovery and practical application of a new type of high energy

density material (HEDM). Nuclear isomers could yield an energy source with a specific energy as much as a hundred thousand times as great as that of chemical fuels and can be adapted to a range of applications. Researchers completed two experiments to verify the reported x-ray-induced decay of the 31-yr HF-178 isomer; they completed work on an analytic model of isomer energy release, which explores the conceptual engineering features of isomer energy supply systems; they installed a microcalorimeter developed by NASA scientists, which has superb energy resolution; and, finally, they accomplished the synthesis of crystalline needles from an Nb-HF-KF aqueous solution, which has the advantage of a greater chemical yield than other growth techniques. (Project #00-123)

# NUCLEAR ENERGY RESEARCH INITIATIVE

## 5. NERI's Impact on University Nuclear Programs

One of NERI's long-term goals is to improve the nation's nuclear science and engineering infrastructure in order to maintain the country's leading position in nuclear energy research. One way of achieving this long-range goal is to focus on the classrooms and research laboratories of colleges and universities around the United States. By cultivating research partnerships among U.S. universities, national laboratories, and industry, NERI is not only helping educational institutions across the country stay at the forefront of science education, but it is also benefiting future nuclear industry and national laboratory endeavors by training the next generation of nuclear scientists.

### University Involvement

DOE believes that funding creative research ideas at the nation's universities and colleges, as well as at national

laboratories and industry, helps solve important issues that the private sector is unable to fund alone due to the high-risk nature of the research and/or the extended period before a return on investment is realized. Participants in NERI's initial planning workshop recommended that NERI be viewed as a "seed program" where new nuclear-related technological and scientific concepts could be investigated.

Based on this research philosophy, NERI has provided universities and colleges with a competitive, peer-reviewed research program that allows faculty and students an opportunity to conduct innovative research in nuclear engineering and related areas. Since 1999, twenty-eight U.S. universities have received research awards as lead investigators and collaborators. Of the 93 projects conducted in the NERI program, 75 percent involved U.S. colleges and universities. Figure 3 provides a map and complete listing of the universities and colleges involved.

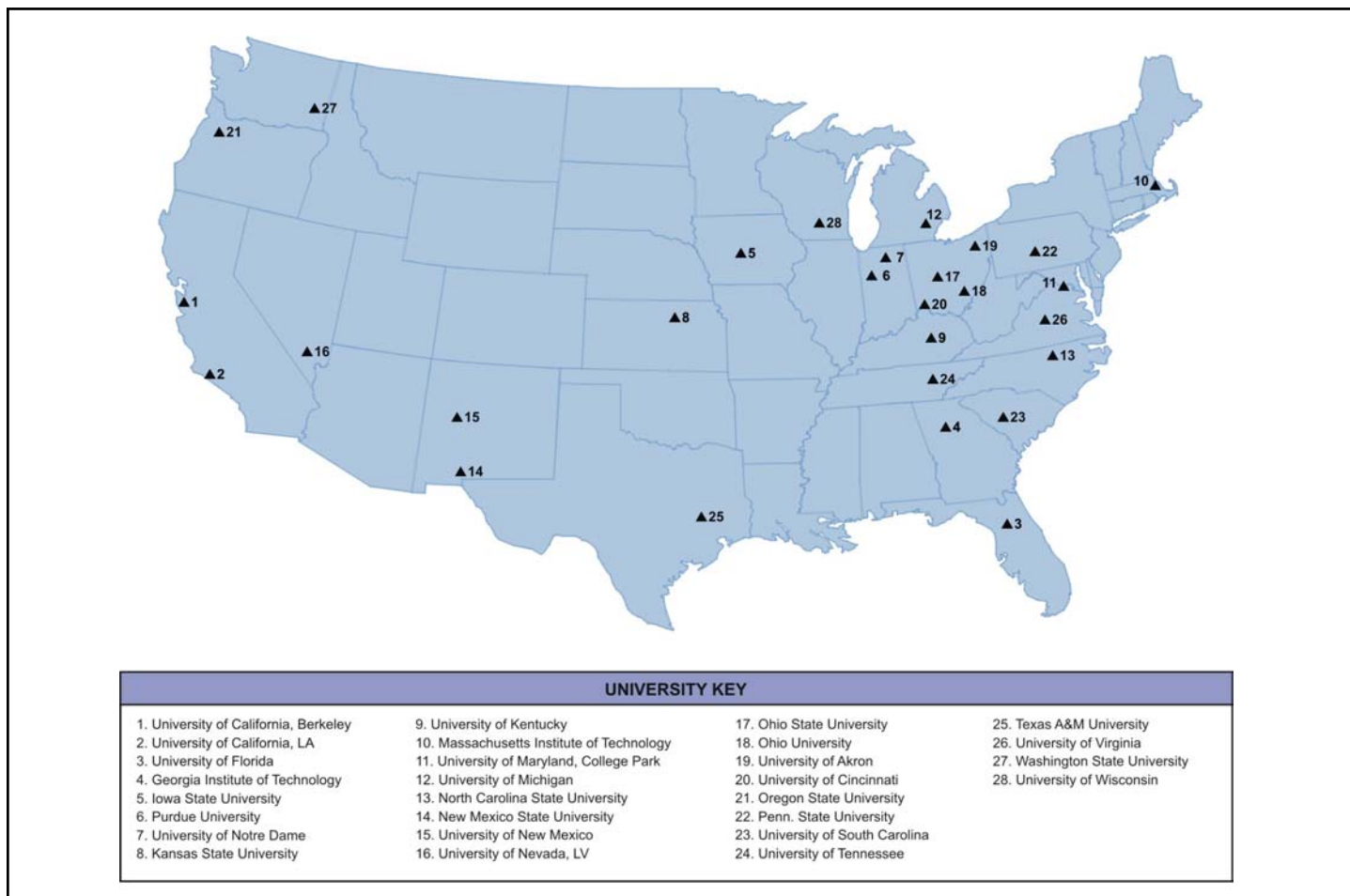


Figure 3. Locations of universities and colleges participating in NERI projects.

## Student Participation

One great success of NERI and other DOE programs is that nuclear-related educational opportunities at the universities have significantly increased. Universities have benefited from increased research dollars which have served as incentives for new student recruitment. As a result of this involvement, student interest in nuclear engineering has been revitalized. In 1998, only 500 students were enrolled in U.S. universities seeking degrees in nuclear engineering; today, 1,300 students are enrolled in nuclear engineering programs.

This student participation includes all levels—undergraduates and those students performing masters and doctorate level work. A total of 359 students have participated in the 93 projects funded since the program's inception. The distribution of participation between undergraduate, graduate, and doctorate students is noted in Figure 4. In addition, numerous post-doctoral fellows at universities have been involved in these NERI research projects. Over the past few years, graduates of these programs have had higher than normal grade point averages, showing that these programs are training highly qualified individuals that will sustain the future growth of the nuclear power industry.

NERI has provided U.S. universities and colleges an opportunity to work closely with industry and DOE national laboratories and it has introduced these researchers to other nuclear energy-related government programs. In addition to research on the Advanced Fuel Cycle Initiative, the Generation IV Nuclear Energy Systems Initiative, the Nuclear Hydrogen Initiative, and the Nuclear Power 2010 program, NERI's activities are coordinated with other

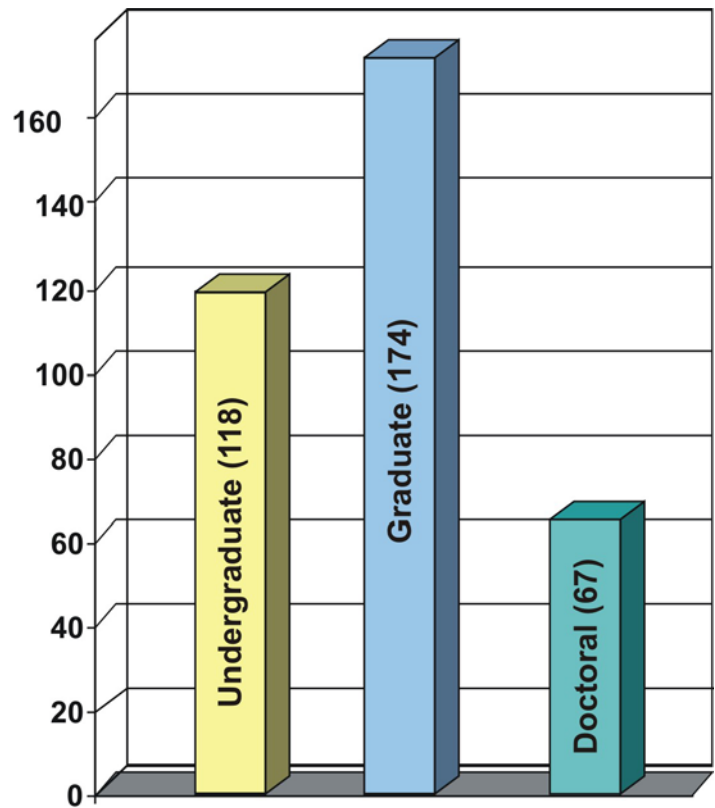


Figure 4. University student distribution among the degree programs.

relevant DOE energy research programs in the Office of Science, and the Office of Energy Efficiency and Renewable Energy, and the Nuclear Regulatory Commission. Furthermore, the Department leverages NERI program resources by encouraging no-cost collaboration with international research organizations and nuclear technology agencies. In this way, universities are also given the opportunity to gain experience with international research interests and capabilities.

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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## 6. Advanced Nuclear Energy Systems

This program element includes 27 research projects of which 8 were awarded in FY 2000, 7 in FY 2001, and 12 in FY 2002. It includes the investigation and preliminary development of advanced concepts for reactor and power conversion systems. These systems offer the prospect of improved performance and operation, design simplification, enhanced safety, and reduced overall cost. Projects may involve innovative reactor, system, or component designs; alternative power conversion cycles for terrestrial applications; new research in advanced digital instrumentation and control and automation technologies; hydrogen production from nuclear reactors; and identification and evaluation of alternative methods, analyses, and technologies to reduce the costs of constructing, operating, and maintaining future nuclear power plants.

Additionally, this element includes research projects to improve the intrinsic proliferation-resistant qualities of advanced reactors and fuel systems. Possible technology opportunities and subjects of investigation include alternative proliferation-resistant reactor concepts, systems that minimize the generation of weapons-usable nuclear materials (e.g., Pu-239) and waste by-products, or systems that increase energy extraction from the utilization of plutonium and other actinide isotopes generated in the fuel.

Projects under this program element specifically address the characteristics, feasibility, safety features, proliferation-resistance, and economic competitiveness of advanced reactor systems. Research focuses on advancements in light water reactor technology to achieve higher performance as well as on development of other higher temperature advanced reactor designs for higher efficiencies.

Other research under this program element focuses on developing compact or modular reactor designs suitable for transport to remote locations and alternative energy production or co-generation reactor applications. Desirable features include long-lived reactor cores that minimize or avoid the need for refueling, and concepts that maximize fuel burn-up or employ advanced energy conversion technology.

Finally, this program element includes research and development to identify and evaluate innovative concepts for producing hydrogen using nuclear reactors. This research includes investigating hydrogen generation processes that are compatible with advanced reactor systems and developing integrated systems that are efficient and cost effective.

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# NUCLEAR ENERGY RESEARCH INITIATIVE

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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Study of Cost-Effective, Large, Advanced Pressurized Water Reactors that Employ Passive Safety Features

PI: James W. Winters, Westinghouse Electric Company LLC

Project Number: 00-023

Project Start Date: August 2000

Collaborators: None

Project End Date: September 2003

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### Research Objectives

On December 16, 1999, the United States Nuclear Regulatory Commission (NRC) issued a Design Certification for the AP600 standard nuclear reactor design. This culminated an eight-year review of the AP600 design, including its safety analysis and probabilistic risk assessment. The AP600 is a 600-MWe reactor that utilizes passive safety features. Once actuated, these features depend only on natural forces such as gravity and natural circulation to perform all required safety functions. Not only do passive safety systems result in increased plant safety, they also significantly simplify plant systems and equipment, resulting in simplified plant operation and maintenance. The AP600 meets NRC deterministic safety criteria and probabilistic risk criteria with large margins.

The large safety margins of the AP600 can be attributed to the performance of the passive safety systems in response to accidents. An extensive AP600 test program was performed to provide confidence in the ability to adequately predict the performance characteristics of the passive safety systems, as required by 10 CFR 50. This test program consisted of separate effects and integral systems tests of the passive safety systems and is well documented in *NUREG-1512, Final Safety Evaluation Report Related to Certification of the AP600 Standard Design*. Westinghouse used the test programs to develop analytical computer codes that can predict, with adequate certainty, the performance of the passive safety systems in response to design basis and beyond design basis accidents. In addition to the extensive test program conducted by Westinghouse, the NRC also performed confirmatory tests and analyses at both the Advanced Plant Experiment (APEX) test facility at Oregon State University and the ROSA test facility at the Japan Atomic Energy Research Institute. As a result, the Westinghouse computer codes were validated as sufficient for use in performing accident analyses in accordance with the requirements of 10 CFR Part 50 and Part 52. In

addition, the NRC performed independent analyses of the AP600 using different analysis codes to confirm the adequacy of the AP600 design as well as the AP600 safety analysis presented in the *AP600 Standard Safety Analysis Report*. These independent analyses also confirmed the large safety margins exhibited in the AP600.

Westinghouse is developing a larger version of the AP600 called the AP1000. The AP1000 design is based largely on the AP600. It employs passive systems that operate in the same manner as in the AP600. The AP1000 is being designed to meet NRC regulatory criteria in a similar manner to that found to be acceptable for the AP600; it is also being designed to meet NRC deterministic safety criteria and probabilistic risk criteria with large margins.

Westinghouse intends to certify the AP1000 standard plant design under the provisions of 10 CFR Part 52. To that end, Westinghouse submitted an application for Design Certification of AP1000 to the NRC on March 28, 2002. This NERI program provided support for development and analysis of some areas of the design that are included in the Design Certification application. AP1000 design features, as they relate to Design Certification, are included in the *AP1000 Design Control Document (APP-GW-GL-700)*.

### Research Progress

AP1000 uses a canned motor pump for its reactor coolant pump. Canned motor pumps are used in the United States naval nuclear program and are part of the AP600 design as well. The pump and motor size required for AP1000 is an extension from current practice. The plant designers worked with the pump designers to develop a pump specification that met plant requirements while minimizing the pump design extension.

AP600 was designed and certified based on a version of the ASME Code and other applicable national consensus

standards. AP1000 should be based on more current versions of those standards. This NERI project partially supported a study to determine which version of the ASME Code will be the basis for AP1000 and the technical basis that was provided to NRC to justify use of this version.

The steam generators for AP1000 are larger than those for AP600 and are based upon the replacement units for Arkansas Nuclear Unit 1. Researchers prepared a unique specification to account for the AP1000 thermal hydraulic operating conditions and for the channel head mounted reactor coolant pumps.

Researchers on this project also prepared safeguards data packages to perform safety analyses. This NERI project helped support analysis in two areas. The results of all safety analyses are included in the *AP1000 Design Control Document*.

In 2002, the NRC prepared and transmitted to Westinghouse 700 Requests for Additional Information (RAIs). This completed the generation of RAIs and Westinghouse answered them all by December 2, 2002. A large number of these RAIs related to safety analysis. NRC requested additional information on code development, analysis techniques, model development, assumptions, relevant equations, applicability of tests, and other details. There are no RAIs that question the basic safety of AP1000. These NRC/Westinghouse interactions culminated in an in-person NRC review of AP1000 thermal/hydraulic calcula-

tions during the week of November 17, 2003.

Westinghouse performed the safety analyses necessary to answer RAIs from the NRC. Phase 3 activities were in the areas of Loss of Coolant Accident (LOCA) analysis, non-LOCA analysis, and containment response analysis. A final report was issued outlining the NERI-supported, safety-related analysis performed for AP1000.

In conclusion, this NERI project provided support for representative design certification activities. These activities are unique to AP1000, but are representative of research activities that must be driven to conclusion to realize successful licensing of the next generation of nuclear power plants in the United States.

## **Planned Activities**

This NERI project has been completed.



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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Design and Layout Concepts for Compact, Factory-Produced, Transportable, Generation IV Reactor Systems

PI: Fred Mynatt, University of Tennessee

Project Number: 00-047

Collaborators: Massachusetts Institute of Technology, University of Tennessee, Westinghouse Electric Company LLC, Oak Ridge National Laboratory, Northrop Grumman Newport News

Project Start Date: August 2000

Project End Date: November 2003

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### Research Objectives

The purpose of this research project was to develop design and layout concepts for a compact Generation IV nuclear power plant. The potentially small footprint of this system offers the opportunity for maximum factory fabrication and optimal packaging for transportation and siting. Barge mounting was an option to be considered that would offer flexibility for siting including floating installation, on-shore fixed siting, and transportation to nearby inland sites. Railroad and truck transportation of system modules was also considered in this work. The project utilized the work of others including previous work, concurrent Generation IV work, and a previously funded NERI project to develop standards and guidelines for cost-effective layout and modularization of nuclear power plants.

This interdisciplinary project was comprised of three university-led nuclear engineering teams identified by reactor coolant type (water, gas, and liquid metal). The University of Tennessee (UT) led the teams for two types of reactors (water and liquid metal) and the Massachusetts Institute of Technology (MIT) led the team for the gas-cooled type. The industry and laboratory participants were Westinghouse Science and Technology for the light water reactor (LWR) team and Oak Ridge National Laboratory for the high-temperature gas reactor (HTGR) team. Northrop Grumman Newport News (formerly Newport News Shipbuilding) provided comments on the effectiveness of modular manufacturing. A fourth industrial engineering team, led by UT, studied computer simulation and optimization of the factory fabrication processes. Each team consisted of a professor and a graduate student who performed most of the work; review and consultation was provided by industry and laboratory partners. This interdis-

ciplinary arrangement enhanced the opportunity to satisfy DOE objectives for advancing state-of-the-art nuclear technology while strengthening nuclear science and engineering infrastructure in the United States.

### Research Progress

This project was funded as a grant to the University of Tennessee and a subgrant to MIT. The first phase of the project began with the acquisition and review of available designs and requirements for each reactor type. Based on that work, the project team selected three reactor types. These included a modular pebble bed, helium-cooled concept developed at MIT; the Westinghouse International Reactor, Innovative and Secure (IRIS) water-cooled concept developed by a team led by UT; and a lead-bismuth-cooled concept also developed by UT.

Development of plant layout and modularization concepts requires an understanding of both primary and secondary systems. MIT's work to develop the modular pebble bed reactor (MPBR) included the initial concepts for both these systems. The IRIS project did not have a conceptual design for a secondary system. The lead-bismuth concept did not have conceptual designs for either the primary or secondary system. The second phase of this project focused on further developing the MPBR concept, developing a secondary system and integrated plant concept for IRIS, and developing a lead-bismuth-cooled integrated plant concept. The second phase also included increased interaction between the IRIS development team for the LWR concept, the Oak Ridge National Laboratory for the MPBR concept, and several individuals working on the lead-bismuth-cooled reactor concepts.

The primary effort in the third phase of this project was to simulate and analyze the fabrication and manufacturing

of a modular reactor. The task was performed by an industrial engineering student and professor at UT with assistance and input from the professors who led the development of the modular reactor concept. The focus was on evaluating economies of factory fabrication versus economies-of-scale of large, site-constructed plants. A related effort evaluated whether the modular approach really works and whether it is feasible and cost effective to build modules in the factory and assemble them at the site. Northrop Grumman Newport News performed this task based on their experience with modular construction of ships and submarines.

**LWR Concept.** In this project, researchers developed a conceptual design and balance-of-plant (BOP) for a Generation IV nuclear power plant using the Westinghouse IRIS. The preliminary BOP design was presented as a basis for a Science Thesis in Nuclear Engineering at UT in May 2002. In a following effort, modifications were made to the preliminary design to include an increased and more conservative cold side inlet temperature for the condenser, a corrected condenser duty, more accurate condenser models, and changes to the sizes for the feedwater heaters. The feedwater heaters were also reoriented to a vertical configuration in order to achieve better maintenance and repair conditions. The system output is 1,000 MW thermal and approximately 345 MWe. It has six feedwater heaters and dual reheat with one high-pressure and one low-pressure tandem compound turbo-generator unit. Researchers estimated the sizes and weights of the components and associated piping. The final layout of the plant has a footprint that is 100 meters long by 40 meters wide, and weighs approximately 7,047 tons. Figures containing visualizations of plant components layout and solid modeling have been developed. In order to develop an example of barge mounting and transportation, the footprint was constrained by modularity requirements as the plant needed to be transportable by barge from the mouth of the Mississippi River to desired sites along the Tennessee River and its tributaries. This required that the components fit on a barge no larger than 400 feet long by 110 feet wide with a draft less than 9 feet. Researchers searched navigation charts for the Mississippi River from its mouth to the mouth of the Ohio River, and for the Tennessee River from its mouth to Knoxville, Tennessee. They tabulated detailed listings of all potential obstructions (bridges, overhanging cables, locks, and dams) and their relevant clearance parameters (height, width, etc.), as well as channel depth limitations. The final concept depicted in Figure 1 meets these criteria.

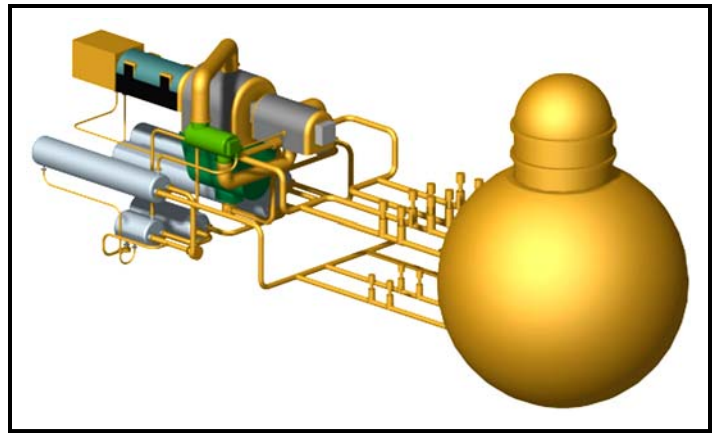


Figure 1. Visualization of the IRIS containment and BOP.

**MPBR Concept.** The modular pebble bed reactor concept was developed closely with another NERI project at MIT that designed the major components including the intermediate heat exchange, turbines, compressors, recuperators, precoolers, and intercoolers. Together, the teams established layout options using the actual conceptual designs that were being developed. The MPBR design power level is approximately 100 MWe.

The modularity and packaging studies used to develop the modular BOP system for this concept were divided into several tasks:

1. System layout and design (physical layout and packaging of the plant components).
2. System concept design for increased modularity and decreased cost.
3. Advanced component design concepts for future implementation.

The first task involved defining the physical layout of the power plant and any transportation issues involved in its construction. The second task involved making high-level trade studies of the actual system, such as the number of intercoolers, limiting temperatures, and other system parameters. The third task involved searching for advanced component concepts that would aid in the other two tasks by making individual components simpler, cheaper, or more fault tolerant.

The proposed modular BOP system uses components and component carriers sized to fit within the limitations of truck transportation. These component carriers are steel space-frames that encapsulate each component. Using this method, all the BOP components can be built in factories and easily assembled on-site. Using the integral matrix structure of steel space-frames, all the necessary access

hardware (e.g., catwalks, valves, and flanges) can be built in the factory, further minimizing on-site assembly. Figure 2 is a drawing of the MPBR BOP.

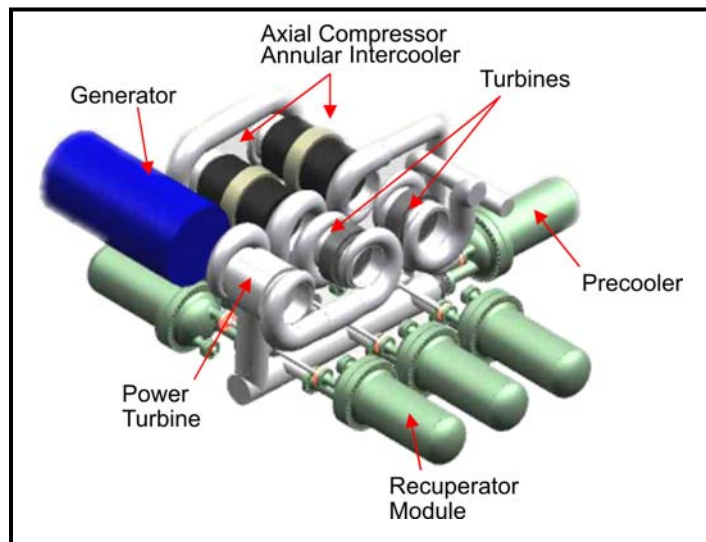


Figure 2. A three-dimensional model of the MPBR balance-of-plant.

**Lead-Bismuth (PbBi) Concept.** Liquid metal breeder reactors hold particular promise for future energy supply since they offer sustainability of energy production by effectively utilizing fertile and fissile materials. They also can be used to recycle nearly all of the actinide radioactive waste produced by current nuclear reactors—using this waste for energy production. Many breeder reactors have been designed and a few have been built and operated. However, most designs have an inherent problem with positive coolant voiding reactivity coefficients; thus, they may present more risk than many would prefer to accept. Results from calculations indicate that proper choices of thorium (Th), plutonium (Pu), and uranium (U) fuels, along with some changes in geometry, permit a PbBi-cooled reactor to operate with a negative PbBi voiding reactivity coefficient. This means that a reactor can be designed that has considerably more inherent safety than previous designs.

One significant advantage of using PbBi as a coolant is that the reactor spectrum is relatively hard, thus permitting significant quantities of actinides to be used as fuel, which eliminates the need to dispose of them as waste. The nuclear characteristics of this design also permit operation for at least five years without refueling, or reshuffling, since the conversion ratio can be maintained very near unity. The time between refueling is limited by the performance of the fuel materials rather than by the ability to sustain the

chain reaction. Proliferation resistance is improved relative to the reactors in current commercial use since the Pu-239 inventory can be held constant or be diminished, depending on fuel management choices.

In order to accomplish the size limitation for reactor components, the proposed design is constrained by a reactor vessel size that will be transportable on a standard rail car. This limits the height and width to about 12 feet, the length to about 80 feet, and the weight to about 80 tons. This should be adequate for producing 300 to 400 MW of electricity, depending on the optimization of the primary and secondary systems' performance, while satisfying all licensing requirements.

This project determined that a PbBi-cooled fast reactor that produces 310 MWe can be designed with primary system components that are all rail transportable. It was also determined that a cylindrical, PbBi-cooled reactor that uses only Pu as fuel and that has a negative voiding coefficient probably cannot be designed without the use of leakage-enhanced fuel assemblies. However, results to date indicate that a relatively high leakage slab core that uses a combination of Pu, U, and Th for fuel does have a negative coolant voiding coefficient. The reference system design uses steam generators coupled to the secondary system BOP that was designed for IRIS as part of this NERI project. This has an overall efficiency of about 35 percent. The efficiency could probably be increased to about 40 percent with additional design effort. A PbBi-cooled fast reactor provides a long-term option for sustainable nuclear power, and it can be operated to produce very little transuranic waste. Figure 3 shows the PbBi concept.

#### Simulation and Optimization of Manufacturing.

The purpose of the third phase of this project was to use recently developed industrial engineering methods to simulate the factory fabrication of these reactor concepts and perform analyses to reduce costs. Simulation of factory fabrication requires detailed data on materials, labor, and fabrication processes, and it was determined that simulating an entire reactor fabrication was far beyond the scope of this project. In order to address the key issues, researchers performed a detailed simulation of the fabrication of a heat exchanger, a ubiquitous component that represents much of a reactor's BOP. This work was joined with a much broader study in which the experience in the modular construction of nuclear submarines was used to evaluate the potential cost savings by modular design of the MPBR concept.

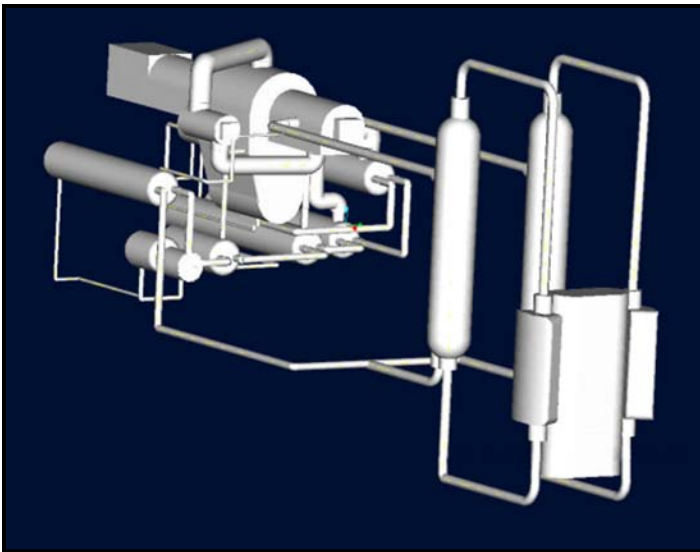


Figure 3. The PbBi concept.

In the factory fabrication study, researchers developed a simulation model that mimics the current and desired production processes for shell-and-tube heat exchanger manufacturing. They also developed a costing model to determine the product cost associated with variations in manufacturing simulations. When the fabrication and costing models were complete, researchers performed a variations-of-parameters study analysis for a 2x4 matrix. The four factors chosen for the study were annual demand, equipment reliability, learning curve, and quality. Two levels were considered for each factor, thereby making the 2x4 matrix. The study showed that demand and learning curve are the dominant influences to cost. In order for the learning curve to take effect, the factory must use a flow-process rather than the usual job-shop process manufacturing. This, in turn, depends on demand quantity and certainty. These improvements can result in significant cost savings, approximately 20 percent, which is large considering the high material costs for these components, which were held constant.

In the second part of this phase, experts in modular submarine construction at Northrop Grumman Newport News reviewed the design of the MPBR concept and evaluated the potential cost savings from modular design and fabrication. Experience in modular submarine construction has shown that reductions in labor costs for fabrication and installation are as much as an order of magnitude. However, the same experience shows that overall labor costs are reduced about a factor of two because of increased engineering costs, planning time, and investment in fabrication and assembly equipment.

Further cost reductions are possible by making the modules and components more amenable to automated fabrication and by using manufacturing processes that result in near nominal production dimensions. The two most important aspects of successful modular construction are:

1. Devising a connecting scheme for the modules that allows for adjustment in all six degrees of freedom during connection, and
2. Developing construction processes that result in the module connection points always being at nominal dimensions.

The final report on this project includes several recommendations on how to achieve these two important criteria.

## Planned Activities

This NERI project has been completed.

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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Integrated Nuclear and Hydrogen-Based Energy Supply/Carrier System (STAR-H2)

PI: David Wade, Argonne National Laboratory

Project Number: 00-060

Collaborators: Texas A&M University

Project Start Date: October 2000

Project End Date: September 2003

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### Research Objectives

The objective of this project was to devise a nuclear energy system intended for the mid-21st-century global energy market conditions where electricity and hydrogen are employed as complementary energy carriers. The resulting concept is a secure, transportable autonomous reactor for hydrogen production (STAR-H2), which is a small, 20-year refueling interval reactor that manufactures hydrogen and potable water sufficient to meet the entire energy and water needs of a city of 25,000 in a developing country. The STAR-H2 fuel cycle is based on full transuranic recycle and regional fuel cycle centers to achieve a sustainable, proliferation-resistant, nuclear-based energy supply suitable for widespread, worldwide deployment.

### Research Progress

#### Identification of Mid-Century Energy Needs.

Researchers on this project evaluated global energy demand forecasts for the 21st century. They projected massive growth in demand for energy services and showed that the dominant capacity additions by 2030 and beyond will occur in the currently developing economies. The global reach of the nuclear client base will expand and so will the range of demanded energy products; there will be an emerging need for process heat conversion of water or hydrocarbon feedstocks to hydrogen. Manufacture of potable water will also be needed as cities increasingly outsource municipal water supply contracts to profit-making entities. By mid-century, population and energy demand will be focused primarily in cities.

**Configuring Nuclear to Meet the Needs.** Because much of the future growth will be in cities of developing nations, market conditions facing future nuclear deployment will be different from the historical conditions where deployment occurred primarily in industrialized countries under regulated electricity market conditions. The STAR-H2

concept was devised specifically to attain Generation IV sustainability goals by responding to the foreseen mid-century needs and market conditions. It is targeted for urban centers, particularly in developing countries, and is designed to fit within a hierarchical hub-spoke architecture. This concept uses nuclear fuel and hydrogen as the long-distance energy carrier and distributed electricity generation as the local carrier to mesh with urban energy distribution infrastructures that uses grid delivery of electricity, hydrogen, potable water, and communications (and sewage return) through a common grid of easements.

The system's small-to-mid size is ideal for incremental deployments where capital financing is not readily available and/or indigenous infrastructure is at an early stage of development. To facilitate rapid assembly and revenue generation, the STAR-H2 concept uses modular construction, factory fabrication, and delivery of a turnkey heat source reactor to the client's site where a non-safety-grade balance-of-plant (BOP) has already been placed. These strategies are intended to achieve economy of mass production to replace the historical economy of scale. The concept also employs extensive levels of passive safety to be consistent with a worldwide deployment of many thousands of plants.

This system has a long (20-year) refueling interval and full core cassette refueling supported from consortia-owned regional fuel cycle (front and back end) service centers, operating under international oversight. This is intended to make nuclear-based energy supply available in countries that do not want to place an indigenous front-to-back fuel cycle infrastructure. The regional centers, infrequent cassette refueling, and full transuranic recycle (such that both reload and spent fuel cassettes meet the spent fuel standard of self protection) are intended to provide appropriate barriers to the possibility of misusing the materials and facilities for military purposes. Full transuranic multi-

recycle is employed to both extract the full energy content of the uranium ore, and to consign only fission products (and trace recycle/refabrication losses) to waste.

The resulting STAR-H2 energy supply architecture will provide centuries of energy security via a hierarchical hub/spoke arrangement using an ordered sequence of energy carriers: (nuclear fuel → hydrogen → electricity) based on their power-carrying capacity. The architecture will employ non-carbon-emitting technology and nuclear fuel recycle to achieve sustainable ecological closure. If successfully deployed, such an arrangement can meet all elements of the broad definition of sustainability for global energy supply.

**The Reactor Heat Source.** STAR-H2 is a Pb-cooled, fast neutron spectrum, 400-MWth reactor operating at low power density with natural circulation cooling, passive load following, and passive safety response characteristics. The 400-MWth sizing retains a rail-shippable reactor vessel size and allows for passive decay heat removal. The lead coolant enables a low power density, high coolant volume fraction fuel pin lattice. This allows natural circulation to remove the heat at full power. Its neutron reflection properties and hard neutron spectrum permit fissile self-regeneration in the core lattice, which achieves zero burnup reactivity loss over the 20-year burnup interval and minimal reactivity vested in control rods. These characteristics are key to enabling passive load following/passive safety. Passive safety/passive load following in turn enables use of a balance-of-plant having no safety function; this allows for the indigenous construction and operation of the balance-of-plant, using the local work force and institutional conditions prevalent during the initial stages of industrialization and providing local jobs for economic growth. The reactor has been designed and shown to meet its long life and passive safety/passive load following requirements.

**The Balance of Plant (BOP).** The STAR-H2 balance-of-plant is comprised of three cascaded cycles (water cracking, Brayton cycle, desalination) operating at successively lower temperatures. The heat rejected from each cycle is used to drive the succeeding cycle. The reactor supplies 400 MWth of heat between 800°C and approximately 650°C to the BOP through a flibe (fused salt) intermediate loop. The strategy of this BOP plant design is to use the heat as follows: use as much of the heat as possible to maximize hydrogen production; use only as much of the heat to make electricity in the Brayton cycle as is required to run the BOP; use whatever heat is finally left over to desalinate water.

The Ca-Br water cracking cycle has three main segments: an endothermic "water cracking" segment where  $\text{CaBr}_2$  and steam react to make HBr and CaO; an exothermic Ca rebromination segment where CaO and bromine react to regenerate  $\text{CaBr}_2$  for recycle and release heat and oxygen; and a plasma chemistry HBr cracking segment where electrical driven radio frequency (RF) energy cracks HBr to regenerate bromine for recycle and to release hydrogen. The plasmatron is followed by a pressure swing absorption cascade that cleans and pressurizes the hydrogen to meet pipeline delivery specifications.

In the segment for regeneration of  $\text{CaBr}_2$  from CaO, heat at 600°C is rejected. It is used to help drive the SC- $\text{CO}_2$  Brayton cycle. After expanding in the Brayton cycle turbine, the SC- $\text{CO}_2$  passes through a high-temperature and a low-temperature recuperator. It exits the low-temperature recuperator at 125°C. Heat is rejected from the SC- $\text{CO}_2$  in the Brayton cycle cooler, which cools the SC- $\text{CO}_2$  to 31°C in preparation for its compression.

Seawater provides the cooling fluid for the cooler, and the resulting 100°C seawater delivers heat and seawater feedstock to the desalination plant. The desalination plant is a feed forward multi-effect-distillation (MED) design, which produces 8,000 m<sup>3</sup>/d of potable water. Finally, heat at a temperature slightly above ambient exits the plant in the form of heated brine tailings from the desalination process.

The BOP has been designed and shown to achieve about 44 percent conversion of heat to H<sub>2</sub> lower heating value (LHV)—making 160 MWth-days/day of H<sub>2</sub> (LHV) and 8,000 m<sup>3</sup>/day of water—enough to support a city of 25,000.

**The Fuel Cycle.** The reactor uses uranium/transuranic nitride fuel and operates on a 20-year, whole-core cassette refueling interval; it is fissile self-sufficient with an internal core conversion ratio of one. The fuel recycle technology is based on electrometallurgical recycle and remote vibropack refabrication of the uranium/transuranic N-15 enriched nitride fuel. The recycle technology produces a co-mixed stream of all transuranics and removes incomplete fission product such that the transuranic materials during processing and during fresh and used cassette shipping are always at least as unattractive for military use as is light water reactor spent fuel. All fuel cassette shipments and used cassette returns are conducted by Regional Center personnel who bring the refueling equipment with them and take it away with the spent cassette. No refueling equipment remains at the site.

The fuel cycle feedstock is natural or depleted uranium, and multi-recycle through sequential cassette reload cycles achieves total fission consumption of the feedstock; only fission product waste forms (and trace losses of transuranics) go to a geologic repository.

**Institutional Innovations.** The nuclear industry will have to undergo significant structural changes in order to support an expanding STAR-H2 segment of nuclear energy supply. The business would likely become one analogous to the airplane and automobile sales businesses where risk is transferred from client to supplier; where customers receive a standardized commodity product, prelicensed and ready to use; and where suppliers make significant up-front investments in factories and fuel cycle facilities to supply a large volume of sales. Conceptual business plans have been identified.

## Planned Activities

This three-year project was completed in September 2003. Fuels, materials, and chemical plant R&D is required to progress further with this design. STAR-H2 is a member of the Gen-IV Small Pb-Alloy Reactor Concept family, which is one of the six concepts selected for further R&D work under the Gen IV Initiative. The Ca-Br cycle is a backup option included in the draft *Generation IV Hydrogen R&D Plan*.





# NUCLEAR ENERGY RESEARCH INITIATIVE

## Development of Design Criteria for Fluid-Induced Structural Vibrations in Steam Generators and Heat Exchangers

PI: Ivan Catton and Vijay K. Dhir, University of California-Los Angeles

Project Number: 00-062

Collaborators: None

Project Start Date: August 2000

Projected End Date: November 2003

### Research Objectives

- a) **Single-Phase Flow:** For this research area, the objectives were to 1) measure velocities and pressure distributions in square and triangular arrays with different pitch-to-diameter ratios for rigid and flexibly mounted tubes, including several heated tubes to determine the relationship between instability avoidance and heat transfer penalty, and 2) determine the entrance length and develop a stability map.
- b) **Two-Phase Flow:** For this research area, the objectives were to: 1) determine fluid-elastic instability conditions on tube arrays and single tubes in rigid arrays held at different orientations to the flow; 2) based on that data, develop an instability map; 3) conduct single tube steam-water flow and stability tests and compare results to air-water data; 4) measure flow and stability when the tubes are heated to cause boiling; 5) establish the differences between air-water and steam-water flow and stability characteristics.
- c) **Theoretical Development:** Under this task, the objectives were to: 1) develop numerical algorithms for solving the governing equations using the vorticity transport equation as a first approximation, 2) use data from the measurements of pressure differences in an array of rigid cylinders to check the validity of pressure variation assumption, 3) develop an energy equation for use in steam-water studies, 4) begin the development of models to describe the instabilities, 5) initiate development of tools to model the entrance region, 6) improve the constitutive relations and models needed for flow and stability modeling, 7) incorporate basic design data (tube material, diameter, wall thickness, length, type of support and internal flow and heat transfer) into the models, and 8) develop a relationship between tube supports used in experiments and prototypic supports.

### Research Progress

**Single-phase Flow.** The main focus of this work was studying the influence of two different parameters on the onset of the fluid elastic instability. In particular, researchers conducted different sets of experiments on two array configurations: normal square and normal triangular (Figure 1). During this period, they conducted and analyzed a complete set of experiments for the normal triangular array configuration, where the natural frequency of vibration of the tubes has been set to three different values: 12, 16, and 20 Hz. These natural frequencies correspond exactly to those used for the normal square array configuration. After investigating normal square array configuration, researchers chose to provide a data set of the normal triangular pattern for comparison. The pitch-to-diameter ratio of the triangular array is equal to that of the square array, allowing for a single parameter to be isolated so they could investigate the effect on the fluid-elastic instability (FEI) onset independently.

The first important measure was to identify and quantify the onset of fluid-elastic instability. Researchers used two methods (interpolation, correlation) to analyze the motion of seven adjacent tubes in the normal triangle configuration (as was done for the five tubes in the normal square array). The tubes were labeled according to the figure shown below.

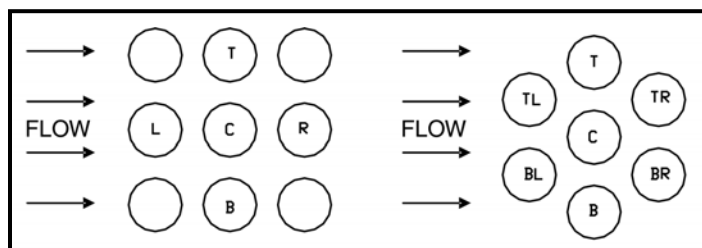


Figure 1. Normal square array (left) and normal triangular array (right). T=Top, C=Center, B=Bottom, R=Right, L=Left, TR= Top Right, TL=Top Left, BR= Bottom Right, BL=Bottom Left.

For each reduced velocity, researchers recorded a time series of 600 images, which corresponded to a time period of 5 seconds. The first data set (set 0) was taken for a reduced velocity equal to zero, in order to determine the static equilibrium position of the tube. For each configuration and calibration frequency, a different number of points

were taken. Both the interpolation and correlation methods were applied to each data set; since the two methods showed a good agreement, only results from the correlation method are reported. Figures 2 through 4 show the behavior of the tubes vibration amplitude at different flow speed for the normal triangular array calibrated at 12, 16, and 20 Hz.

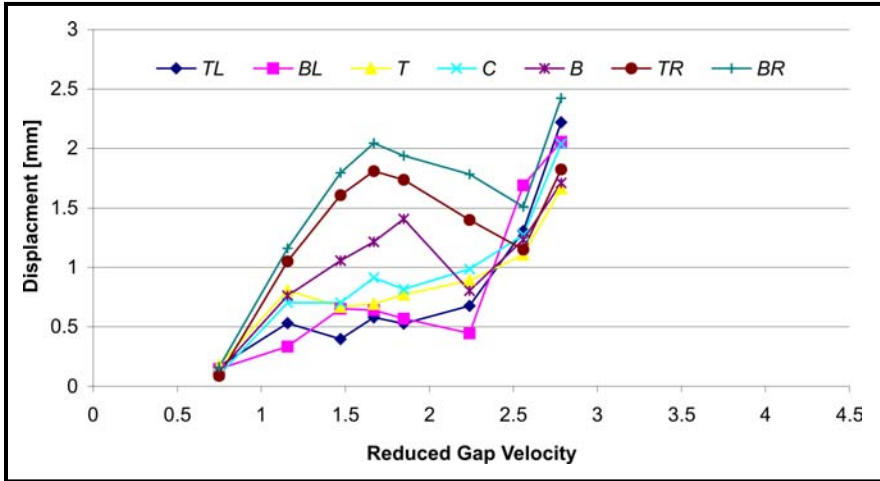


Figure 2. Mean relative vibration amplitude for normal triangular, 12Hz.

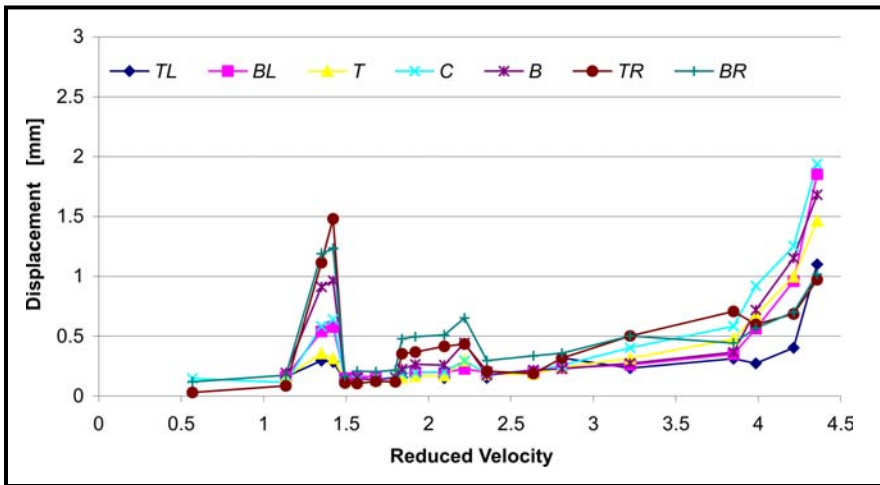


Figure 3. Mean relative vibration amplitude for normal triangular, 16Hz.

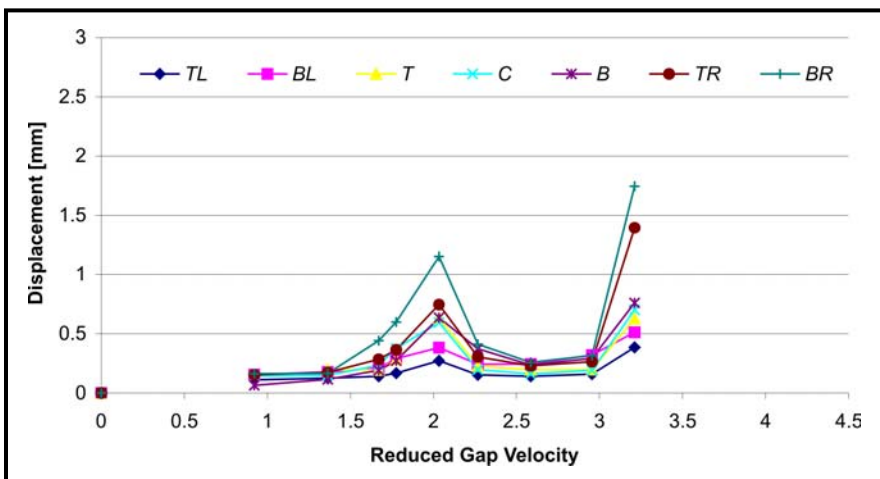


Figure 4. Mean relative vibration amplitude for normal triangular, 20Hz.

Several features of the tube array vibration may be noted from the figures. The first figure of the series (Figure 2) shows a gradual increase in the vibration amplitude and a subsequent decrease occurring in a reduced velocity range related to the "vortex shedding" phenomenon. In this case, the energy associated with this particular mode of vibration is much larger and the phenomenon is not as sudden as the one occurring when the array is calibrated at higher frequencies.

Figure 3 shows that, at a specific reduced velocity of about 1.4, there is a sharp increase in the average magnitude of vibration of the tubes; as noted before, this feature corresponds to vortex shedding. The magnitudes of these vibrations varied greatly from tube to tube in the array. Researchers noted that the two tubes farthest downstream were the most excited, while the vibration magnitude of the top and top left tubes was less than 20 percent of this magnitude. The downstream tubes may have been more excited due to the vortices originating from the upstream vibrating tubes. However, until researchers determine the velocity field of the flow around the flexible tubes, they will not be able to conclude the exact reason for this behavior. It is nonetheless useful to know that, in this array configuration, the downstream tubes were indeed more susceptible to vortex-induced vibration.

Researchers compared the experimental results with similar results available from literature. From this, researchers developed an instability map where the onset of fluid elastic instability, regarded as the flow critical reduced velocity, was plotted against the mass damping parameter. Figure 5 provides a sampling of data from other

experiments (Weaver et al., 2000) in single-phase flow. Figure 5 also shows the suggested design guidelines, labeled "suggested limit," as recommended by the ASME Boiler Code (Section III, Appendix N) and the median curve that best interpolate the experimental data overall. The black squares on the chart correspond to the points that mark the onset of instability for the normal square array experiments. All the points corresponding to the triangular array lie above the mean curve, thus indicating that two different criteria should be used for the two different geometries that were investigated.

The "suggested limit" curve appears to be too conservative when applied to the normal triangular configuration. This is because, compared to the normal square configuration, the normal triangular array is less susceptible to the onset of fluid-elastic instability at the same levels of mass damping. Although the suggested limit curve may apply to the normal square array configuration, applying such a strict design for the normal triangular array may result in a lower efficiency for the heat exchanger, therefore causing economic losses.

**Two-phase Flow.** The objective of the two-phase flow experiments was to determine the differences between experiments conducted with steam-water mixtures and air-water mixtures that have commonly been used to simulate fluid-elastic instability. A number of differences exist between these two fluid systems. A growing body of literature calls for researchers to carry out more experiments with steam-water mixtures. To this end, in the previous project period (September 2001-September 2002), researchers conducted and reported on a two-phase flow loop capable of producing air-water and steam-water

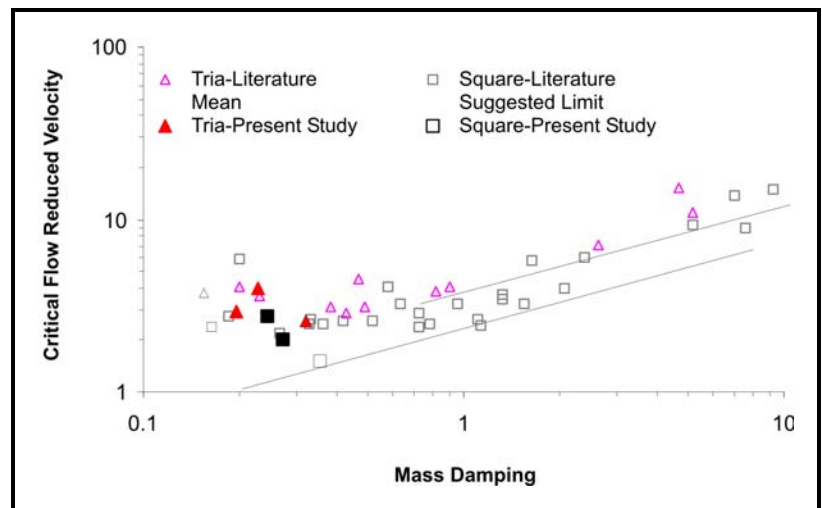


Figure 5. Instability map for single-phase flow experiments; comparisons.

mixtures. During this period, they also demonstrated and reported on using the strain gauges to predict unstable vibration of a prototypical tube.

In this period, researchers carried out two-phase flow experiments with air-water flow in a normal square fully flexible array and compared the results with those conducted in an array consisting of a single flexible tube in a rigid array. The differences between the sets of experiments performed in this study and those used for comparison are listed in Table 1. The experiments in the present study were compared with those of Pettigrew et al. (1989), who provided one of the most comprehensive datasets available on air-water flow, and those of Joo and Dhir (1995), both of which were conducted previously in this laboratory. All experiments have been carried out with air-water and are different mainly in the way the tubes were made flexible.

Researchers	Variable	Pettigrew <i>et al.</i> (1989)	Joo and Dhir (1995)	Present study
	<b>Array Geometry</b>	Normal square	Normal triangular	Normal square
	<b>P/D range</b>	1.47	1.4	1.4
	<b>Void fraction (%) range</b>	5 - 99	0 - 50	0 - 50
	<b>Method of suspension</b>	Cantilevered tube, clamped at one end	Cantilever-beam suspension	Piano wire suspension
	<b>Rigid/Flex. array</b>	Fully Flexible array	Flexible tube/Rigid array	Fully flexible array
	<b>Damping ratio</b>	Flexible tube in rigid array	Flexible tube in rigid array	Tube in fully flexible array
	<b>Void-fraction measurement</b>	Homogeneous model	Gamma-densitometry	Gamma-densitometry
	<b>L/D</b>	46	9	13.125

Table 1. Summary of test conditions for air-water fluid-elastic instability tests.

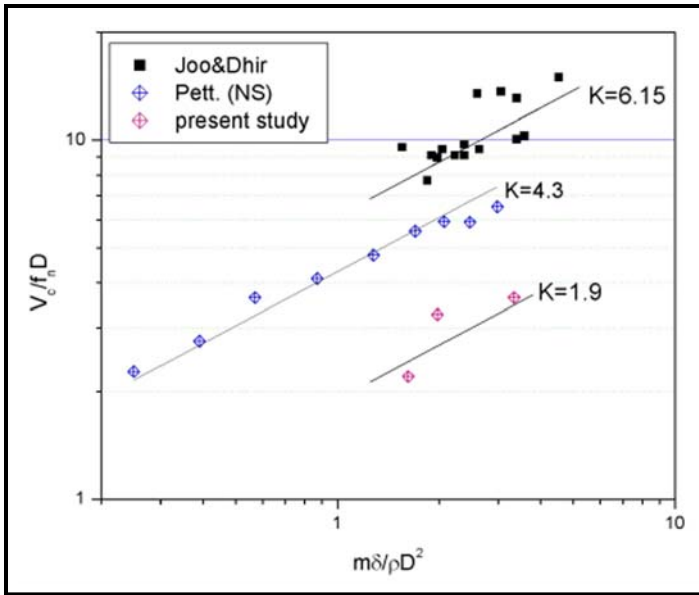


Figure 6. Results of air-water flow experiments plotted on Connors' criterion plot.

**Theoretical Development.** Researchers plotted the results using the Connors' criterion. This criterion relates the non-dimensional reduced flow velocity to the mass damping parameter as

$$\frac{V_c}{f_n D} = K \left( \frac{2\pi m \zeta}{\rho D^2} \right)^{0.5}$$

where  $V_c$  is the critical two-phase flow velocity;  $f_n$  is the natural frequency of the tube;  $D$  is the tube diameter;  $m$  is the mass/length of the tube;  $\zeta$  is the damping ratio of the tube in two-phase flow;  $\rho$  is the fluid density; and  $K$  is the instability constant. The three data sets follow yield for three distinct values of  $K$  indicating that parameters (structural and flow) not appearing in the Connors' criterion lead to differences and these need to be accounted for in a correlation predicting fluid-elastic instability.

Researchers carried out a limited number of tests on steam-water flow. The main difficulties with performing these experiments were in controlling the void fraction of the mixture by controlling the flow rates and temperatures of the two phases. Figure 7 shows the results from a steam-water two-phase flow test at a water flow rate of  $Q_j=20$  gpm compared to an air-water flow test at a water flow rate of  $Q_j=30$  gpm. The results of the amplitude of tube vibration show that the instability is achieved earlier in steam-water flow. Researchers investigated this effect by using improved test methods for performing steam-water flow experiments and by investigating the differences between air-water and steam-water systems.

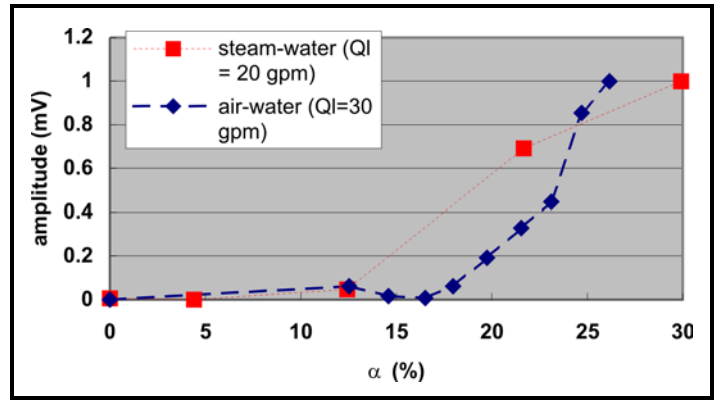


Figure 7. Comparison of tube vibration amplitude for air-water and steam-water flow.

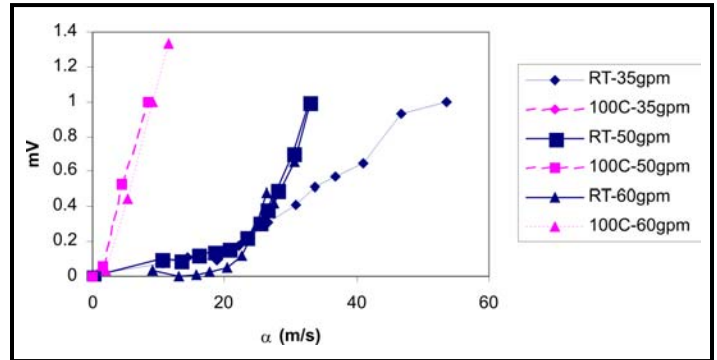


Figure 8. Comparison of rms amplitudes for air-water flow tests at room temperature and elevated temperature.

In order to understand this effect in a better manner, experiments were proposed with air-water flow at near saturation temperatures (elevated temperature air-water flow). In these experiments, a single flexible tube in a rigid normal square array was used. In these experiments, the bulk water was heated to 99°C and air at room temperature was introduced into the air line. Since the air was at room temperature, the air expanded as it reached the higher bulk water temperature to form the two-phase mixture. This was accounted for in the calculation of the corrected air-flow rate. The results from tests carried out at base water flow rates of 35, 50, and 60 gpm are shown in Figure 8 along with the results from the air-water flow tests at room temperature. As in the case of the steam-water flow experiments, it is seen that the tubes become unstable at a very low void fraction. Clearly, differences exist between the fluid systems. More systematic experiments are needed to resolve the differences in experimental results observed in the three cases.

### Planned Activities

This NERI project has been completed.

# NUCLEAR ENERGY RESEARCH INITIATIVE

## An In-Core Power Deposition and Fuel Thermal Environmental Monitor for Long-Lived Cores

PI: Don W. Miller, The Ohio State University

Project Number: 00-069

Collaborators: Westinghouse Science and Technology Center

Project Start Date: September 2000

Projected End Date: December 2003

### Research Objectives

The primary objective of this program was to develop a constant temperature power sensor (CTPS) for the core of the reactor. This sensor would provide a detailed map of local nuclear power deposition and coolant thermal-hydraulic conditions during the entire life of the core. In DOE Generation IV reactor cores, this could include normal operation, post-accident operation, and monitoring after the core is placed in permanent storage. The sensors used in this instrumentation must have a lifetime comparable to the core and be compatible with the neutronic and thermal conditions expected over the range of proposed Generation IV reactor designs. The sensors must be robust and capable of operating even with extensive material degradation and, if required to achieve this objective, they must provide for *in situ* calibration and performance monitoring.

The CTPS concept was based on maintaining a constant temperature in a small mass of actual reactor fuel or fuel analogue by adding heat through resistive dissipation of input electrical energy. Researchers used a feedback control loop to provide the exact amount of input electrical energy needed to keep the fuel mass at a specified constant temperature, well above the coolant bulk temperature, regardless of the nuclear energy deposited in the mass. Energy addition to the fuel mass and fuel temperature feedback to the controller were both provided by a simple resistive heating element embedded in the fuel mass. The electrical energy required to maintain a constant temperature provided a measure of the actual nuclear energy deposition, since they are inversely related.

### Research Progress

The majority of the effort over the last year has focused on completing sensor prototypes. Screen printed sensors with a planar geometry had a higher potential for developing CTPS and constant heat flux power sensors (CHFPS) than comparable sensors with cylindrical geometry. That is why researchers on this project focused on screen-printed planar CTPS and CHFPS. This sensor design is shown in Figure 1.

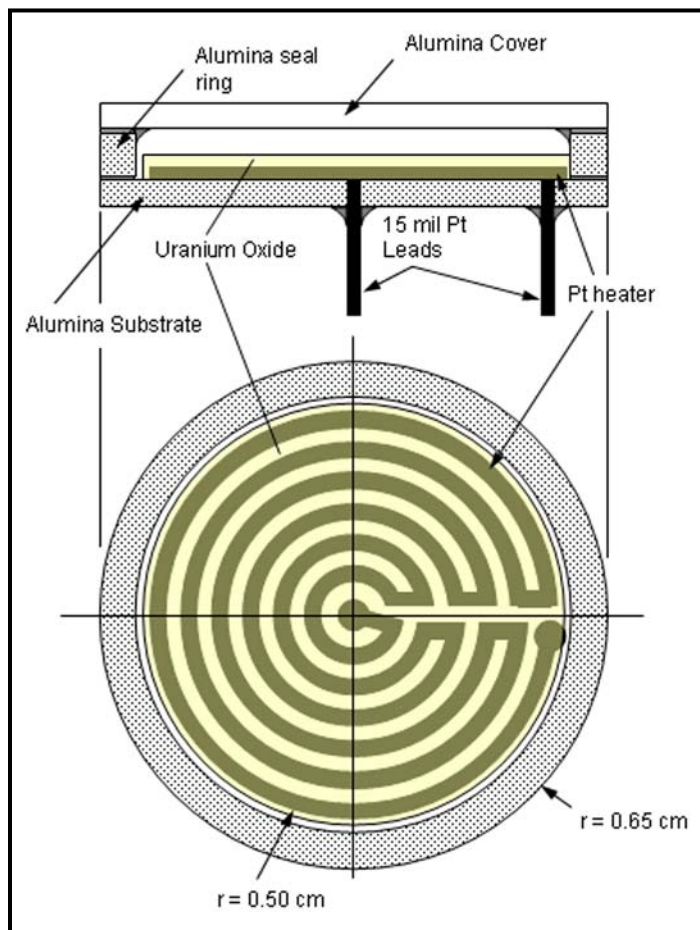


Figure 1. Planar, screen-printed sensor design.



Researchers produced four different variants and four sensors of each type. The leads on this group of sensors were 15 mil platinum wires. The heavier wire solved the lead fragility problem observed in an earlier set of sensors made with 6 mil platinum leads. Each sensor contained 17.8 mg of  $U^{235}$ . The uranium oxide used contained 97 percent  $U^{235}$  and 3 percent  $U^{238}$ . After fabrication, researchers leak tested all sensors by vacuum impregnation with distilled water. Leakers gained substantial weight, due to the imbibed water, and could easily be distinguished from sensors that were sealed. Researchers successfully sealed leaking sensors by coating the circumference with feldspar paint and firing a final time at 1,250°C in forming gas. All leaks were confined to the joints between the substrate and sealing ring or to the joints between the top cover and the sealing ring. No leaks were observed in the seals around the lead wires. Several sensors had transparent sapphire ( $Al_2O_3$ ) covers so that researchers could examine the inside of the sensors after testing them in the reactor. Sensors of each type are available for performance evaluation at the Ohio State University's nuclear reactor.

Completion of this research provided technical information regarding the benefits of incorporating constant temperature power sensors and constant heat flux power sensors in the instrumentation and control (I&C) systems in both operating and Generation IV nuclear power plants, such as the Westinghouse IRIS. It also provided insight into the additional research and development required to develop a viable commercial product.

### **Planned Activities**

This NERI project has been completed.

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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Design and Construction of a Prototype Advanced On-Line Fuel Burn-up Monitoring System for the Modular Pebble Bed Reactor

PI: Bingjing Su, University of Cincinnati

Project Number: 00-100

Collaborators: North Carolina State University,  
Massachusetts Institute of Technology

Project Start Date: August 2000

Project End Date: December 2003

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### Research Objectives

The overall goal of the project was to conceptually design, construct, and test an advanced on-line fuel burn-up monitoring system for the next-generation modular pebble bed reactor (MPBR). The MPBR is a high-temperature, gas-cooled nuclear power reactor currently under study as a possible Generation IV system. In addition to its inherently safe design, a unique feature of this reactor is its multi-pass fuel cycle in which the graphite fuel pebbles are randomly loaded and continuously cycled through the core until they reach their prescribed end-of-life burn-up limit (approximately 80,000 MWD/MTU). An on-line measurement system is needed to accurately assess whether a given pebble has reached its end-of-life burn-up limit. The monitor would provide an on-line, automated go/no-go decision on fuel disposition on a pebble-by-pebble basis.

This project investigated approaches to analyzing pebble bed fuel in real time using gamma spectroscopy and possibly using passive neutron counting of spontaneous fission neutrons to provide the speed, accuracy, and burn-up range required for the MPBR. The project involved all phases necessary to develop and construct a burn-up monitor, including a review of the design requirements of the system, modeling and development of potential designs, and, finally, the construction and testing of an operational detector system.

### Research Progress

The project had four major tasks. Progress in each task is briefly summarized.

**Task 1: Identification of the System Requirements.** The objective of this task was to determine the design requirements for an on-line burn-up

monitoring system to be used with the MPBR plants. This task involved collecting the most recent design parameters from the MPBR design effort underway at Massachusetts Institute of Technology (MIT), the Idaho National Engineering and Environmental Laboratory (INEEL), and South Africa's ESKOM. Based on the information collected, the research team determined the required availability of the burn-up monitor, pebble throughput rates, burn-up ranges of interest, cool-down time for pebbles prior to measurement, and other basic physical parameters that are needed for the design of an on-line burn-up monitor.

#### **Task 2: Finding Correlations Between Fuel Burn-up and Radiation Emission from a Pebble.**

The objective of this task was to accurately model the buildup of fission products and transuranic elements in irradiated fuel pebbles and to identify correlations between types, amounts, and spectra of radiation emitted from a fuel pebble and the fuel burn-up level of the pebble. To this end, the team used the ORIGEN2.1 code to perform the fuel depletion calculations and investigated the utilization of passive gamma-ray spectrometry and neutron counting methods to establish a power-history and cooling-time insensitive burn-up measurement approach, which relies on the relationship between the burn-up and the radiation emitted by the fuel pebble from fission products or heavy actinides that have built-up during its passing through the reactor core.

In the case of gamma-ray measurements, researchers found that accurate and predictable correlations between activity and burn-up can result if Cs-137 and Eu-154 are used as burn-up indicators. The activity of these radionuclides exhibited a behavior that is highly independent of the cooling time and the in-core power history (i.e., the pebble's path in the core). Variations in the predicted discharge burn-up are about 3 to 5 percent when the

cooling time is varied between 0 and 7 days and the power is varied between 50 and 150 percent of the nominal thermal core power.

In addition, researchers studied the option of using artificially introduced dopants (e.g., Co-59) as burn-up monitors. The use of such dopants may be desirable because they can provide intense and high-energy gamma rays to improve signal-to-noise characteristics, and, therefore, can improve the accuracy of the measurement. Results indicated that the relative activity ratio of Cs-134 to Co-60 is resistant to power variation and thus is a potential indicator of discharge burn-up that is accurate to within 5 percent. Furthermore, using a relative burn-up indicator eliminated the need for an absolute efficiency calibration of the gamma ray detector and thus minimized the contribution of a detector calibration error in the final uncertainty analysis of the burn-up monitoring system.

Researchers also investigated the use of passive neutron counting as a method for measuring burn-up. After a pebble is taken out of the reactor, neutrons are produced either by the spontaneous fission of heavy actinides or from the ( $\alpha$ , n) reactions that take place within the pebble. The depletion calculations indicated that the ( $\alpha$ , n) component is negligible compared to the contribution of spontaneous fission at a high burn-up level. Moreover, the spontaneous fission component is dominated by the contribution from Cm-244 that has a half-life of 18.1 years. This allowed the establishment of a correlation between neutron emission from a pebble and its burn-up. Results showed that total neutron emission can be used as a burn-up indicator. However, this emission/burn-up correlation is less resistant to power history variation than that of Cs-137 and is usable only at high burn-up range (such as greater than 60,000 MWD/MTU) due to low production rate for neutron emitters. In addition, this correlation is reactor-type dependent and is sensitive to spectral averaged cross sections used in the ORIGEN depletion calculations. Therefore, the neutron emission/burn-up correlation obtained by using ORIGEN2.1 could have a large degree of uncertainty.

**Task 3: Study on the Detectability of Selected Burn-up Indicators and Related Issues.** Although the work of the previous task concluded that passive gamma-ray spectrometry of selected fission products and passive total neutron counting have the potential to be developed as credible methods for on-line burn-up measurement, the feasibility of using any of these approaches must take into account other considerations. Paramount among these is the ability to perform the measurements within the realistic requirements of throughput and the overall system reliabil-

ity. That was the focus of this task. The objectives of this task were to establish signal-to-source response functions for candidate detector systems, detector selection and optimization, and conceptual system design. Following is a description of the major accomplishments and conclusions of this task.

MCNP was used to simulate the signal-to-source response functions for several candidate gamma-ray spectrometers that are based on either cryogenically cooled or room temperature high-purity germanium (HPGe) detectors. In addition, the Gaussian broadened spectra for these detector responses were produced by using the full-width at half-maximum vs. energy relation generated by SYNTH. For Cs-137, the activity measurement was performed using the 662 keV gamma line, which is found to be significantly interfered by the 658 keV line of Nb-97. This spectral interference cannot be completely resolved—even when using high-resolution germanium detectors. Detailed analysis revealed that this spectral interference may cause 10 to 30 percent uncertainty in determination of the Cs-137 peak area.

Researchers computed the minimum detectable activities of candidate fission products. Results indicated that for gamma spectrometry measurements, Cs-137, Cs-134, and Co-60 are radioactively strong enough to be detected. With approximate values for the detection efficiency, the expected measurement time that would allow a statistically accurate result for burn-up measurement varies between 30 to 60 seconds. This will be sufficient to meet a circulation rate of one pebble every 30 seconds, especially if a multi-detector system with enhanced detection efficiency is used.

Because the measurement is expected to be conducted under high counting rate conditions, the pulse pileup effect in gamma spectrometry measurement was also studied. The team developed a Monte Carlo algorithm to simulate the pile-up behaviors of both an analog and a digital gamma-ray assay system. Results showed that the pileup effect caused significant distortion to gamma spectra. They also showed that below 2-3 MeV the digital system is more resistant to pileup than the analog system. More importantly, researchers concluded that any counting setup for a proposed assay device must use, in addition to other aspects, a count-rate-dependent response of the system. The count ratio of Cs-134/Co-60 was found to be more resistant to the pileup effect than the Cs-137 count.

On the neutron counting approach, the team investigated the use of BF<sub>3</sub> tube, fission chamber, Gd converter, SiC detector, He-4 proportional counter, He-3 counter, and



an active neutron counting method for the on-line burn-up determination for fuel pebbles. The difficulties with the on-line neutron measurement included the following: low neutron emission rate (approximately  $10^4$  neutrons per second at the discharge burn-up), short measurement time (30 seconds), and extremely high gamma noise (greater than  $10^{13}$  gammas per second). Through their analyses and MCNP simulations, researchers found that most of the neutron measurement methods were unsuitable for this on-line application due to either the low detection efficiency, or the incapability of discriminating gamma rays, or both. However, two methods were identified to potentially meet the on-line measurement requirements.

One method is to use a multiple-fission-chamber detection system. Fission chambers can effectively discriminate gamma rays because the electrical pulses produced by neutron fission reactions appear above 50 MeV, much greater than the pulse energies produced by various gamma interactions. However, the detection efficiency of a single (conventional) fission chamber is not high enough for the application. To improve the detection efficiency, the team designed a multiple fission chamber system, which can lead to hundreds of neutron counts within 30 seconds by the system when a pebble's burn-up is greater than 60,000 MWD/MTU. The other method is to use a He-3 neutron detection system, which includes gamma shield, neutron moderator, and three He-3 gas counters. Studies showed that the detection efficiency of the system is higher than the requirement, and the gamma exposure rate inside each He-3 chamber is lower than the typical operation limit of 10 Rad/h.

**Task 4: Set up of a Burn-up Measurement System and Experimental Testing.** In this task, the team constructed a high-resolution gamma spectrometry detec-

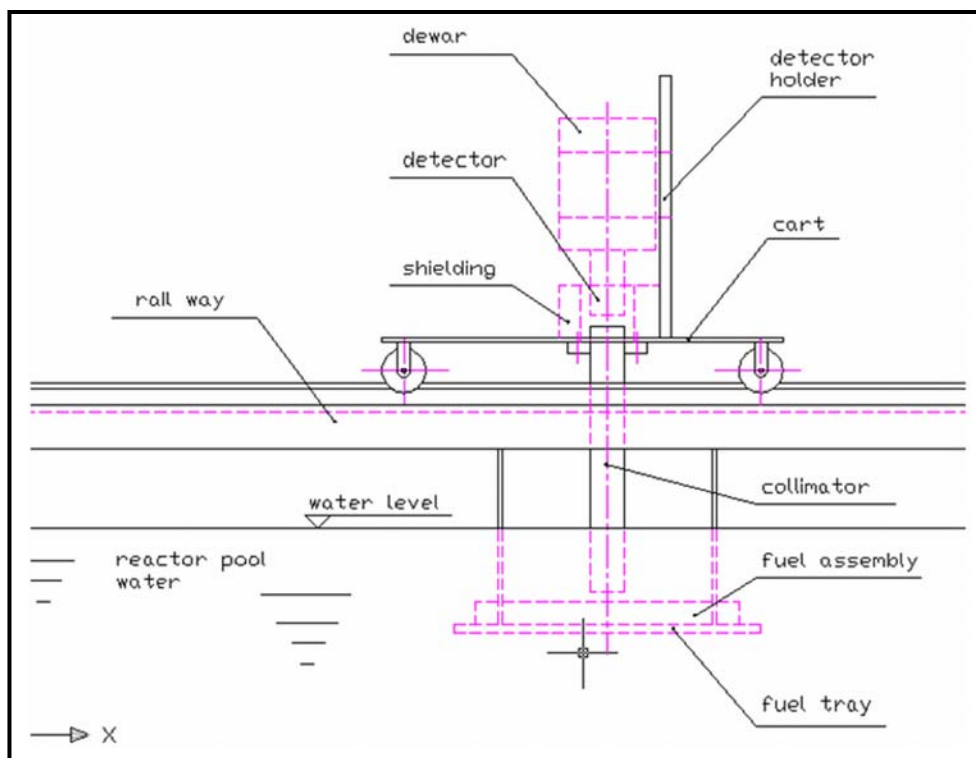


Figure 1. Fuel measurement setup at the NC State PULSTAR reactor.

tor system as a burn-up monitor. The main components of the system are a 40-percent n-type, coaxial HPGe (resistant to neutron damage); a digital gamma-ray spectrometer; and a data acquisition computer. Researchers calibrated this burn-up monitor system and completed preparation for the fuel measurements at the NC State PULSTAR reactor. The team plans to utilize this system and the fuel of the PULSTAR ( $UO_2$  enriched to 4 percent in U-235) to experimentally study issues related to the on-line gamma spectrometry assay. Figure 1 shows the setup designed to perform the measurement. The group working on this task is currently in the process of performing the measurements and will prepare a final report of the results.

## Planned Activities

The remaining activities include 1) conducting experiments at the North Carolina State University's PULSTAR Reactor Laboratory to evaluate fundamental gamma spectrometry issues that may affect the burn-up measurement, and 2) preparing a final report documenting the research performed and main conclusions of this project.



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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Balance-of-Plant System Analysis and Component Design of Turbo-Machinery for High-Temperature Gas Reactor Systems

PI: Ronald G. Ballinger, Massachusetts Institute of Technology

Project Number: 00-105

Collaborators: Northern Engineering & Research

Project Start Date: August 2000

Project End Date: September 2003

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### Research Objectives

The purpose of this project was to develop a conceptual design and systems analysis tool for evaluating turbo-machinery and balance-of-plant (BOP) power conversion in high-temperature, gas-cooled reactor systems. Current concepts for high-temperature, gas-cooled reactor systems call for modular designs with electrical output in the 110 MWe range. Key questions that needed to be addressed to adequately evaluate these systems include: 1) Can a helium power turbine be developed in the 110 MWe range? 2) Can advanced compact heat exchanger technology be used in the design of intermediate heat exchangers (for indirect cycle plants) and/or recuperators (direct and indirect cycle plants)? 3) Can structural and materials issues be adequately characterized to allow for detailed life-cycle analysis? and 4) How do specific component designs impact overall cost?

**Project Design Goals.** Following were the overall design goals of the project.

1. Develop a "reference" plant design that could be built without significant advances in technology. This design needed to satisfy all appropriate codes and standards and should not have required a significant R&D effort on the part of the component vendors.
2. Answer key questions related to the design of the power conversion system. These questions encompass three general categories: 1) intermediate heat exchanger design, 2) turbine and compressor design, and 3) system control.
3. Develop an "advanced" design that allows for prudent and achievable extensions of technology. In this context, "prudent and achievable" is taken to mean that some development effort may be needed but that this development effort should not result in this being a significant fraction, i.e., greater than 20 percent of the cost of the system.

The design team also had to make an assumption as to the nuclear island. While it was not the task of the project to "design" the nuclear island, it was necessary to choose a reference system as the starting point. For this project, researchers chose the current ESKOM pebble bed modular reactor (PBMR) as their reference. This was a reasonable choice for one obvious reason—its design fit with the design criteria in that it represents a Brayton cycle plant that is currently being designed for commercial use and, therefore, will be constrained by the same codes and standards of the BOP design.

### Research Progress

Progress made on this project includes the following:

- Researchers first established a "reference" plant design which can be built with existing technology. However, the thermal efficiency of the plant was sub-optimal due to restrictions on the reactor outlet temperature to 850°C. The BOP design is a 4-shaft design. The number of shafts resulted in an increase in control complexity.
- Based on the initial reference design, researchers identified key issues that needed to be addressed to achieve an advanced design that could be built using current technology but with some additional confirmatory R&D effort.
- Researchers developed the final reference design. In the final design, the reactor outlet temperature was increased to 900°C. This has resulted in an increase in efficiency to approximately 45 percent and a reduction in the number of shafts from 4 to 3.
- Researchers established final "reference" designs for the turbo machinery and heat exchangers, including the intermediate heat exchanger. Two concepts were identified; however, each design would require that active measures be taken to assure safe operation.

- Researchers identified potential vendors for all of the major components and obtained cost estimates for these components.
- Researchers developed a steady-state model for the overall plant; this model was used to optimize the system configuration.
- Researchers developed a transient model, which was also used to optimize the final reference design.

The above project goals imply certain constraints on the design process. The general design constraints were established as follows:

1. Compliance with the ASME Boiler and Pressure Vessel Code, Section III, Class I, for the primary pressure boundary, which includes the reactor vessel and piping and the primary side of the intermediate heat exchanger.
2. Compliance with the ASME Boiler and Pressure Vessel Code, Section VIII, where applicable.
3. Purchasable components.
4. Use of the ESKOM PBMR as the primary heat source.

**ASME Code Compliance.** ASME code compliance places limits on temperature, allowable stress, and materials selection. Section III qualified materials are the most severely limited in the entire ASME code. The requirement of Section III places limits on the intermediate heat exchanger inlet temperature. For advanced materials (9Cr-1MoV or Alloy 625), an allowable inlet temperature of 500°C could be achieved. This allowed an outlet temperature of 880°C, which is compatible with a reactor gas outlet temperature of 900°C. However, at these temperatures, the maximum allowable stresses place severe design constraints on the intermediate heat exchanger. These constraints require that an "operating" curve for this component be established in which time and temperature for a given differential pressure (primary to secondary) accumulation is measured to predict component life and assure safe operation. This meant that for certain accident scenarios both of the primary and secondary sides need to be pressure regulated to minimize differential pressure stresses.

**Purchasable Components.** This design constraint was due to technology limits. For the initial phase of the

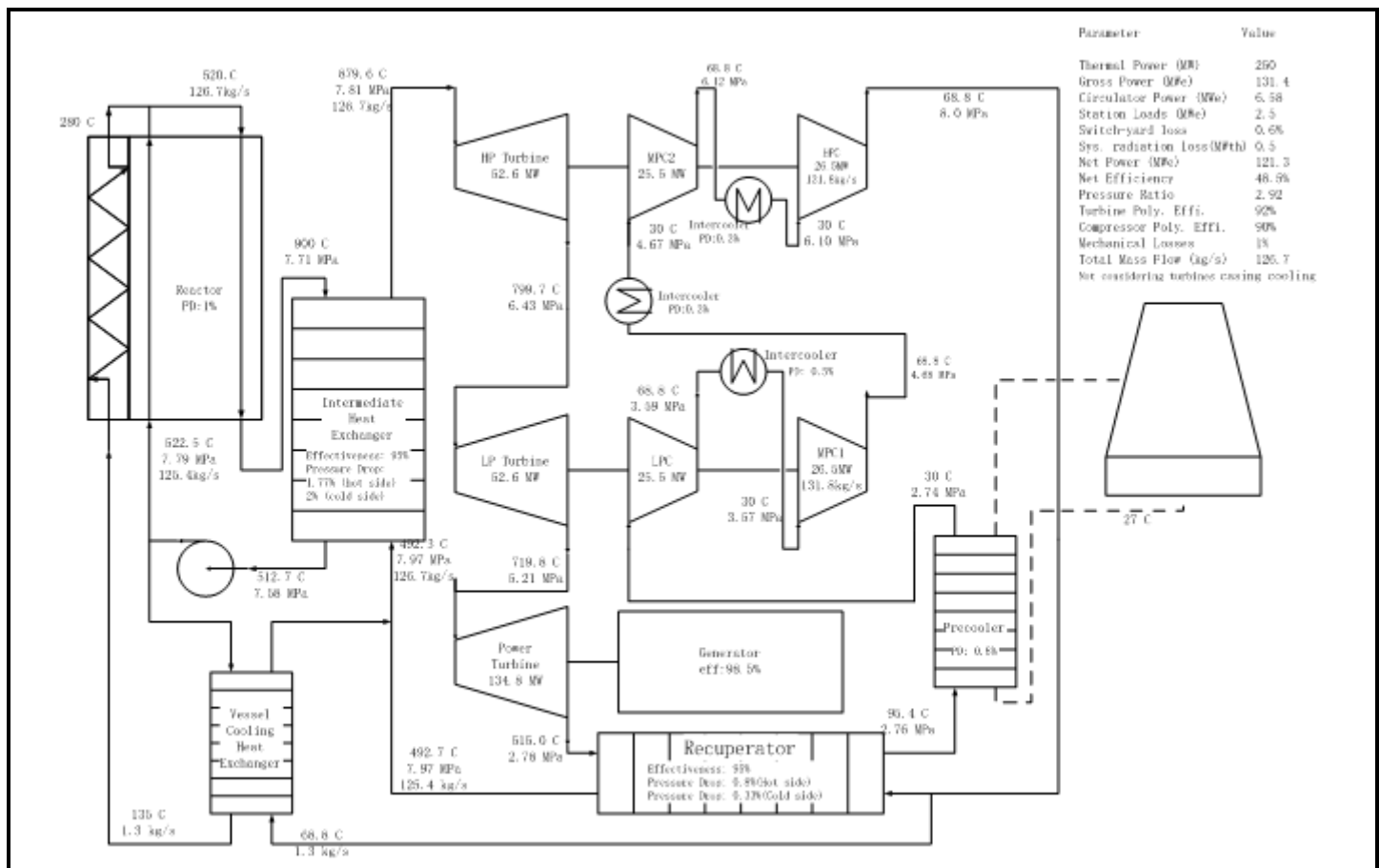


Figure 1. Reference BOP system schematic.

project, there was a limit on the maximum shaft power to approximately 50 MW (70,000 shaft HP). This limit translates into a minimum number of shafts in the BOP system. This, in turn had a direct, and negative, effect on the complexity of the control system for the BOP. The initial design used a 4-shaft BOP with three compressor/turbine sets and a two-set power turbine design. The final reference design, with its higher thermal efficiency and use of higher temperature materials, allowed for a 3-shaft design.

**ESKOM Reactor Limits.** The use of the ESKOM PBMR reactor as the primary heat source carried with it all of the materials limitations for this plant. These include the consequences of using a conventional A508 steel for the pressure vessel and piping. The design also resulted in geometric constraints related to piping configuration and layout.

The use of A508 steel for the pressure vessel placed limits on temperature of 280°C for steady state operation and 350°C for transient, short-time, operation. The high gas outlet temperature, 850°C in the initial and 900°C in the final design, required that an active cooling system be in place during operation. For this design, this also means that the intermediate heat exchanger (IHX) must also have a cooled Section III boundary. Additionally, since the source of cool gas for the ESKOM design is the compressor outlet, using an IHX complicated the design. The design "fix" for this constraint was to include, as either a separate heat exchanger or as a part of the IHX, a compressor outlet gas stream to cool a separate circuit for the pressure vessel and associated piping. Due to the piping cooling requirement, the hot sections of the BOP (to the turbine inlets) had to have cooled pressure boundaries.

**Current Reference Plant Design.** Given the design requirements and constraints, researchers on this project designed and configured a final reference plant. Figure 1 shows a schematic of this design. Temperatures, pressures, and flow rates have been identified.

Key features of the reference system include:

1. The use of a secondary heat exchanger for the reactor vessel and piping cooling system.
2. The use of both inventory and bypass control for system control.
3. The location of bypass control valves on the cold side of the plant.
4. The use of intercooling.
5. The requirement that an IHX differential pressure control system be included in the plant design. This system would likely consist of an inventory control system for both the primary and secondary loops.

The reference plant was a 250-MWth design with a gross power of 131.4 MWe, which yielded a net efficiency of 48 percent. The net plant efficiency achieved the overall project goal of 45 percent when account was taken for the additional cooling gas that would be required and that was not accounted for in the 48 percent estimate. The 45 percent number was consistent with projected values for the ESKOM PBMR plant that was in the final stages of design.

## Planned Activities

This NERI project has been completed.



# NUCLEAR ENERGY RESEARCH INITIATIVE

## Failure Forewarning in Critical Equipment at Next-Generation Nuclear Power Plants

PI: Lee M. Hively, Oak Ridge National Laboratory

Project Number: 00-109

Collaborators: Pennsylvania State University

Project Start Date: August 2000

Project End Date: September 2003

### Research Objectives

The objective of this project was the forewarning of machine failures in critical equipment at next-generation nuclear power plants (NPP). Test data were provided by two collaborating institutions: Duke Engineering and Services (first project year), and the Pennsylvania State University Applied Research Laboratory (PSU ARL) during the second and third project years. New, nonlinear methods were developed and applied successfully to extract forewarning trends from process-indicative, time-serial data for timely, condition-based maintenance. Anticipating failures in critical equipment of next-generation NPP will improve maintenance scheduling to minimize safety concerns, unscheduled non-productive downtime, and collateral damage due to unexpected failures. This approach provided significant economic benefits, and is expected to improve public acceptance of nuclear power.

### Research Progress

The approach used in this project was a multi-tiered, model-independent, and data-driven analysis, which used Oak Ridge National Laboratory's (ORNL) novel, nonlinear method to extract forewarning of machine failures from appropriate data. The first tier of the analysis provided a robust choice for the process-indicative data. The second tier rejected data of inadequate quality. The third tier removed signal artifacts that would otherwise confound the analysis, while retaining the relevant nonlinear dynamics. The fourth tier converted the artifact-filtered time-serial data into a geometric representation, which then was transformed to a discrete distribution function (DF). This method allowed for noisy, finite-length datasets. The fifth tier obtained dissimilarity measures (DM) between the nominal-state DF and subsequent test-state DFs. Forewarning of a machine failure was indicated by several successive occurrences of the DM

above a threshold, or by a statistically significant trend in the DM. This paradigm yielded robust nonlinear signatures of degradation and its progression, allowing earlier and more accurate detection of the machine failure.

Project Year 1 results were as follows. Long-term failure monitoring of operational equipment was not feasible within the scope of this project, since such failures typically take years to occur. Instead, researchers acquired data from a motor-driven pump for two test sequences, initially in nominal operation and subsequently with progressively larger (seeded) faults. Specifically, the experimenters carefully added larger amounts of mass imbalance in one test, and increasing misalignment between the motor and pump in the second test. ORNL's nonlinear measures of condition change correlated well with the experimental level of vibration, both below and above the applicable international standards (ISO 2372 and ISO 3945). The team used a robust implementation of the nonlinear analysis on a desktop computer, not unlike that used at an advanced nuclear reactor.

Project Year 2 work involved acquiring and analyzing

Data Provider	Equipment and Type of Failure	Diagnostic Data	PY
1) EPRI (S)	800-HP electric motor: air-gap offset	motor power	2
2) EPRI (S)	800-HP electric motor: broken rotor	motor power	2
3) EPRI (S)	500-HP electric motor: turn-to-turn short	motor power	2
4) Otero/Spain (S)	¼-HP electric motor: imbalance	acceleration	2
5) PSU/ARL (A)	30-HP motor: overloaded gearbox	load torque	2
6) PSU/ARL (A)	30-HP motor: overloaded gearbox	vibration power	2
7) PSU/ARL (A)	30-HP motor: overloaded gearbox	vibration power	2
8) PSU/ARL (S)	crack in rotating blade	motor power	2
9) PSU/ARL (A)	motor-driven bearing	vibration power	2
10) EPRI (S)	800-HP electric motor: air-gap offset	vibration power	3
11) EPRI (S)	800-HP electric motor: broken rotor	vibration power	3
12) EPRI (S)	500-HP electric motor: turn-to-turn short	vibration power	3
13) PSU/ARL (A)	30-HP motor: overloaded gearbox	vibration power	3
14) PSU/ARL (A)	30-HP motor: overloaded gearbox	vibration power	3
15) PSU/ARL (A)	30-HP motor: overloaded gearbox	vibration power	3
16) PSU/ARL (A)	30-HP motor: overloaded gearbox	vibration power	3
17) PSU/ARL (S)	crack in rotating blade	vibration power	3

Table 1. Summary of test sequences.

additional test data, as summarized in Table 1. Some test sequences involved seeded faults (denoted by "S" in Table 1), with the equipment initially in nominal operation, and subsequently with successively larger (controlled) faults. A second class of *accelerated* failure tests (denoted by "A" in Table 1) also began with nominal operation. The overstressed equipment subsequently experienced a gradual (uncontrolled) degradation, and ultimately failed. For example, the gearbox failed by the breakage of one or more gear teeth. Table 1 also shows the type of diagnostic data that was analyzed for failure forewarning. Researchers obtained electrical motor power from the three-phase motor currents and voltages. They obtained vibration power from tri-axial acceleration data to capture the dynamics from all three acceleration directions. ORNL's patented nonlinear measures showed clear change, as the tests progressed from nominal operation, through degradation, to failure for all nine Project Year 2 test sequences. (Conventional statistical measures and traditional nonlinear measures give little if any forewarning.) Researchers also obtained a statistical criterion to distinguish between the gradual rise in dissimilarity measures and abrupt (additional) increases that give forewarning of failure.

Project Year 3 work involved acquiring and analyzing additional test data, as summarized in Table 1. Items 10-12 during Project Year 3 involved analyzing vibration power, while items 1-3 during Project Year 2 used electrical motor power from the same test sequences. Items 13-16 involved the same test apparatus and protocol as items 5-7 acquired additional test sequences. The Project Year 3 results for items 10-16 showed clear forewarning reproducibility. In particular, four accelerated tests of gearbox failure gave end-of-life forewarning at 93.8-98.5 percent of the final failure time, as well as indication of the failure onset at 99-99.8 percent of the final failure time (see Figure 1). Results showed no false-negative indications (lack of forewarning when a change actually occurred), and no false-positive forewarnings (forewarning when no change really occurred). These results provide compelling evidence for forewarning of failures via the ORNL nonlinear paradigm. During this project, researchers also found that accurate forewarning can markedly reduce failures and improve cost-effectiveness.

Products of this work included U.S. Patents, patents pending, technical publications, oral presentations, software implementation of the nonlinear technology, a cost-benefit analysis of the prognostication approach, and a commercialization roadmap. There are no software deliverables for this project. The ORNL nonlinear forewarning technology has substantial intellectual property protection in the form

of six U.S. Patents and two patents pending. Two of these six patents were obtained during this NERI project, including an objective statistical test for the end-of-life forewarning and the failure onset indication. Both of the patents pending were submitted to the U.S. Patent Office during this NERI project to protect ideas that arose from this work. No licensing agreements presently exist for use of these patents. Researchers on this project have published six technical reports and gave four oral presentations on this NERI work.

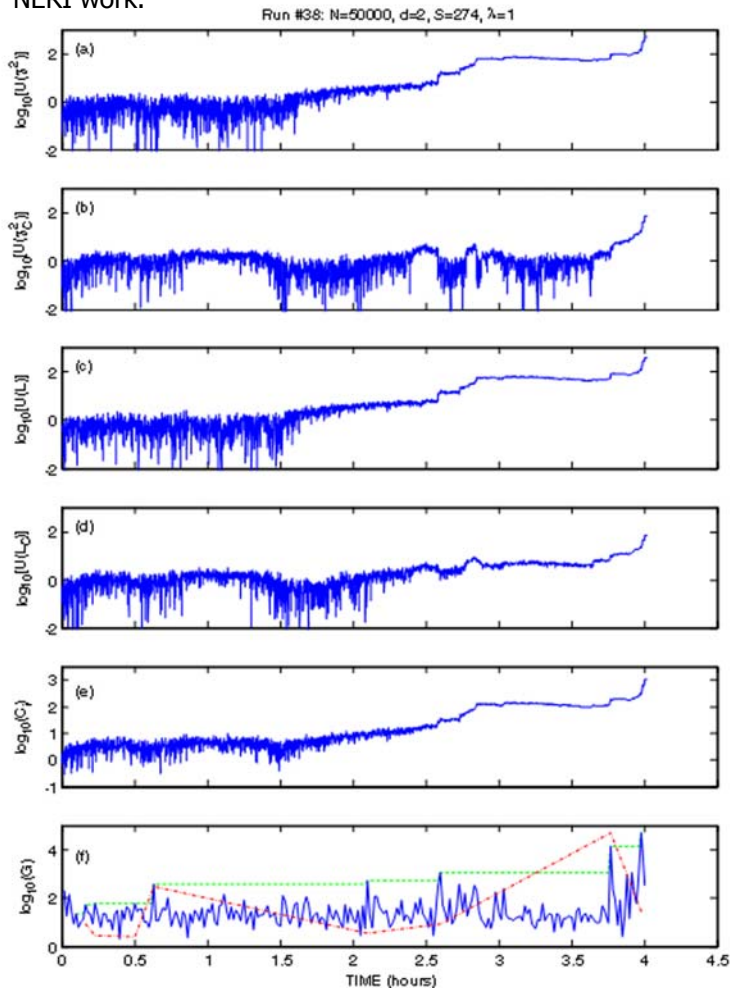


Figure 1. Phase-space dissimilarity measures (PSDM) versus time for the accelerated failure test (Run #38) from vibration power data: (a) - (d) the four renormalized PSDM; (e) composite measure,  $C$ , of the four PSDM; (f) end-of-life indicator,  $G$  (solid), running maximum of  $G$  (dashed), and ratio,  $r$ , of successive maxima (---) in  $G$ . The statistical indicators of forewarning are as follows. The peak in  $G$  at 3.77 hours gives forewarning of the failure, while the peak in  $r$  at 3.98 hours indicates failure onset. Note that the vertical axis is the  $\log_{10}$  of the parameter in subplots (a)-(f), and that  $0.4r$  is plotted in (f) for clarity. The phase-space parameters are  $S=274$ ,  $d=2$ , and  $\lambda=1$ , which are identical to those used for the analysis of the Pennsylvania State University MDTB data in PY2 to show consistency.

## Planned Activities

This NERI project has been completed.



# NUCLEAR ENERGY RESEARCH INITIATIVE

## Feasibility Study of Supercritical Light-Water-Cooled Fast Reactors for Actinide Burning and Electric Power Production

PI: Philip E. MacDonald, Idaho National Engineering and Environmental Laboratory

Collaborators: Massachusetts Institute of Technology, University of Michigan, Westinghouse Electric Corporation

Project Number: 01-001

Project Start Date: August 2001

Project End Date: September 2004

### Research Objectives

The supercritical water-cooled reactor (SCWR) is one of the six reactor technologies selected for research and development under the Generation IV program. SCWRs are promising advanced nuclear systems because of their high thermal efficiency (about 45 percent versus about 33 percent efficiency for current light water reactors [LWRs]) and considerable plant simplification. SCWRs are basically LWRs operating at higher pressure and temperatures with a direct once-through cycle. Operation above the critical pressure eliminates coolant boiling, so the coolant remains single-phase throughout the system. This eliminates the need for recirculation and jet pumps, a pressurizer, steam generators, steam separators, and dryers. The main mission of the SCWR is to generate low-cost electricity. It is built upon two proven technologies: 1) LWRs, which are the most commonly deployed power generating reactors in the world, and 2) supercritical fossil-fired boilers, a large number of which are also in use around the world.

The reference SCWR design for the U.S. program is a direct cycle, thermal spectrum system operating at 25.0 MPa with core inlet and outlet temperatures of 280° and 500°C, respectively. The coolant density decreases from about 760 kg/m<sup>3</sup> at the core inlet to about 90 kg/m<sup>3</sup> at the core outlet. The inlet flow splits—about 10 percent of the inlet flow goes down the space between the core barrel and the reactor pressure vessel (the downcomer) and about 90 percent of the inlet flow goes to the plenum at the top of the reactor pressure vessel to then flow downward through the core in special neutron moderator water rods to the inlet plenum. Here it mixes with the feedwater from the downcomer and flows upward to remove the heat in the fuel channels. This strategy is employed to provide good moderation at the top of the core. The coolant is heated to about 500°C and delivered to the turbine.

The purpose of this NERI project is to assess the reference U.S. SCWR design and explore alternatives to determine feasibility. The project is organized into three tasks, which are discussed below.

### Research Progress

**Task 1: Fuel-cycle Neutronic Analysis and Reactor Core Design.** Researchers assessed an alternative SCWR design that is based on vertical power channels and small hexagonal fuel assemblies (as shown in Figure 1). Sufficient neutron moderation is provided by the feedwater flowing downward in the gap between the channels. The control rods are inserted through the lower head of the reactor pressure vessel. Compared with other approaches like water rods, solid moderators, or heavy water, this

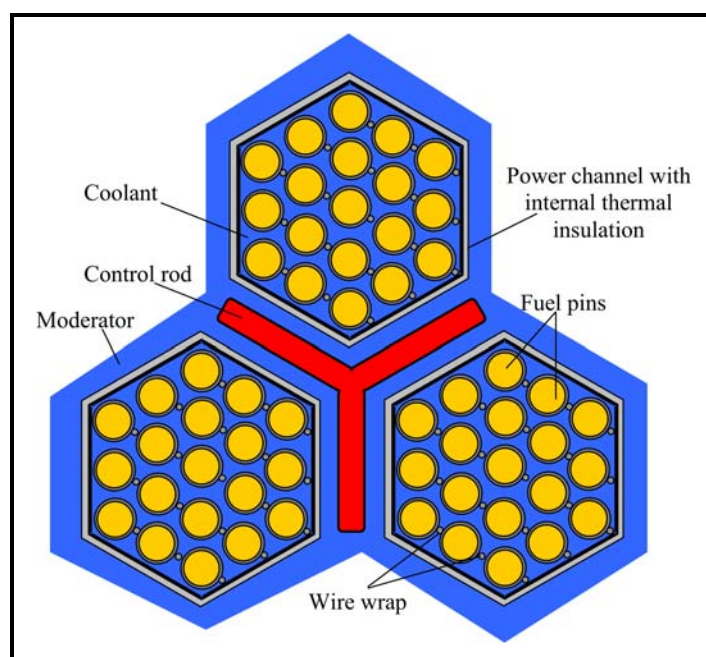


Figure 1. Geometry of the vertical power channel—small hexagonal fuel assembly design.

design has a higher power density and advantages in the area of fuel assembly design and ease of refueling. Based on a simplified thermal-hydraulic and neutronic analysis, it appears that this approach is technically feasible assuming that issues common to all SCWR designs (e.g., development of in-core materials, demonstration of safety, and stability) can be resolved. The estimated fuel-cycle cost is comparable with that of the pressurized water reactor (PWR); the temperature and power distributions are acceptable; and the Doppler and coolant reactivity feedbacks are both negative and within LWR range.

Using the RELAP5/3D computer code, researchers performed steady-state analyses for SCWR designs with water rods and hexagonal power channels. These analyses showed that buoyancy significantly affected the heat transfer rate from the fuel assemblies to the moderator. For example, buoyancy increased the average heat transfer coefficient on the inside of the water rods by a factor of 2.2 in the original design that directed 30 percent of the total feedwater flow to the water rods. Consequently, the current design directs 90 percent of the total feedwater flow towards the water rods to suppress the heat transfer enhancement due to buoyancy. Even with the current design, buoyancy still increased the average heat transfer coefficient by more than 20 percent and, thus, must be accounted for.

The steady-state analyses also showed that both designs had sufficient moderation to achieve acceptable fuel cycle costs. Researchers also found that somewhat lower cladding temperatures could be obtained during normal operation with the power channel design. These lower cladding temperatures were the result of a higher mass flux through the assembly, which increased the heat transfer coefficient and the zirconium-oxide insulation, which reduced the fluid temperature in the assembly. The

analyses also indicated that, although insulation is not necessary for the design with water rod boxes to achieve acceptable fuel cycle costs, insulation is necessary to meet the steady-state thermal limit.

**Task 2: Fuel Cladding and Structural Material Corrosion and Stress Corrosion Cracking.** In Year 2 of the project, the University of Michigan conducted work that provided information on the deformation and stress corrosion cracking behavior of 304L and 316L stainless steels in flowing argon at 500°C, and in deaerated supercritical water at 500°C. This research also provided data on nickel-based Alloy 625 in 500°C deaerated supercritical water and information on oxide layer growth on all the alloys in both argon and water. Researchers compared the stress corrosion cracking results of last year's experiment on 304L in non-deaerated supercritical water with the 304L sample tested in deaerated supercritical water.

The Massachusetts Institute of Technology (MIT) conducted two corrosion tube experiments during Year 2, one with 316L stainless steel and one with Alloy 625. During these experiments, a tube of the alloy to be tested was used as the autoclave, and micro-thermocouples were attached externally along the length of the vessel. Water at an elevated temperature and pressure was pumped into one end and permitted to cool as it traversed the tube. The highest temperature achieved was in excess of 395°C.

The results from the Year 2 testing at Michigan and MIT showed that:

- The stainless steel alloys 304L and 316L are susceptible to intergranular stress corrosion cracking in 500°C deaerated water. The Alloy 304L sample exhibited a higher crack density than did the 316L sample. Alloy 304L stress corrosion cracking is more severe in non-deaerated water than in deaerated water.
- The oxide growths on the 304L and 316L samples tested in deaerated supercritical water were similar in composition. The oxide on the 316L sample was slightly thinner than the oxide on the 304L sample. The oxide thickness on the 304L sample tested in non-deaerated water was significantly greater than the oxide thickness of the 304L sample tested in deaerated water.
- The nickel-based Alloy 625 is susceptible to stress corrosion cracking in deaerated supercritical water (as illustrated in Figure 2). Its yield stress and maximum stress is higher than those for the stainless steel alloys, but the intergranular cracking is more extensive.
- Unstressed Alloy 625 displays significant pitting when tested in 500°C deaerated supercritical water.

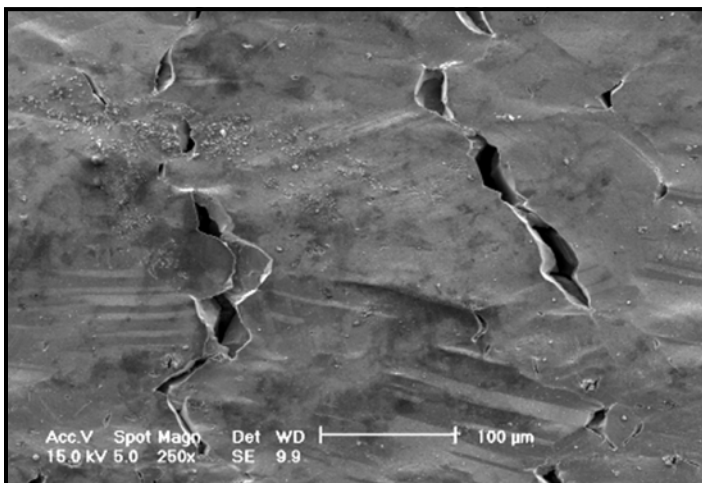


Figure 2. Alloy 625 after failure in deaerated SCW.

### Task 3: Plant Engineering and Reactor Safety

**Analysis.** Researchers modified the VIPRE-W code for supercritical water applications, built a VIPRE-W model of the SCWR core, and performed preliminary sub-channel analyses to investigate the thermal-hydraulic behavior of the SCWR core. The results of the VIPRE-W calculations indicate that the following are essential to lower the hot channel temperatures in a SCWR: multiple enrichments in the fuel assemblies, which result in relatively flat power distributions within each fuel assembly; an optimized assembly geometry for better flow distribution within the fuel assemblies; and orificing to carefully control the coolant flow to each assembly. The effort to minimize local peaking factors in the hot assembly will lead to a complex assembly design, which will require experience in boiling water reactor (BWR) assembly design.

Researchers developed criteria for the design of the fuel rods to assure satisfactory performance in a SCWR. These criteria reflect the acceptance criteria for fuel designs established in the Federal regulations and the NRC Standard Review Plan. Researchers used the FRAPCON-3 computer code to perform a preliminary calculation of the thermal and fission gas release performance of SCWR fuel rods from beginning to end of life (1,350 days and rod average burnup of 77.6 MWd/kgU). The fuel rod design had a relatively large gas plenum volume to better accommodate released fission gases. Nevertheless, the relatively high coolant temperatures in a SCWR result in a release of large amounts of fission gas and in relatively high fuel rod internal pressures. The design of SCWR fuel rods and the power history imposed on the fuel rods need to take into account the effect of higher coolant temperatures on fission gas release.

Researchers performed parametric calculations with the RELAP5/3D computer code to determine the response times and capacities of various safety systems of the SCWR design. The designs used either a solid or water moderator. Moderation by water was achieved with either square water rods or hexagonal power channels. The teams used the calculations to investigate the relative safety characteristics of the designs with water rods or power channels. They simulated transients initiated by loss of feedwater, turbine trip, reactivity insertion, and a step decrease in main feedwater temperature. They also simulated loss-of-coolant accidents (LOCAs).

The parametric calculations showed that the design with solid moderator rods could tolerate a 50 percent instantaneous reduction in feedwater flow without a reactor scram and still meet a transient temperature limit of 840°C.

Transients involving a total loss of feedwater posed a more serious challenge to the reactor. The calculations indicated that acceptable temperature results could be obtained with a 5-second main feedwater flow coast down, a reactor scram, and an auxiliary feedwater flow rate that is 15 percent or more of the initial feedwater flow. The auxiliary feedwater flow would have to be generated within 4.25 seconds of the start of the event to be consistent with the analysis. The rapid initiation of auxiliary feedwater would likely pose a significant challenge for the design. Additional calculations showed that a fast-opening, 100-percent-capacity turbine bypass system could significantly reduce the peak cladding temperature, thus allowing more time to initiate the auxiliary feedwater.

The parametric calculations also showed that the SCWR could meet reactor vessel pressure limits following a turbine trip—provided that the safety relief valve capacity at normal operating conditions is 90 percent or more of the rated steam flow. This safety relief valve capacity is well within typical BWR ranges. The power increase following a turbine trip was much smaller than in a comparable BWR. The parametric calculations also showed that the SCWR could easily tolerate reactivity insertion rates between 5 and 100 pcm/s, provided that the reactor was scrammed at 118 percent neutron power. The peak cladding temperatures were less than 700°C for these transients.

Researchers performed transient analyses for thermal-spectrum SCWR designs with water rods and hexagonal power channels. They initiated the transients by upsetting the main feedwater system through overheating (loss of main feedwater flow) and overcooling (decrease in main feedwater temperature). Because insulation of the water rod boxes or power channels is an important consideration, researchers performed sensitivity calculations with a 1-mm-thick layer of zirconium oxide on the water rod wall. The base designs (water rods without insulation, power channels with 0.5 mm insulation) respond similarly during the loss of main feedwater events. Insulation reduces the maximum steady-state cladding temperature by reducing the fluid temperature of the coolant. However, the insulation retards the flow of heat from the fuel channel to the water rods during an overheating transient, which keeps more of the heat inside the fuel channel, delaying the moderator reactivity effect, and thus resulting in a larger increase in cladding temperature. Consequently, insulation actually increases the peak cladding temperature during the overheating transients studied. (As discussed previously, insulation is required to meet the steady-state temperature limit for the design with water rods.) The peak cladding

temperatures are lower in the design with power channels than in the design with insulated water rods for all three of the transients evaluated. Thus, the overall response to transients initiated by main feedwater upsets is better in the design with power channels.

Researchers evaluated the response of the two designs during LOCAs by determining the time that the maximum cladding temperature reached 1,204°C, which corresponds to the accident limit for current LWRs with Zircaloy cladding. The accident limit was reached more than 300 seconds after the start of the large steam line break and the small feedwater line break. The response of the design with water rods was better for these LOCAs because the accident limit was reached at least 80 seconds later, allowing more time for the safety systems to actuate and mitigate the transient. The larger reactor vessel in this design slowed the depressurization rate and delayed the onset of the nearly adiabatic heatup. The heatup rate was also slower in this design because of its larger fuel rods. The response of the design with power channels was better for the LOCA initiated by a large feedwater line break. In this transient, the heatup was primarily caused by the redistribution of the initial stored energy in the fuel rod, which was lower in the design with power channels because of 1) the insulation and 2) the higher core mass flux during steady-state operation.

A relatively long time is available for safety systems to mitigate the large steam line break and the small feedwater break. Although more time is available for the design with water rods, both designs are considered acceptable for these transients. The large feedwater line break is the most limiting transient because the temperature limit is reached much earlier—26 seconds for the design with water rods and at 57 seconds for the design with power channels. Since the design with power channels has more time available during the most limiting transient, the overall response to LOCAs is considered to be better. Designing safety systems to protect the core during a large feedwater line break will be challenging because of the higher operating temperature of the SCWR and the reduced margin to the temperature limit; however, sufficient time appears available to develop a reasonable safety system design.

The calculated results for the SCWR are sensitive to the choice of heat transfer correlation. Furthermore, the databases of the existing correlations do not cover a sufficiently wide range of thermal-hydraulic conditions to

fully support analysis of the reactor at off-normal conditions and during transients. Researchers should perform heat transfer experiments that are prototypical with respect to thermal-hydraulic conditions and geometry to support analysis of the reactor.

Finally, researchers performed a study to establish the feasibility and general layout of the reactor vessel, focusing on identifying issues associated with operating the reactor with an outlet fluid temperature of 500°C (932°F) and at elevated pressures as compared to current PWRs. The preliminary SCWR vessel design has remained similar to a typical large PWR vessel in many respects, and has used current PWR materials for the pressure vessel boundary. The use of standard PWR vessel design, manufacturing techniques, and materials should prove to be a major economic advantage for the SCWR compared with other Generation IV reactor concepts; the latter will require the use of advanced alloys operating at much higher temperatures. Researchers established the following thicknesses for the vessel wall using minimum thickness calculations based on the ASME Code:

- The vessel shell wall thickness is 0.46 meters (18.0 inches).
- The vessel upper nozzle and closure flange ring-forging wall thickness is 0.63 meters (24.75 inches).
- The vessel lower head wall thickness is 0.30 meters (12.0 inches).
- The vessel upper head thickness is 0.30 meters (12.0 inches).

Researchers at both Westinghouse and Idaho National Engineering and Environmental Laboratory (INEEL) have performed finite element analyses for this preliminary vessel design. These analyses indicate that the vessel is able to meet ASME Code specifications under design pressure. In addition, INEEL has been exploring alternatives to the preliminary design to reduce both peak stress and vessel thickness. INEEL has also started to look at alternative approaches to the outlet nozzle thermal sleeve. Although the team has not yet achieved a satisfactory design for the thermal sleeve, it appears that multiple isolation features will be required to isolate the bulk reactor vessel from the hot leg temperature (500°C).

## Planned Activities

Below is a list of the major activities planned for Year 3 of this project:

- Researchers will use the burnup code MOCUP (which uses the Monte Carlo transport code MCNP and the exponential matrix generation and depletion code ORIGEN2.1) to assess the neutronics of the solid moderator, water rod moderator, and the vertical power channel-small hexagonal fuel assembly designs. Researchers at INEEL will calculate reactivity as a function of depletion, Doppler and void coefficients, and radial and axial power distributions.
- Researchers at the University of Michigan will measure the corrosion, deformation, and stress corrosion cracking behavior of proton irradiated austenitic alloys (304, 316, 625, 690) and one set of ferritic alloys in the unirradiated condition (T91, HT9, T122) in flowing argon at 500°C, and in deaerated supercritical water at 500°C.
- Researchers will develop improved fuel assembly designs and assess this design with the VIPRE-W subchannel analyses code at Westinghouse.
- The Generation IV program is funding the design of SCWR safety systems at Westinghouse. Once details of these designs are available, researchers at INEEL will use the RELAP5/3D computer code to characterize the transient response of the plant. Researchers will simulate transients initiated by loss of feedwater, turbine trip, reactivity insertion, and a step decrease in main feedwater temperature. They will also simulate LOCAs.
- Researchers at Westinghouse and INEEL will develop and analyze designs for the key reactor pressure vessel's internal components.
- A final report will be prepared.



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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Particle-Bed, Gas-Cooled Fast Reactor (PB-GCFR) Design

PI: Temitope A. Taiwo, Argonne National Laboratory

Project Number: 01-022

Collaborators: Brookhaven National Laboratory; Commissariat a L'Energie Atomique, France; University of Rome, Italy

Project Start Date: September 2001

Project End Date: August 2003

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### Research Objectives

The objective of this project was to develop a conceptual design of a particle-bed, gas-cooled fast reactor (PB-GCFR) core that meets the enhanced proliferation-resistant goals of the U.S. Department of Energy's NERI program. The key innovation of this project was to apply a fast neutron spectrum environment to enhance both the passive safety and transmutation characteristics of the advanced particle-bed and pebble-bed reactor designs. The PB-GCFR design was expected to produce a high-efficiency system with a low unit cost. It was anticipated that the fast neutron spectrum would permit small-sized units (approximately 150 MWe) that could be built quickly and packaged into modular units, and whose production could be readily expanded as the demand grows. Such a system could be deployed globally. The goals of this two-year project were as follows:

- 1) Design a reactor core that meets the future needs of the nuclear industry by being passively safe, thus reducing the need for engineered safety systems. This would entail an innovative core design incorporating new fuel form and type.
- 2) Employ a proliferation-resistant fuel design and fuel cycle. This would be supported by a long-life core design that is refueled infrequently, and hence, reduces the potential for fuel diversion.
- 3) Incorporate design features that enable the system to be an efficient transmuted that could burn separated plutonium fuel or recycled light water reactor (LWR) transuranic fuel, should the need arise.
- 4) Evaluate the fuel cycle for waste minimization and for the possibility of direct fuel disposal. The application of particle-bed fuel provides the promise of extremely high burnup and fission-product protection barriers that may permit direct disposal.

### Research Progress

In the first year of the project, the team performed physics calculations in support of a compact, fast-spectrum core based on the pebble-bed design. The results showed that mixed uranium and transuranics (TRU) carbide and nitride fuel forms can enable a long-life core and high-temperature operation. Researchers identified potential matrix materials (titanium nitride [TiN], zirconium carbide [ZrC], and silicon carbide [SiC]) for these fuel forms. The physics studies showed that a long-life core (with conversion ratio greater than one) requires a fuel volume fraction greater than employed in current high-temperature reactor (HTR) designs. A high core fuel-volume fraction (approximately 30 percent) or large core size (power density less than 25 W/cc) is required to reach the desired sustainable design with a high conversion ratio. Researchers indicated that achieving a high fuel volume fraction would require a redesign of the typical coated fuel particles to minimize the volume occupied by the non-fuel components of the matrix.

Using this design knowledge, the team performed core physics studies that were done in the earlier part of the second year on a core design using the promising cold finger device for passive safety. Additionally, researchers performed a study investigating waste amounts in the PB-GCFR fuel cycle. They evaluated the impact of the fuel management scheme on TRU waste minimization, using the lifetime TRU material processed as the figure of merit. A 30-year period was used in the study. Because all the cores had the same power density (50 W/cc) and because of the constraint on the maximum TRU enrichment (20 percent), researchers preferred the long-life core. This design resulted in the lowest amount of radiotoxic transuranics to be processed and sent to the repository.

Those earlier studies were for TRU breakeven cores, which are consistent with Generation IV nuclear system sustainability goals. It is conceivable, however, that Generation IV reactor systems might be deployed early in their lifetimes to burn the TRU contained in spent nuclear fuel, which accumulates in spent fuel pools and dry storage at power plants. During the second year, researchers evaluated the feasibility of configuring the PB-GCFR as a TRU burner. They also investigated the performance of a non-fertile fuel core. The findings of this study formed the basis of a deliverable report.

It is known that the safety case for fast spectrum reactors employing gas as a coolant is complicated by the poor heat transfer properties and low thermal inertia of the gas coolant. The ability of this reactor type to survive a scrammed depressurization accident with a concurrent loss of electrical power, without undue hazard to the public, is clearly an attractive feature of an advanced GCFR of the Generation IV class. This NERI project explored a number of concepts that could potentially provide this safety feature through passive means. First, the team performed a fundamental assessment of heat transfer modes and the implications of the decay heat curve. They carried out scoping thermal calculations. The study revealed that natural convection at one atmosphere cannot be relied upon for the available selection of primary coolant gases, and that radiation through the core would dominate above 1,000°C. Below this temperature, the better alternative may be providing conduction pathways. For the period immediately following scram, substantial core thermal inertia is needed, as heat transfer on this timescale is not adequate for the core materials of the near future. To improve the feasibility of the passive core concept, it would be prudent to reduce the reactor power envelope to below 300 MWt. Researchers investigated three types of basic core elements that could possibly provide core configurations with the desired passive core safety feature: 1) block/plate, 2) pin/tube, and 3) pebble/particle. After the initial investigation, the team decided that the major focus of the work would be on the pebble/particle fuel element and, in particular, on the pebble-bed core configuration.

In the first year, the team investigated various concepts to promote passive safety in a 300 MWth PB-GCFR core and introduced a unique concept to increase the heat storage capacity of the fuel pebble. This concept uses fuel spheres in which the center is filled with a material that does not contain fuel and which can melt and absorb heat as latent heat of fusion. While workable temperatures (maximum fuel temperature less than 1,630°C) during normal opera-

tion and transient conditions (severe depressurization accident) were obtained, the permissible core power density of 23 W/cc was low and uneconomical for a fast reactor. Therefore, researchers investigated other concepts for passive decay heat removal in the event of a severe depressurization. These included: 1) prompt unloading of the pebble fuel, 2) extended flow coastdown, and 3) tube reactor with a tank. These approaches were primarily using heat removal by passive conduction or radiation heat transfer. It was found that these individual approaches could not adequately remove the heat for the relatively high power density of interest in the project. Consequently, the team conceived and developed the cold finger concept, which combined two heat removal approaches.

The cold fingers served dual purposes, both as reactivity-control devices as well as a passive decay-heat removal mechanism during severe depressurization. In addition to core physics, researchers investigated thermal-hydraulic and safety assessments and mechanical design issues (flow instability and flow-induced vibration). Core designs using cold fingers provide a potential solution to passive decay heat removal. However, the cold fingers will occupy a significant portion of the core volume, thus, leading to core designs with relatively low power density (approximately 25 W/cc). Additionally, the mechanical design and structural integrity of the cold fingers could be a major issue. Finding materials that could withstand the fluence, temperatures, temperature gradients, and pressure-induced stresses that the cold finger could be subjected to is a serious challenge. Therefore, researchers investigated alternatives to these devices. The idea is that if a low power density is the maximum that can be tolerated from a passive safety viewpoint, then it might be possible to come up with a design that is less demanding.

The alternative designs explored two new approaches for decay heat removal. These are autonomous systems and natural convection in a pebble bed core. For direct-cycle plants, both concepts require one or more additional primary flow loops. These loops would contain heat exchangers that either power the autonomous systems or merely dump decay heat, as in the case of natural convection. These extra loops require check valves to help prevent reverse flow that could cause a significant portion of the main coolant flow to bypass the reactor core. Researchers found that using natural convection at the low power density as the primary means for removing decay heat might work in a helium-cooled PB-GCFR, provided a coolant pressure greater than 10 atmospheres is maintained following severe depressurization. Researchers on



this project investigated approaches for ensuring this pressure level. A leading approach is to provide a pressurized guard containment around the reactor vessel. Researchers also investigated a semi-passive autonomous approach for passive decay heat removal. Such systems use the decay heat from the shutdown reactor core to provide the pumping power that forces the flow for decay heat removal. Results using these two devices were positive. However, additional investigations are required before conclusive statements about them can be made. It is conceivable that a combination of two systems might be needed. The resolution of these items would require more refined models (than used for these conceptualization studies) and balance-of-plant considerations that were beyond the scope of this work.

Researchers performed a literature review to identify candidate fuels and materials for developing a GCFR that meets Generation IV system criteria. Much of the effort was devoted to identifying sources of pertinent information, collecting material properties, and reviewing current gas-cooled reactor fuel designs, as well as evaluating space-reactor development efforts of the 1960s. The review evaluated fuel and material compatibility issues, high-temperature mechanical and thermal properties, and performance issues expected by operation in a fast neutron spectrum ( $E > 0.1$  MeV). The study recommended mixed carbide and nitride fuels as preferred fuels for the PB-GCFR. Titanium nitride (TiN), silicon carbide (SiC), and zirconium carbide (ZrC) were identified as possible matrix materials. More conclusive selection of the PB-GCFR materials requires additional investigation.

In a similar manner, researchers collected and assessed property data for industrially available, structural materials that had well-established manufacturing technologies to identify candidate materials for various components of the PB-GCFR. Since detailed design information about these components do not presently exist, researchers first considered materials and materials production systems that were evaluated in other reactor development projects. Based on this evaluation, recommendations for structural materials have been made for structures in the vicinity of the fuel zone (ceramics such as SiC, SiC/SiC composites, ZrC, TiC, MgO, Zr(Y)O<sub>2</sub>, TiN, Si<sub>3</sub>N<sub>4</sub>); for the pressure vessel (2¼ Cr-1Mo and 9-12Cr steel); for cooling system components (Inconel 718, Inconel 800, and Hastelloy X); for the shielding and thermal barriers (borated Type 304 and 316 stainless steel, ferritic HT9 and various vanadium alloys); and for the reflector zone (uranium, tungsten, iron, stainless steel, Nb-1Zr, and Zr<sub>3</sub>Si<sub>2</sub>).

This project has remained cognizant of fuel and material activities under the GCFR I-NERI project led by Argonne National Laboratory and the Commissariat à l'Énergie Atomique (CEA), and pertinent activities under the Generation IV and Advanced Fuel Cycle Initiative (AFCI) programs.

The project has accomplished its objectives by investigating fuel cycle and safety issues for a pebble-bed gas-cooled fast reactor core:

- Researchers conceived and designed core designs with passive/semi-passive safety features.
- Researchers conducted a preliminary literature review of materials for use in high-temperature and fluence environment.
- Researchers considered proliferation-resistant fuel/core designs (systems with no blanket and long-life core designs).
- Researchers assessed systems for waste minimization and for TRU burning, by considering long-life core designs, feasibility of non-fertile fuel, and utilization of coated fuel particles.

The project has also developed a core group of experts in gas-cooled fast reactor issues and has incorporated a post-graduate student and a fresh Ph.D. holder in the efforts. In addition, the project has been able to leverage its activities with those of the U.S. Department of Energy-CEA I-NERI project on the GCFR. The expertise developed in both the NERI and I-NERI activities has also contributed significantly to the progress of the Generation IV GCFR system design, including development of international and U.S. program plans. Finally, the GCFR being considered in the project or its variant could be utilized for the AFCI mission of burning transuranics and providing benefits to the geologic repository.

## Planned Activities

This two-year NERI project has been completed.



# NUCLEAR ENERGY RESEARCH INITIATIVE

## Miniature, Scintillation-Based, In-Core, Self-Powered Flux and Temperature Probe for HTGRs

PI: David E. Holcomb, Oak Ridge National Laboratory

Project Number: 01-039

Project Start Date: September 2001

Collaborators: The Ohio State University

Project End Date: September 2004

### Research Objectives

The objective of this project is to develop a miniature, scintillation-based, in-core, self-powered neutron flux and temperature probe. The probe is intended to be generally applicable to any reactor technology, but is specifically designed for the higher temperatures of high-temperature gas reactors (HTGRs). The scintillation assembly consists of a uranium layer placed against a thick film scintillator layer. The fission fragments resulting from neutron interactions in the uranium produce light in the scintillator. The light from the scintillator is guided out from the core using a hollow core optical fiber. Both the converter layer and the scintillator are segmented. A scintillator of one wavelength is collocated with a lightly  $^{235}\text{U}$ -enriched uranium layer. A scintillator with a different characteristic wavelength is placed against a higher  $^{235}\text{U}$ -enrichment uranium layer (2 percent and 4 percent, for example). The scintillators produce different wavelength light allowing independent readout of the scintillation. Neutron flux is indicated by the total amount of light produced by either scintillator; the ratio of the different amount of light at the different waveband intensities serves as a burn-up monitor. Researchers use multi-wavelength pyrometry to measure temperature.

### Research Progress

Researchers on this project have produced the primary sensor components. System testing and refinement is currently underway. Researchers have developed the scintillation deposition technique and selected a set of phosphors for use in-core. They have also developed an electrochemical technique for depositing uranium films onto nickel disks. They have developed both a silvered glass version of the light guide tube and a polished titanium light guide tube for in-core use. They have produced both a wavelength-dependent light measurement system as well as a pulse-based photon measurement system coupled to the proximal end of the light guide tubes. Researchers have completed a high-temperature, near-core, test environment chamber and a gamma dose chamber.

Most recent activity has centered around two tasks: 1) the development of a mechanically sturdy and high light-throughput tube to convey light from the end that contains the neutron absorber and the phosphor layers to the optical detection system outside the reactor and 2) the development of electrodeposition techniques for segmented uranium films on nickel substrates. Additionally, researchers completed the near-core, high-temperature, testing

facility at the Ohio State University (OSU) Research Reactor during the past quarter and finalized the light measurement apparatus. Researchers have developed high light throughput fused silica light guides with silver-mirrored interior coatings. For more mechanically rugged applications, researchers have also fabricated a refractory metal light guide—essentially a highly

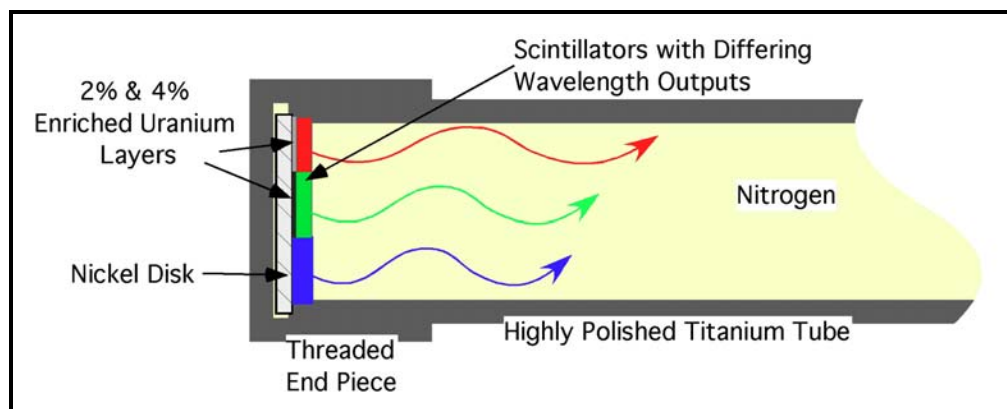


Figure 1. Conceptual layout of scintillation-based neutron flux and temperature probe.

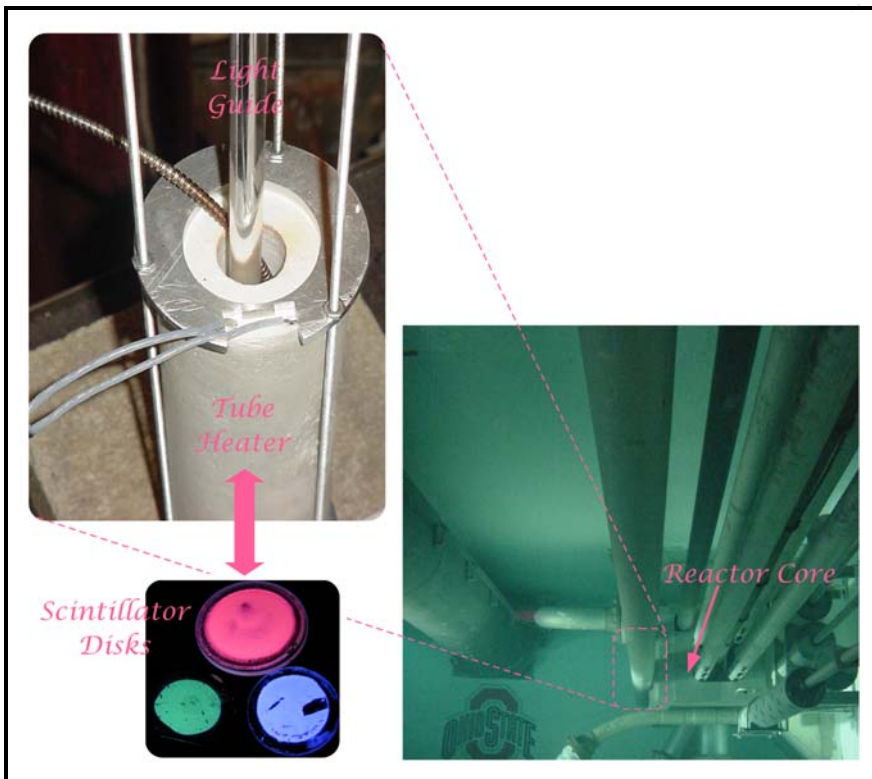


Figure 2. Measurement System Layout - Reactor core with adjacent dry tube, tube heater and light guide, and scintillation disks for deployment at the tip of the light guide.

polished titanium tube. The polishing protocol consisted of passing a rotating rod, driven by a drill motor, and coating the last 3 inches with Tygon™ tubing repeatedly through the titanium tube. The Tygon tubing was used to support, in sequence, grit paper of 600; 800; 1,200; 2,400; and 4,000 grade. The polishing was finished with a silk coating saturated with one-micron diamond suspension. Researchers attempted to increase the reflectivity (light throughput) of the polished tube by depositing a palladium-silver alloy interior coating. They were, however, unsuccessful in this. The silver appears to alloy with the titanium forming a dark coating. Future efforts to implement a light guide would incorporate a niobium tube instead of titanium since it does not form alloys with silver and could incorporate a reflective coating.

The approach to the signal-processing task has followed two parallel and complementary paths. One involves using a PC-card type optical spectrometer to characterize the wavelengths and relative intensities of the scintillator light output, while the other utilizes an optical analysis system for selected wavelengths of output light, including photomultiplication of the light signal and high-speed pulse shape analysis of the amplified signal. To these ends, researchers have obtained the required instrumentation components and have assembled them for evaluation.

They have designed and fabricated a light-tight mechanical coupler for attaching the light guide to the spectrometer input. The upper portion light guide for spectrum-based signal processing consists of a collimating lens and a large core communication grade optical fiber.

Researchers have invested considerable effort in adapting electrodeposition techniques used for the bioassay of actinides in environmental and personnel monitoring samples to the deposition of relatively thicker uranium films. The uranium is required as a neutron absorber which, upon fission, releases energy that is converted into light through the intervention of an overlying layer of an appropriate phosphor. Relatively thick, about one micron, adherent films of uranium oxide can be deposited on nickel cathode plates following procedures similar to those used in bioassay for trace amounts of actinides. Uranium electrodeposition results from reducing a starting uranyl

salt to uranium dioxide. The deposition is incidental to water splitting and, as such, is highly dependent on experimental parameters such as the pH and concentration of the supporting electrolyte as well as the nature of the cathode surface both in terms of the material used and its roughness. Researchers on this project are currently preparing a publication giving the details of the developed technique.

## Planned Activities

The main tasks for the next year are to 1) initiate reactor testing of the developed system, 2) complete development of the segmented scintillation disks, and 3) finalize the pulse mode signal processing apparatus. Researchers will initially complete bench-top testing and system check-out with standard light sources and black-body radiation. Low radiation environment measurements will follow at ambient temperature conditions. Elevated temperature tests at high neutron and gamma radiation levels in the OSU Research Reactor will comprise the final measurements and will complete the performance evaluation of the self-powered, neutron/temperature sensor and its process analysis system. Current fabrication efforts are centered on the deposition of uranium on segmented portions of the cathode. This is being accomplished through the use of appropriate masks.

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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Generation IV Nuclear Energy System Construction Cost Reductions Using Virtual Environments

**PIs:** Timothy Shaw, Anthony Baratta,  
Penn State University

**Project Number:** 01-069

**Collaborators:** Panlyon Technologies,  
Westinghouse Electric Company, Burns and Roe  
Enterprises

**Project Start Date:** August 2001

**Project End Date:** July 2004

### Research Objectives

The objective of this project is to demonstrate the feasibility and effectiveness of using full-scale virtual reality simulation in the design of future nuclear power plants. Specifically, this project will test the suitability of Immersive Projection Display (IPD) technology to allow engineers to evaluate the potential cost reductions that can be realized in Generation IV Nuclear Energy Systems installation and construction sequences. The intent is to see if this type of information technology can be used to improve arrangements and reduce construction and maintenance costs, as has been done by building full-scale physical mockups.

Development, testing, and evaluation of the virtual environment technology have been divided into five tasks, to take place over three years. For the first task, researchers will create and review a full-scale virtual mockup of a selected space within an advanced nuclear power plant design for use as an experimental testbed. During the second task, researchers will use this testbed to study the effectiveness of the technology to support the development and evaluation of the installation sequence for the selected space. In the third task, researchers will develop the methodology and the required tools to perform a prototypical maintenance task using the virtual mockup. The actual maintenance activity study will be performed as task four. Finally, the team will investigate the lessons learned during the first four tasks as they apply to a Generation IV design.

### Research Progress

The first year of the project focused on the development of the full-scale virtual mockup. Three-dimensional CAD models prepared by Westinghouse were successfully converted to a format that could be recognized by the immersive virtual environment system, which allows the models to be projected in stereoscopic 3-D in full scale. Room 12306 within the Westinghouse Advanced Passive (AP 600/1000) plant, shown in Figure 1, was chosen as a testbed for the virtual mockup due to its relative complexity. The room is designed to contain multiple modules and piping assemblies, which are composed of piping from ten different fluid systems.

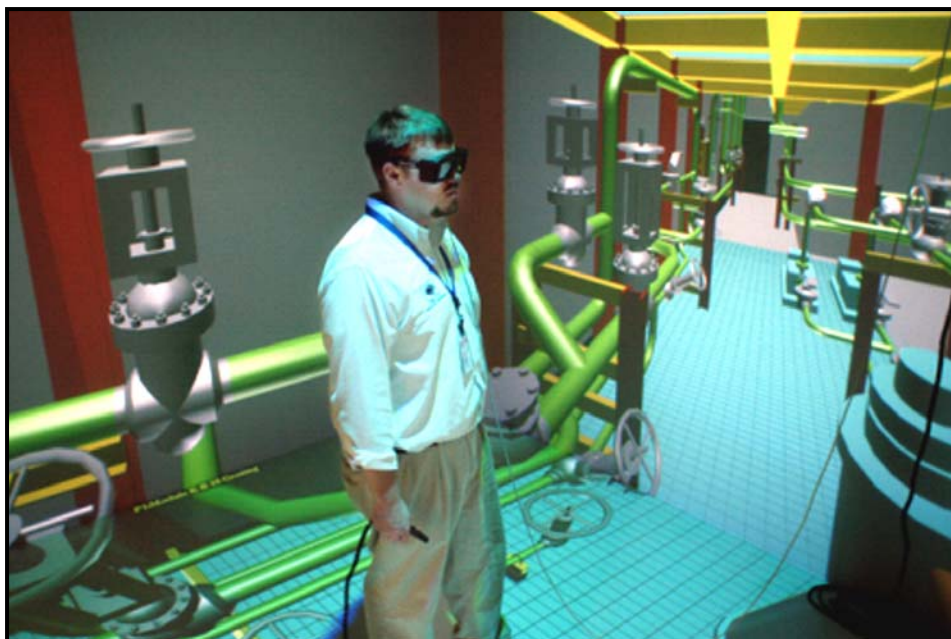


Figure 1. Virtual mockup of room 12306 in the AP600.

After the virtual mockup was completed, construction personnel reviewed the space to determine whether or not the technology provided sufficient realism, therefore providing a potential design tool. A survey was completed by the participants, which compared the virtual mockup to computer models (3-D CAD) and physical mockups. The virtual mockup scored well in categories where good spatial correlation and visualization are critical, including space perception, interference analysis, access, operability, maintenance, ensuring construction requirements are met, illumination evaluation, demonstration of equipment removal, analysis of proposed design modifications, advanced reactor design development support, and evaluation of previous designs.

The second year of research focused on evaluating the full-scale virtual reality mockup of a room in the AP600 nuclear power plant, developed during Year 1, for the development and review of installation sequences for modular construction. Because most of the next-generation nuclear power plant designs utilize some form of modular construction to speed construction and improve quality, a study of potential methods for developing and analyzing these techniques is also beneficial.

Researchers performed two experiments to test the use of immersive virtual reality for developing and reviewing construction sequences for a next-generation nuclear power plant. Two groups of Penn State construction management students used the virtual environment to interactively develop reasonable installation sequences for Room 12306 in the Westinghouse AP600 nuclear power plant. In a second experiment, two groups of experienced construction superintendents from Burns and Roe Enterprises used 3-D isometric paper drawings to develop a construction plan for Room 12306. Their construction plans were translated into a 4-D virtual model that was projected in an immersive virtual environment. The superintendents viewed the construction plans in the virtual environment and suggested a number of changes to their construction plans. The superintendents also collaborated to develop an optimum construction sequence using the immersive virtual environment. The experiments demonstrated that the virtual reality technology could be used to assist construction planners in developing and optimizing installation sequences for equipment in future nuclear power plants, possibly resulting in shorter, more efficient plant construction schedules.

Once researchers completed the experiments and associated analysis of the installation sequences, work on Task 3 was initiated. Task 3 entails developing new capabilities so that the immersive virtual reality system could be used to simulate a maintenance activity in a nuclear power plant. The first capability investigated was the development of a rudimentary radiation dose model so that a worker's radiation doses could be measured as they performed maintenance tasks in the immersive virtual environment. The dose model is designed to simulate the functionality offered by survey meters used by radiation protection personnel and electronic dosimeters worn by radiation workers. Virtual radiation sources of known energy and known source strength can be placed anywhere in the virtual environment.

In order to proceed further with Task 4, collaborators selected steam generator sludge lancing as the maintenance task activity to simulate. The necessary equipment is currently being modeled in the full-scale virtual reality model of the steam generator compartment of the AP1000 so that student workers will be able to simulate this task.

## Planned Activities

In the coming months, the report detailing the research performed under Task 2, the installation sequencing study, will be completed. Researchers will test radiation dose model, developed for Task 3, against actual data to ensure that it simulates realistic (or at least conservative) dose measurements. They will also continue developing the virtual tools necessary to perform steam generator sludge lancing. Trained student workers will perform the maintenance task, and the task will be analyzed. Finally, the project team will study and report the feasibility of applying the immersive virtual reality technology and the lessons learned from the four previous activities to one of the Generation IV power plant designs such as the gas-turbine modular helium reactor (GT-MHR) or the pebble bed modular reactor (PBMR).



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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## On-Line NDE for Advanced Reactor Designs

PI: Norio Nakagawa, Ames Laboratory

Project Number: 01-076

Collaborators: Westinghouse Electric Company  
LLC

Project Start Date: October 2001

Project End Date: September 2004

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### Research Objectives

The extended refueling interval of Generation IV (Gen IV) nuclear reactors creates new maintenance challenges. Current commercial reactors achieve high levels of availability and reliability by employing outage-based maintenance (i.e., performing methodical, periodic, off-line inspections; preventive maintenance; and component repair/replacement during planned refueling periods). Compared to the traditional 1- to 1.5-year refueling cycle, Gen IV reactors use extended refueling intervals, such as four years and beyond. New approaches are required to keep maintenance from interrupting operation. The key strategy of this effort is to replace/augment current outage-based maintenance with on-line structural health monitoring to ensure the current level of safety.

The project's specific objectives are to:

- 1) Determine, based upon regulatory requirements and commercial reactor experience, the most appropriate inspection through a comprehensive review of each component of the Gen IV reactor design.
- 2) Determine which inspections provide the greatest economic benefit when implemented as in-situ monitoring, considering the inspection requirements and reduced off-line inspection opportunities.
- 3) Optimize mechanical design parameters to simplify inspection.
- 4) Develop the concept of a built-in structural integrity monitoring system using electromagnetic, ultrasonic, or radiation detectors, to be integrated into the design for Gen IV nuclear power systems.
- 5) Evaluate and characterize the performance of conceptual sensor systems by using physics-based simulation models.

- 6) Enhance the capabilities of the simulation models to meet the challenges posed by unique power system environments.
- 7) Select sensor types and materials, find their compatibility with hazardous environments, and examine their possible degradation.

In summary, the objective of this project is to propose a shift for future power systems from outage-based maintenance to on-line inspection and monitoring. Researchers on this project have identified several prototypical Gen IV reactor components that can receive the maximum benefit of on-line monitoring with the appropriate NDE methodologies. Conceptual developments of on-line NDE methods have been generated.

### Research Progress

This project, now in its second year, involves the design and development of on-line monitoring systems. The on-line monitoring systems incorporate nondestructive evaluation (NDE) sensors, and can be applied to next-generation nuclear power systems of integral reactor design. The project aims to advance nuclear power system safety and economy by proactively using what researchers know about NDE. This will also impact advanced reactor designs as they are being developed. By identifying the potential failure modes for each of the critical reactor components, researchers can modify the design to ensure that conditions leading to component failure can be reliably detected and addressed before they reach a critical stage.

Through the first and second year, researchers on this project thoroughly examined a representative integral reactor design, i.e., the International Reactor Innovative and Secure (IRIS), and identified several in-vessel components where on-line integrity monitoring can provide

maximum benefits, as shown in Table 1. In Year 1, researchers focused on the steam generator (SG) integrity, while this year they paid significant attention to monitoring the integrity of the reactor coolant pump (RCP) and the primary coolant flow. In Year 3, the team will examine other areas, such as the structural integrity monitoring of pump attachments and the reactor-head penetration welds.

Table 1 also lists the candidate NDE methodologies that the team has identified. The use of eddy current testing (ECT) and ultrasonic testing (UT) via the electromagnetic acoustic transducer (EMAT) were conceived in Year 1, while the coolant flow monitoring methodology was conceived this year, with preliminary, model-based performance estimation. Figure 1 schematically illustrates the locations of the target in-vessel components and candidate on-line NDE sensor placements.

Among the list of on-line NDE methods, the coolant flow monitoring method is based on detection of gamma rays from nitrogen-16 (N-16). For stable reactor operation, the primary coolant should maintain its steady and uniform flow inside the reactor pressure vessel (RPV). The coolant is regulated at a constant speed by the RCP. Therefore, a

Component	Monitoring Needs	NDE Method
Steam Generators	Magnetite deposits <ul style="list-style-type: none"> <li>• inside tubes</li> </ul>	EC, EMAT UT
	Tube/Header attachment	EMAT UT
	Tube integrity <ul style="list-style-type: none"> <li>• tubes themselves</li> </ul>	EC, EMAT UT
Coolant Pumps	Coolant flow	<sup>16</sup> N/ $\gamma$ -ray detector
	Structural attachment	EMAT UT
Penetration Welds	Degradation	EMAT UT

Table 1. Identified monitoring needs and applicable on-line NDE methods: reactor pressure vessel (RPV), eddy current (EC), electromagnetic acoustic transducer (EMAT) ultrasonic testing (UT).

measurement of the flow rate provides a measure of RCP performance. The N-16 method monitors the coolant flow rate on-line. This is based on the following principle:

The radioactive N-16 isotope is produced by neutron reactions with oxygen in water in the reactor core, and decays with a characteristic 7.13-sec half life while traveling from the core to the SG. The constant flow rate results in a constant travel time (nominally 12 sec for IRIS), and consequently leads to a steady N-16 abundance at the SG (down by the factor  $2^{-12/7.13}=0.31$ ). Therefore, fluctuation of the N-16 gamma count rate at the SG location will provide a measure of potential flow disturbance.

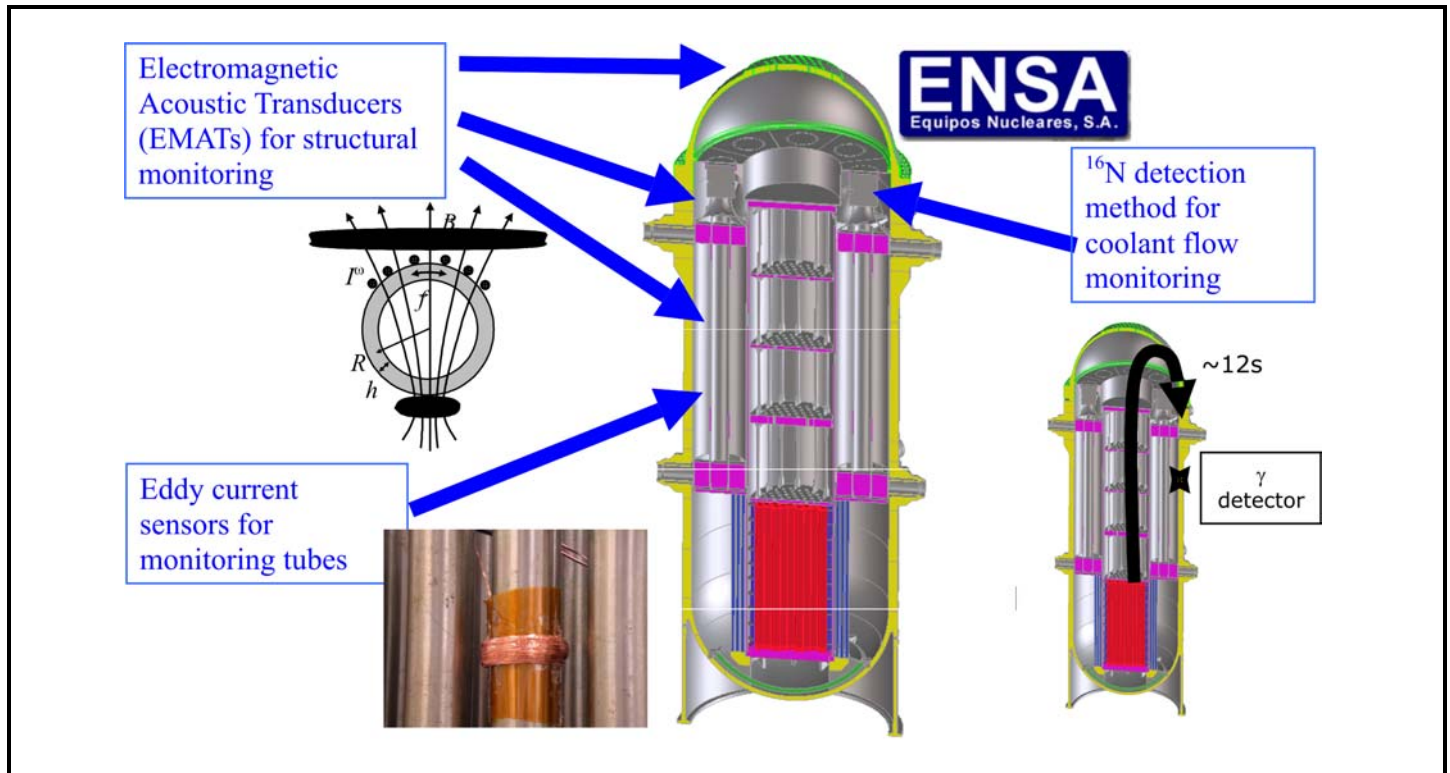


Figure 1. Integral reactor coolant system: Use of the on-line NDE methodologies at target in-vessel locations are shown schematically.



Researchers have evaluated this concept with Monte Carlo and shielding calculations. Specifically, they have estimated the N-16 production rate, as well as its abundance within a SG, using the current IRIS design parameters. The calculation predicts that the N-16 count rate will be of the order of 300 cps for the 6,129-keV peak based on an assumed detector/collimator configuration. The background, due mainly to cobalt-60 from crud, was also estimated, and a favorable signal/background ratio can be anticipated for detection of N-16.

Researchers have made progress in developing NDE modeling capabilities. In Year 1, researchers used the ECT modeling to estimate the magnetite deposit detection signals for an encircling coil. This year, the model has been extended to allow other sensor coil configurations, such as rectangular coils inserted between tubes. Researchers calculate the electromagnetic eigenmodes for tube geometry, which is used to form Green's function for the geometry. In Year 3, researchers will perform the numerical computation of the deposit signal for the various coil configurations.

A significant effort has been made in the area of EMAT UT modeling. The focus in this area has been on the mathematical formulation of the guided wave generation, propagation, and detection in tubing geometry. The most recent progress made has been in calculating the transmission/reflection coefficients for scattered guided wave modes, scattered by a crack-like defect from an incoming guided wave. The research team has nearly completed development of the overall computational procedure, and the first computational result is about to emerge for a pressure-wave mode. In Year 3, this work will follow with signal predictions for guided wave modes, particularly torsional modes, with the previously conceived EMAT design.

The development of the deterministic transport equation code is at its critical stage. The code aims to provide an efficient alternative to Monte Carlo codes for complex radiation flux calculations suitable for hard gamma rays where the photon-charged-particle couplings are significant. The charged-particle sector of the code is being developed and integrated into the existing photon transport code. Researchers plan to complete the code in Year 3, and to apply it to parametric studies needed for, for example, detector optimization for improved S/N ratio.

## Planned Activities

**Task 1: Design Review.** As NDE sensor concepts develop, researchers will consider adaptations of proposed on-line NDE methodologies, as required. The goal is to transfer the sensor designs and their inspectability predictions to the reactor design team. In addition, researchers will continue to monitor the evolution of IRIS design to identify additional areas where on-line monitoring may be beneficial. The research team will also attempt to identify opportunities for applying the NDE technologies being developed to existing nuclear plant systems.

**Task 2: Radiation Monitoring.** Researchers will further examine the method for monitoring reactor coolant flow via N-16 radiation through calculations and measurements. Specifically, they will calculate N-16 activity concentrations and evaluate the impact of background radioactivities in IRIS, determine the optimal detector type and location, evaluate candidate detectors for N-16 detection, address the effect of ambient temperature (approximately 290°C) conditions at detector location on detector operation, improve collimator design for the detector, evaluate the effect of filters on signal/background ratio of the N-16 peaks, and evaluate detector response to transient events involving the reactor coolant pump. In addition, they will complete development of the charged-particle transport equation model. The resulting code will give predictions to the charged-particle corrections to gamma flux intensities. It will also provide an efficient, alternative, flux intensity calculation method for detector optimization.

**Task 3: Eddy Current Sensors.** Researchers will give inspectability predictions to the conceived electromagnetic on-line sensors for steam generator tubing inspections. Specifically, this will be done by calculating eddy current signals from magnetite deposits for realistic coil configurations, namely finite encircling coils and/or rectangular coils inserted between tubes.

**Task 4: Ultrasonic Sensors.** Researchers will predict inspectability of conceived on-line EMAT sensors for steam generator and other RPV structural inspections. First, they will complete guided, ultrasonic wave calculations to apply to SG tubing integrity monitoring. This will require researchers to compute transmission/reflection coefficients by defects such as cracking and deposit buildup for selected incoming guided wave modes. Furthermore, they will consider using EMATs for other structural integrity monitoring, such as at the coolant-to-vessel pump mounting points.



# NUCLEAR ENERGY RESEARCH INITIATIVE

## Supercritical Water Nuclear Steam Supply System: Innovations in Materials, Neutronics, and Thermal-Hydraulics

PI: Mark Anderson, Michael Corradini, Kumar Sridharan, and Paul Wilson, University of Wisconsin

Project Number: 01-091

Project Start Date: September 2001

Collaborators: Argonne National Laboratory

Project End Date: September 2004

### Research Objectives

In the 1990s, researchers considered supercritical light-water reactors (SCWR) in conceptual designs. A nuclear reactor cooled by supercritical water would have a much higher thermal efficiency with a once-through direct power cycle, and could be based on standardized water reactor components (light water or heavy water). The theoretical efficiency could be improved by more than 33 percent over that of other water reactors and could be simplified with higher reliability, for example, a boiling water reactor without steam separators or dryers.

To make such a system technologically feasible, advances are required in high-temperature materials with improved corrosion and wear resistance (cladding and pressure structural boundaries), in neutronics to improve fuel-cycle versatility with these advanced materials, as well as in neutronics and thermal-hydraulics to insure efficient heat removal and passive safety and stability. The research objectives of this project are:

- To employ innovative, plasma-based, surface modification techniques, including ion implantation, energetic-ion-induced near-surface alloying, and surface homogenization to improve material compatibility under supercritical conditions. These techniques are being applied to cladding and structural materials with proven bulk properties in order to mitigate surface-initiated degradation phenomena of corrosion, oxidation, and wear under supercritical thermal-hydraulic conditions.
- To perform neutronics analyses to identify ranges of alternative fuel cycles, including variations in enrichment, refueling schedules, recycling, and conversion/breeding. These analyses, using quantitative metrics, would focus on coolant density effects at supercritical conditions to verify passive safety from the standpoint of fuel burnup, flexibility, proliferation resistance, as well as sustainable development.

- To perform thermal-hydraulic studies focusing on heat transfer and flow stability issues associated with coolant density changes for natural and forced circulation of supercritical water. Scaled simulated experiments are to be designed and performed to provide heat transfer and stability data to be used in developing predictive tools.

### Research Progress

**Task 1. Materials Science and Corrosion in Supercritical Water Corrosion Loop.** Argonne National Laboratory (ANL) and University of Wisconsin (UW) researchers have made substantial progress this year with investigating three plasma surface treatment approaches: high energy ion implantation of gaseous species, film deposition and surface alloying, and heavy inert gas ion bombardment. The treatments listed in Table 1 were performed this year on three alloy classes: Zircaloy, stainless steel, and Inconel.

Plasma surface treatment approach	Species incorporated or deposited on alloy flats
Method I: High energy ion implantation	N <sup>+</sup> , O <sup>+</sup> , and C <sup>+</sup>
Method II: Inert ion bombardment	Xe <sup>+</sup> and Ne <sup>+</sup>
Method III: Film deposition	Yttrium and Si-O-C*

\*Performed using a hexamethyl-disiloxane (HMDSO) precursor

Table 1. Plasma-based surface treatment performed on multiple samples of the three alloys.

The activities involved 1) plasma surface treatment of test flats of Zircaloy-4, Inconel 718, and 316 austenitic stainless steel; 2) corrosion testing and characterization in supercritical water loop at 350, 400, and 500°C, 25MPa and oxygen concentration of approximately 10ppb for 3, 5, and 7 days; and 3) analysis of materials samples for the given time-and-temperature of residence in the supercritical water reactor loop, using scanning electron microscopy (SEM), auger, and scanning microprobe. Table 2 summarizes the material samples tested with surface modifications.

	Stainless Steel 316	Inconel 718	Zircaloy-4
<b>3-Day Test Run</b>			
Untreated	X	X	X
<b>5-Day Test Run</b>			
Untreated	X	X	X
Method 1 (N <sup>+</sup> )	X	X	X
Method 2 (Xe)		X	
Method 3 (Yt)	X		
<b>7-Day Test Run</b>			
Untreated	X	X	X
Method 1 (N <sup>+</sup> )	X	X	X
Method 2 (Xe)		X	
Method 3 (Yt)	X		

Table 2. Summary of the corrosion testing performed under supercritical water conditions.

Researchers first analyzed the corrosion test specimens with the SEM to allow a qualitative examination of the sample surface as well as a cross-sectional examination along a sectioned edge. The same test flats were then more quantitatively examined via the scanning microprobe and the auger microprobe. Results, as expected, indicated more substantial corrosion for the untreated samples, with Zircaloy the most corroded. In contrast, when all the samples were surface treated with the plasma-ion implantation, the amount of corrosion was reduced substantially, with the stainless steel samples least affected, even at 500°C.

**Task 2. Neutronics Analysis of Coolant Density and Cladding Materials on Fuel Cycle.** To mitigate design issues of the SCWR (i.e., bottom skewed axial power shape, local power-peaking problems, positive void coefficient, etc.), researchers developed a conceptual design of the mixed spectrum SCWR (MS<sup>2</sup>) core using the SOLTRAN code. Its potential benefits were presented at the Ameri-

can Nuclear Society (ANS) annual meeting in June 2003 at San Diego. In the MS<sup>2</sup> core, the coolant first passes through an outer thermal zone and then an inner fast zone. By separating the thermal and fast zones radially, the MS<sup>2</sup> concept provides potential advantages of simple axial power shape and actinide burning in the fast zone. To optimize the fuel assembly design, researchers performed Power Density (P/D) sensitivity calculations using HELIOS code. After optimizing the design parameters (i.e., P/D value, fuel composition, etc.), researchers are comparing the nuclear characteristics of the MS<sup>2</sup> core with the thermal SCWR cores proposed by Idaho National Environmental and Engineering Laboratory (INEEL). Researchers will also evaluate the performance of the cladding materials (Figure 1) and fuel cycle analysis based on the MS<sup>2</sup> core.

**Task 3. Natural Circulation Heat Transfer and Flow Stability Studies.** The ANL natural circulation loop of supercritical carbon dioxide is now operational. This loop (named SNAC for Supercritical CO<sub>2</sub> Natural Circulation) will provide fundamental data on natural circulation heat transfer and flow stability associated with the SCWR system.

Figure 2 shows the calculated mass flux and heater outlet temperature versus input power at a loop operating pressure of 80 bar and heater inlet temperature of 20°C. The peak in the mass flux curve, shown in Figure 2, corresponds to the power necessary to raise the bulk fluid temperature above the pseudo-critical temperature (35°C) and past the region of increased fluid heat capacity. Once past the region neighboring the pseudo-critical point, the

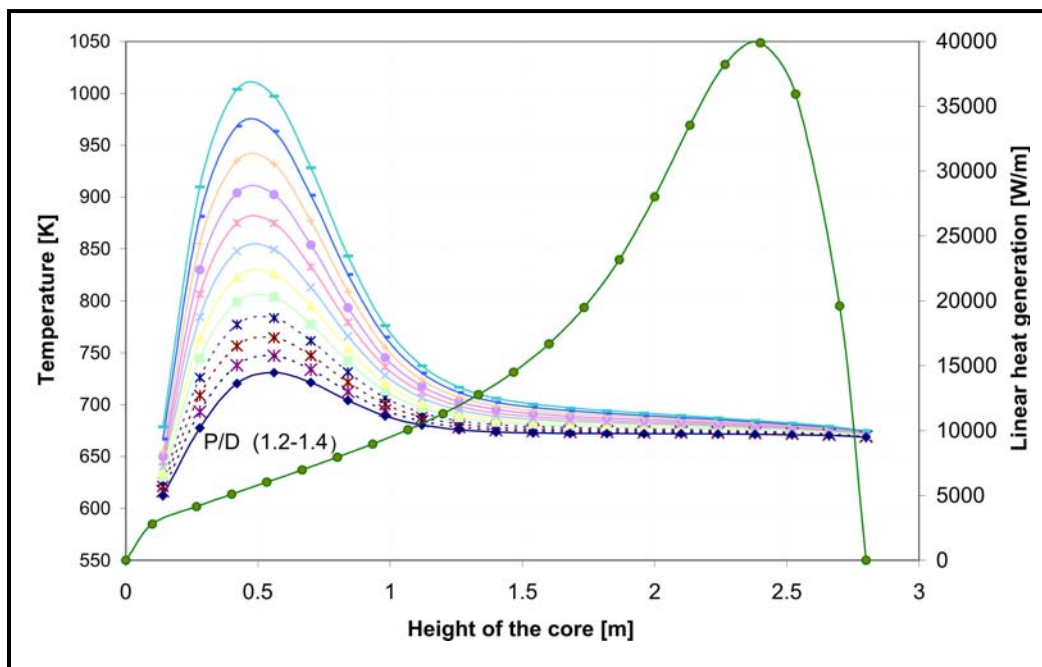


Figure 1. Axial cladding surface temperature in outer core of MS<sup>2</sup> reactor design.

fluid temperature and specific volume rise rapidly with input power, which boosts friction losses in the hot leg and suppresses the loop mass flow rate. For comparison, researchers included the initial test data in the plot. The measurements were made during steady-state operation at a pressure of roughly 80 bar and an inlet temperature of 25°C. The data agreed well with the calculations, which did not include the effects of density change on flow losses. There were no significant flow instabilities observed during these initial

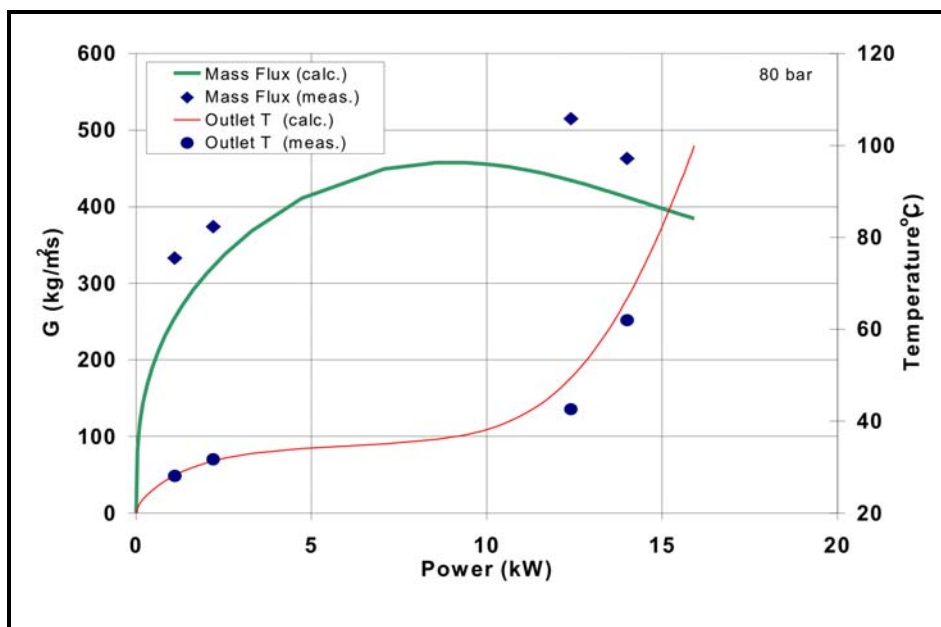


Figure 2. The calculated mass flux and heater outlet temperature versus input power at a loop operating pressure of 80 bar and heater inlet temperature of 20°C.

experiments. This is an intriguing result that requires more investigation. The development of a complete steady-state model for this natural convection loop with a complete equation of state for the supercritical fluid indicates that the presence or absence of flow instabilities is a function of loop geometry. Researchers on this project are now in the process of applying more sophisticated frequency-domain and time-domain models to determine when instabilities occur.

## Planned Activities

In the last year of this research grant the team plans to:

1) **Complete corrosion tests with the three metal alloys with and without plasma surface modifications.** During the past two years, researchers have successfully designed, fabricated, and began corrosion testing in a supercritical water loop. Three metal alloy

classes (Zircaloy, stainless steel, Inconel) were tested with three different types of plasma surface treatments. In the final year, the team will focus on AISI 316 austenitic stainless steel and Inconel 718 with and without these surface treatments over longer corrosion periods (10–20 days). These longer test times will allow researchers to correlate the corrosion rate and growth of the oxide layer with the documented improvements by plasma surface treatments. Actual boiler tube corrosion will be compared.

2) **Complete a neutronic and thermal-hydraulic design for the MS<sup>2</sup> reactor design.** Researchers

will complete their effort for a novel

mixed spectrum reactor core design with neutronics and thermal-hydraulics analyses. In addition, the ANL-UW researchers have developed a versatile computational tool for more general use in the design of advanced water reactors.

3) **Complete flow instability experiments and associated steady-state and transient T-H model.**

The ANL supercritical CO<sub>2</sub> loop is a versatile new facility to investigate natural circulation and forced circulation flow instability phenomena. The ANL-UW team will develop a comprehensive database for steady flow natural circulation, while identifying the conditions under which the flow instability is initiated. In addition, the team will extend the steady-state and transient model used in test analysis (CO<sub>2</sub> and water) to consider not only fixed heat flux and fixed temperature boundary conditions, but also power-flow feedback for reactor applications.



# NUCLEAR ENERGY RESEARCH INITIATIVE

## Testing of Passive Safety System Performance for Higher Power Advanced Reactors

PI: José N. Reyes, Jr., Oregon State University

Project Number: 01-094

Collaborators: Westinghouse Electric Company, LLC

Project Start Date: August 2001

Project End Date: July 2004

### Research Objectives

The primary objective of this project is to assess the cooling performance of the AP1000 passive safety system core under high decay power conditions for a spectrum of breaks located at a variety of locations in the APEX test facility. In addition, researchers will compare predictions of the integral system data to the measured results using a reactor systems thermal hydraulic computer code. This project will provide insights into new passive safety system concepts that could be used for Generation IV higher power reactors.

### Research Progress

During the past two years, excellent progress has been made in meeting the primary objective of assessing the performance of the AP1000 passive safety systems. Researchers have successfully conducted five integral system tests and have issued seven reports documenting the APEX-1000 test facility scaling analysis, its design, and the results of testing.

Figure 1 shows the modified APEX-1000 integral system test facility. It is a ¼-height-scale test facility that includes a complete primary system, all of the passive safety systems and their corresponding safety actuation logic. The test facility has been audited by DOE, Westinghouse, and the U.S. Nuclear Regulatory Commission (NRC) to assess its adequacy for use in plant design certification.

As shown in Table 1, researchers have successfully conducted six integral system tests in the APEX-1000 facility thus far. The tests are primarily Design Basis Accident scenarios specifically selected to examine the important

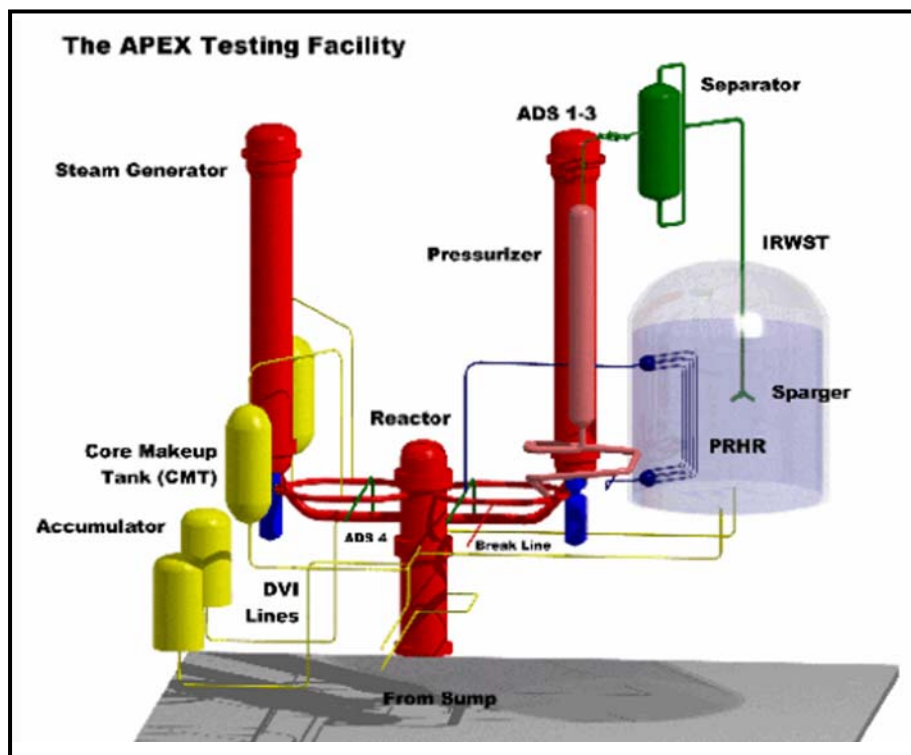


Figure 1. APEX-1000 Integral System Test Facility at Oregon State University.

Test ID	Test Description	Date
DBA-01-D	Double-Ended DVI Line Break with Failure of 1 ADS-4 valve on Loop 2. (Flow Nozzles)	2/28/03
TR-01-D	Full-Pressure ADS-4 Blowdown to Onset of IRWST Injection with No Reserves. Constant power (600 kW) and Failure of 1 of 4 ADS-4 valves.	3/18/03
DBA-03-D	Double-Ended DVI Line Break with Failure of 1 ADS-4 valve on Loop 1. (Reduced ADS-4 Line Resistance Venturi Nozzle)	5/1/03
DBA-04-D	Double-Ended DVI Line Break with Failure of 1 ADS-4 valve on Loop 2. (Reduced ADS-4 Line Resistance Venturi Nozzle)	5/15/03
DBA-05-D	2-Inch (5 cm) Cold Leg Break with Failure of 1 ADS-4 valve on Loop 2.	7/01/03
TR-02-D	Full-Pressure ADS-4 Blowdown to Onset of IRWST Injection. Initial Pressure-100 psia; High Decay Power, Failure of 1 ADS-4 Valve.	7/09/03

Table 1. APEX-1000 integral system tests completed thus far.

operational characteristics of the AP1000 passive safety systems. The results of these first six tests have been used to guide the balance of testing, which will focus on assessing the performance of the fourth stage of the Automatic Depressurization System (ADS4). Researchers have transmitted all of the data obtained to date to Westinghouse for their review and analysis as part of the AP1000 plant certification process.

## **Planned Activities**

Researchers will conduct five tests in the next fiscal year to better understand the long-term cooling and sump recirculation phases of an AP1000 transient. In particular, researchers will take detailed measurements of ADS-4 line pressure drop, vapor quality, and liquid entrainment rates for a wide range of core decay powers. They will assess existing two-phase pressure drop and liquid entrainment rate models using this new data. Non-proprietary and proprietary reports shall be issued for potential use in the AP1000 certification design process.



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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Engineering and Physics Optimization of Breed and Burn Fast Reactor Systems

PI: Michael Driscoll, Massachusetts Institute of Technology

Project Number: 02-005

Collaborators: Argonne National Laboratory-West, Idaho National Engineering & Environmental Laboratory

Project Start Date: September 2002

Project End Date: September 2005

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### Research Objectives

The goal of this project is to develop a practical implementation of breed and burn operation in hard spectrum fast reactors. In the present context, "breed and burn" refers to cores for which reload fuel has a significantly lower enrichment than that required to sustain criticality: for example < 5 w/o U-235. In the ideal case, no recycle is required (but not precluded) to still achieve natural uranium utilization significantly higher than current light water reactor (LWR) units.

The general concept dates back to the late 1950s; but, despite sporadic interest since, has not generated much top-level interest because of the unresolved challenges that are the subject of the present research: the need for a large, low-leakage core with minimal non-heavy-metal fuel diluents, plus high power density and burnup to accelerate and sustain fissile buildup such that one moves quickly to an equilibrium fuel cycle.

In contrast to the contemporary effort in Russia on a lead-cooled reactor of this type, the present project centers on the use of gas-cooled units. This requires addressing attendant performance issues, most notably, the provision of highly reliable post-shutdown decay heat removal, with, preferably, a significant contribution by passive means. Achieving overall economical plant design may warrant adoption of the innovative supercritical CO<sub>2</sub> power cycle, which develops high efficiency (approximately 45 percent) at temperatures less than 650°C and permits use of metal cladding. Nevertheless, fuel integrity is another priority focus because of its high burnup, high fluence, and time-at-temperature.

Finally, researchers are investigating fuel re-use employing non-separative reprocessing technology (e.g., AIROX: successive oxidation reduction) with two more goals in mind: 1) the refabrication and re-insertion of gas-cooled

fast reactor (GCFR) fuel if its integrity is not adequate for single-campaign service, and 2) the recycling of the fuel into LWRs to improve overall economics and spoil the plutonium isotopic mix for potential diversion to weapons uses. This information is also highly relevant to accident sequence assessment, for example, post loss-of-coolant accident (LOCA) air ingress or the interaction of CO<sub>2</sub> with fuel having cladding defects.

### Research Progress

The first year of this project's efforts has been devoted to downselection among the myriad of options open to consideration. Table 1 summarizes the end-state arrived at, which is also the starting point for Year 2 work. Most of the plant-related issues are self-explanatory and follow directly from the requirements for meeting the goals; that is, providing competitive economics and assuring ultra-reliable shutdown and emergency core cooling, within the stringent constraints imposed by the physics performance of a breed and burn reactor.

Researchers carried out a wide-ranging survey of generic GCFR core performance under simulated breed and burn conditions for pin, block, and pebble-type cores. Figure 1 shows representative unit cell results for ceramic fuels starting with an equivalent, core-average 10 percent U-235 enrichment in pin geometry with HT-9 clad and He coolant. As shown in the figure, UC and UN-15 are significantly superior in terms of bred-in reactivity, and UO<sub>2</sub> is so inferior as to be impractical. Researchers performed similar studies for a variety of metal alloy fuels and several cladding candidates. While neutronically attractive, metal fuels were eliminated based on their restrictive operating temperature constraints, and the need for liquid metal bonding. Studies using four-assembly colorset clusters and four batch staggered reloading, starting with 5 a/o U-235

Core		Comments:	
Fuel:	Reference:	UC	UO <sub>2</sub> not viable neutronically
	Alternate:	UN-15	Reaction of UN and UC with CO <sub>2</sub> and O <sub>2</sub> if clad is breached is an issue
Clad:	Reference:	ODS	ODS may be able to resist creep adequately up to ≈700°C
	Alternate:	HT-9	Proven LMR fast reactor clad
	Advanced:	SiC	SiC is focus of GFR INERI with CEA
Coolant:	Reference:	He, Indirect Cycle	He is inert chemically
	Alternate:	CO <sub>2</sub> , Direct cycle	Simpler, cheaper plant, higher efficiency: no IHX, primary blower
Plant			
Power Cycle:	Reference:	Supercritical CO <sub>2</sub> , indirect	S-CO <sub>2</sub> cycle is efficient at lower T than He direct which requires >800°C Indirect Cycle reduces LOCA initiators
	Alternate:	Supercritical CO <sub>2</sub> , direct	S-CO <sub>2</sub> cycle is compact and simple; cheaper than He Brayton or Steam Rankine
Reactor Vessel:	Reference:	Prestressed Cast Iron Vessel (PCIV)	PCIV is modular, more T resistant than concrete, accommodates large core, envelopes IHX and shutdown loops
	Alternate:	Prestressed Concrete Reactor Vessel (PCRIV)	Proven in GCR service
Shutdown Cooling System: (combined shutdown & emergency)	Reference:	<ul style="list-style-type: none"> <li>3 x 50% capable forced convection loops, electric + pneumatic (accumulator) powered</li> <li>Water-boiler heat rejection</li> </ul>	PRA-guided design supports this selection (basically same No. loops as GCFRs of the 1970s)
	Alternate:	4 x 50% capable forced convection loops with measures taken to reduce common-cause failures	PRA shows potential reduction in CDF by >3x
Containment:	Reference:	PWR type sized to keep post-LOCA pressure ≈5 atm	Combined with CO <sub>2</sub> injection this permits decay heat removal solely by natural convection
	Alternate:	Filtered-Vented like HTGR and some European PWRs	For cost reduction; OK if very high decay heat removal reliability is achieved.

Table 1. Key features of breed and burn GFR concept.

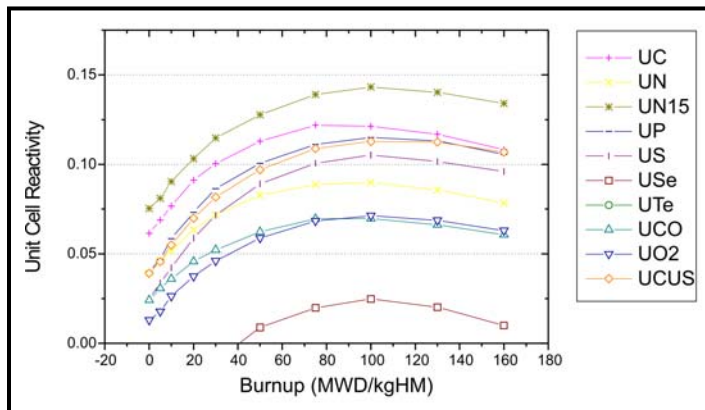


Figure 1. Reactivity histories for ceramic fuels.

enrichment, confirmed these screenings under more realistic conditions.

Researchers made calculations for spent fuel re-fabricated and used directly as pressurized water reactor (PWR) reload fuel to confirm the basic feasibility of this concept. One interesting finding is that rare earth fission product

buildup during GCFR burnup leads to a strong burnable poison effect in the PWR.

Chemistry lab experiments showed that UC can be oxidized to UO<sub>2</sub> using CO<sub>2</sub>—thus confirming that a "CARDIO" process similar to the more familiar AIROX/OREOX/DUPIC process is feasible. However, it also shows that fuel having clad defects would be attacked if CO<sub>2</sub> is used as a reactor coolant. Researchers would have to show that reaction kinetics is slow enough to make the progression tolerable, allowing removal of the defected fuel before serious consequences arise.

### Planned Activities

Year 2 activities will complete the downselection and related performance assessment phases of the effort.

In the physics and fuel cycle area, the focus will be on the use of oxide dispersion strengthened (ODS)-clad UC; but, in view of intense interest in UN-15, a comparative evaluation of this advanced fuel will be carried along. A key feasibility/economic issue is whether fuel pins must be treated or refabricated at mid-life because of clad fluence, fission gas pressure, and clad creep limitations. Efforts will be intensified on the optimization of the design of a PWR lattice employing AIROX-processed spent GCFR fuel. The Year 1 AIROX studies will be broadened to assess ways to reconstitute UC for GCFR re-insertion following mid-life re-cladding, should this prove necessary.

In the closely coupled thermal-hydraulic and plant design subtasks, the major emphases will be on enhancing and confirming the reliability of active and semi-passive mode decay heat removal and on whole-core thermal-hydraulic analyses. The goal will be to increase steady-state power density to 200 kW/l (i.e., closer to that of the GA GCFR of the 1970s). This will require ultra-reliable shutdown/emergency cooling systems, which appears feasible if common cause failure modes can be reduced to an absolute minimum.

Fuel design will focus on coping with the high burnup, high fluence, high temperature (for metal clad) service required of breed and burn fuel. Researchers will analyze the reference UC/ODS fuel in increasing depth, and they will also assess potential alternative/advanced fuels and clad to include UN fuel and SiC clad.

In Year 3 (the final year), researchers on this project will focus on the best overall combination of design features with a strong emphasis on assessing engineering performance relative to key factors such as fuel durability and post-LOCA core cooling. Another major goal is assessing the economic viability of the breed and burn GCFR in a future, sustainable, nuclear economy.

# NUCLEAR ENERGY RESEARCH INITIATIVE

## Evaluation of Integral Pressurizers for Generation IV PWR Concepts

PI: David Felde, Oak Ridge National Laboratory

Project Number: 02-018

Collaborators: Westinghouse Electric Company

Project Start Date: September 2002

Project End Date: September 2005

### Research Objectives

The objective of this project is to build a knowledge base that will enable designers to better appraise the pros and cons of the possible pressurizer designs for integral primary system reactors (IPSR). As part of this process, it is the intent of the project to map the performance of integral pressurizers as a function of their design parameters (gas content, vapor volume, and interface with the primary system). Based on the detailed analysis of pressurizer performance, researchers aim to propose new design solutions that will allow the reactor system to be simplified or withstand more severe accident scenarios.

### Research Progress

Work during the first year focused on developing a description of a reference reactor design based on the International Reactor Innovative and Secure (IRIS) concept that will be used as the basis of the remainder of these studies. Researchers developed a detailed description of that design, which is being used to guide model development and pressurizer design. They developed the RELAP5-3D model of the reference reactor design based on the IRIS reactor. During this project, researchers assembled a three-dimensional thermal hydraulic model, and carried out some initial steady state calculations.

Efforts have focused on developing specific requirements for pressurizer operation. Westinghouse developed a full set of requirements for further use in the IRIS design certification process. In addition, researchers drafted an implementation document discussing the process of deriving practical criteria for implementing the Functional Requirement into the IRIS design. This draft is under consideration by the team members for final acceptance.

Researchers have defined the limiting transients necessary for formulating the limiting in/out surge flows. They consist of the following six event types and address the critical design parameters related to specification of overall pressurizer liquid and gas volumes.

1. Loss of Heat Sink
2. Decrease of Reactor Flow
3. Feed Water System Malfunction
4. Inadvertent Steam Leak
5. Loss of Offsite Power
6. Reactor Trip

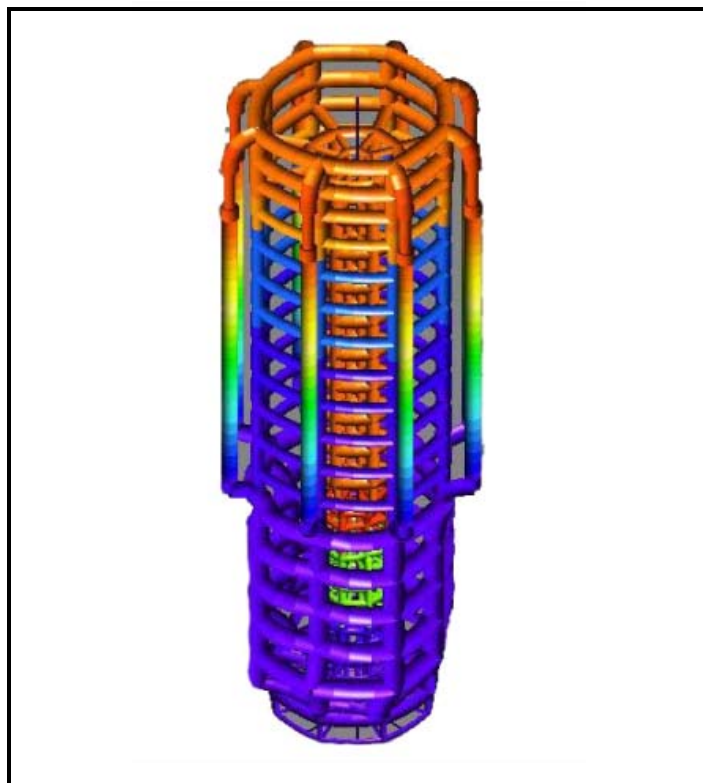


Figure 1. The Graphical User Interface (GUI) generated steady state temperature distribution.

Design Parameter	Value
Overall Volume	77.15 m <sup>3</sup> (2724.52 ft <sup>3</sup> )
Spherical Head Inner Diameter	6.223 m (20.417 ft)
Pressurizer Height, Total	4.4915 m (14.736 ft)
Inverted Top Hat	
Height	1.181m (3.875 ft)
Internal Diameter, Lower Plate	2.900 m (9.514 ft)

Table 1. IRIS PRZ design characteristics.

Based on the results of the transient analyses, Westinghouse completed the conceptual steam pressurizer design. The IRIS pressurizer volume is determined by the space available in the vessel upper head; therefore, it will not impact the overall dimensions of the pressure vessel. All the relevant data required for a mechanical design of this component are provided in Table 1; the conceptual design is depicted in Figure 2.

Two summer interns from Texas A&M University have initiated preliminary work on computational fluid dynamics (CFD) modeling that will be needed for Year 2 of the project. During this effort the researchers have identified nitrogen diffusion coefficients and equilibrium concentration information that will be needed for modeling the gas pressurizer system. In addition, they have developed simplified CFD models that will help in understanding pressurizer and primary system performance.

Oak Ridge National Laboratory (ORNL) has been working with Westinghouse on benchmarking the core physics methods and on the core design. They have developed an initial core design for the first IRIS fuel cycle and are performing ongoing studies to optimize the design and to

determine the equilibrium fuel loading patterns. The RELAP-3D model utilized for the pressurizer analysis will be based on this initial, first cycle design, which will be representative of any future designs. Researchers on this project will develop cross sections libraries for the whole fuel cycle. Collaboration with Penn State University has been established to explore an advanced method for introducing transient cross sections in the RELAP code. Currently, a Ph.D. student at Penn State is working on the required programming associated with these code modifications.

### Planned Activities

Transient analysis will continue focusing mostly on Anticipated Transients without Scram (ATWS). In addition, emphasis will be placed on developing a 3-D neutronic core model to be used in performing these analyses. Work will also focus on finalizing the conceptual gas pressurizer design and evaluating the differences in performance between the gas and steam pressurizer options.

Specific tasks include:

- Developing a detailed CFD model of the pressurizer/reactor interface.
- Performing pressurizer studies using the CFD model.
- Designing/fabricating/installing experimental equipment.
- Performing a transient system evaluation for a specific pressurizer/reactor.

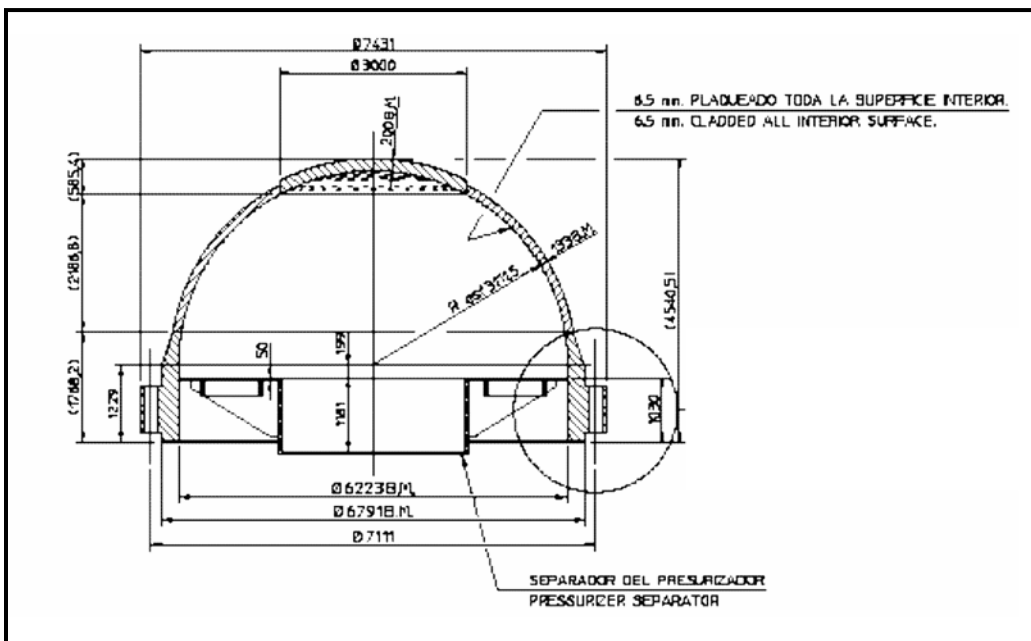


Figure 2. Conceptual PRZ drawing.

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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Nuclear-Energy-Assisted Plasma Technology for Producing Hydrogen

PI: Peter Kong, Idaho National Engineering and Environmental Laboratory

Project Number: 02-030

Collaborators: None

Project Start Date: October 2002

Project End Date: September 2005

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### Research Objectives

The objective of this project is the research and development of a nuclear-energy-assisted plasma process to produce hydrogen carrier materials. The focal point of this research is to develop a plasma electrolysis technology to convert sodium metaborate to sodium borohydride using nuclear-energy-generated electricity to operate the plasma reactor. Using plasma electrolysis to convert sodium metaborate to sodium borohydride is a new idea—no current technologies are similar to this concept.

Sodium borohydride is a safe, concentrated hydrogen carrier compound that can store an impressive amount of hydrogen. For example, 1 liter of 44-weight percent sodium borohydride solution at 1 atmosphere can release about 130 grams of hydrogen. Sodium borohydride releases more hydrogen than other sources of hydrogen. In addition, sodium borohydride has a higher density of hydrogen than other sources. For example, cryogenic liquefied hydrogen has a density of 70 gm/liter. Hydrogen pressurized to 6,000 psi has a density of only 36 gm/liter. Rare-earth-nickel alloys can store hydrogen up to a density slightly higher than liquid hydrogen but less than sodium borohydride. This alloy is very expensive and not as easily handled as a liquid. The borohydride solution is much easier and safer to handle than liquid or high-pressure hydrogen. Current gasoline distribution infrastructure for automobiles can be easily converted to dispense "sodium borohydride fuel" for hydrogen vehicles.

Sodium borohydride can be produced from sodium borate. However, to date, no known technology exists to do so economically. A successful nuclear-power-assisted plasma technology to convert sodium borate to sodium borohydride transportation fuel will have a long-term, significant, economical benefit to the nuclear power industry. During peak operation, nuclear power reactors will

generate electricity to meet peak commercial demand. During off-peak operation, the nuclear reactor will supply electricity and nuclear process heat to produce sodium borohydride. Producing sodium borohydride during off-peak hours will increase the demand for the nuclear industry.

### Research Progress

Sodium borohydride,  $\text{NaBH}_4$ , is a chemical hydride with impressive hydrogen content. This material releases hydrogen when it reacts with water. Half of the hydrogen released is derived from water,  $\text{NaBH}_4 + 2\text{H}_2\text{O} \rightarrow 4\text{H}_2 \uparrow + \text{NaBO}_2$ . When sodium borohydride dissolves in 4-wt% sodium hydroxide solution, hydrogen will not be released until the solution comes in contact with a catalyst. Conceptually,  $\text{NaBH}_4$  can be regenerated by the electrolysis of the spent material, sodium metaborate ( $\text{NaBO}_2$ ) solution. The reaction to regenerate  $\text{NaBH}_4$  is shown in the chemical reaction,  $\text{NaBO}_2 + 2\text{H}_2\text{O} + \text{electricity} \rightarrow \text{NaBH}_4 + 2\text{O}_2 \uparrow$ . During the regeneration, oxygen is given off and hydrogen is extracted from water to form the borohydride. During electrolysis, if oxygen gas liberation can be enhanced and hydrogen gas liberation suppressed at the respective anode and cathode, then the reaction should proceed to borohydride formation. This concept seems straightforward and simple. However, the development of an electrolysis process to suppress hydrogen gas liberation at the cathode could become very challenging. The proof of concept research in FY 2003 centers on four main tasks.

#### **Task 1: Identify and test suitable materials for optimum oxygen gas liberation from the anode.**

This task involved a search for metals with low oxygen overpotentials that are desirable to operate as anodes because oxygen gas can liberate from the electrode more readily at lower voltages. Researchers used a cyclic voltametry (CV) cell to measure the anodic half-cell poten-



tials against a HgO reference electrode. Researchers tested four metals, gold (Au), platinum (Pt), iridium (Ir), and stainless steel (SS), in the CV cell for oxygen gas evolution. Figure 1 shows the test results. The right branch illustrates oxygen liberation. Among the metal tested, a stainless steel anode showed the lowest overall voltage for oxygen gas generation indicating that it is a good anode candidate material.

**Task 2: Identify and test suitable materials for maximum hydrogen gas suppression from the cathode.** Contrary to the anode, the cathode must have a high hydrogen overpotential to suppress hydrogen gas formation in this process. If hydrogen gas liberation cannot be minimized or suppressed, then borohydride formation might not be feasible. Researchers tested several metals, tin (Sn), zinc (Zn), indium (In), platinum (Pt), rhenium (Re), selenium (Se), and Tellurium (Te), as cathodes for hydrogen suppression in the CV cell. Sn, Zn, In, Pt, and Re cathodes all showed hydrogen liberation. However, metals Se and Te showed no hydrogen gas evolution (Figure 2). The result showed that both metals Se and Te are good anode candidate materials.

**Task 3: Conventional electrolysis to evaluate suitable anode and cathode materials for the process.** Researchers constructed a conventional electrolysis reactor as part of the first-year research effort.

This reactor was used to evaluate the electrode material properties of anode and cathode materials, which included a number of different metals and alloys. Researchers identified candidate anodes and cathodes during the electrolysis of a borate solution. Figure 3 shows the test of Te during a hydrogen gas suppression process. It is clearly seen that no hydrogen gas evolved from the cathode while oxygen is liberated from the anode. However, the material tested in this case was unstable and disintegrated under high negative voltages.

**Task 4: Development of a bench scale plasma electrolysis system.** The conventional electrolysis reactor was successfully converted to the pseudo plasma electrolysis system. In the pseudo plasma electrolysis mode, the anode was non-submerged while the cathode was submerged in the solution. Researchers applied a high dc voltage between the electrodes to initiate and sustain the arc. In Figure 4, the arc is sustained above the solution. A foamy layer formed beneath the surface of the arc. This foamy layer was formed by the evolution of very fine bubbles in this layer. The arc appeared yellowish orange due to the presence of sodium ions. Researchers also observed gas generation with the SS cathode. A fine suspension was seen forming in the cathode cell during electrolysis. This layer of suspension would dissolve after the electrolysis was terminated. This task demonstrated that pseudo plasma electrolysis is an operable process.

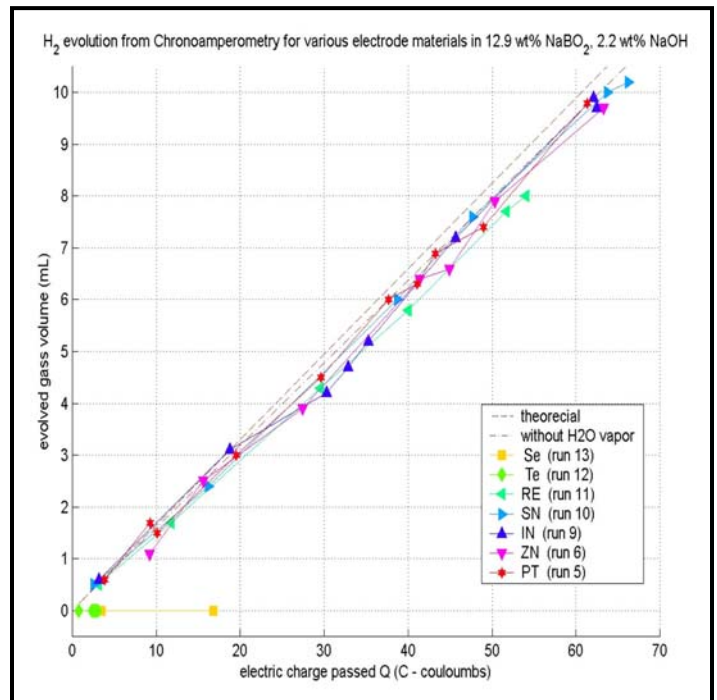
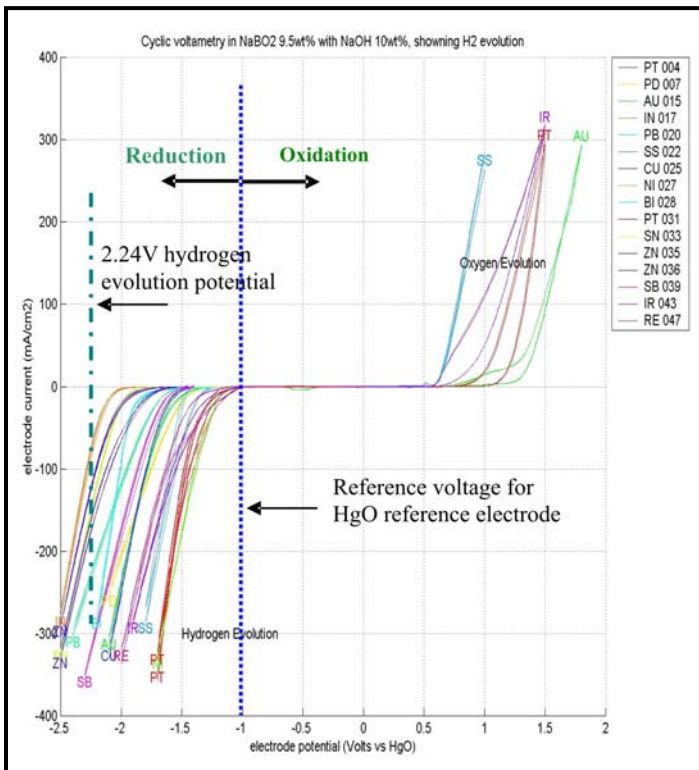


Figure 1. Cyclic voltammetry test for electrode testing.

Figure 2. Measurement of hydrogen evolution for several cathode materials during conventional electrolysis.

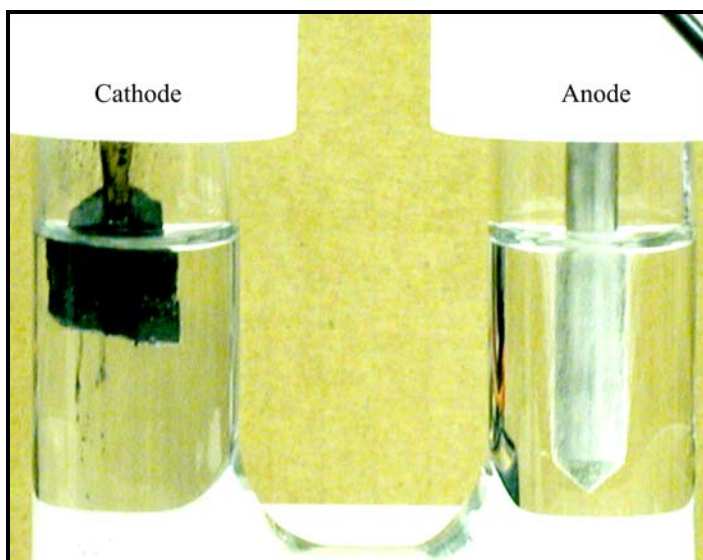


Figure 3. Test of Te as cathode for hydrogen generation suppression.

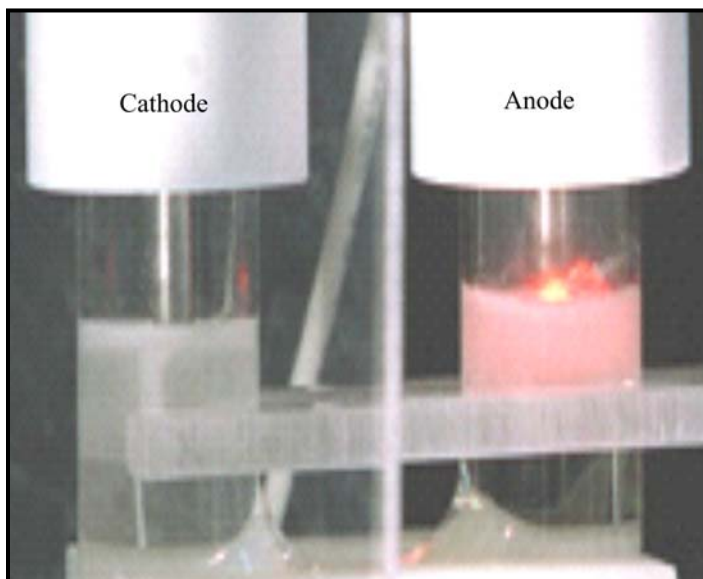


Figure 4. Anode is the plasma electrode and cathode is submerged.

## Planned Activities

- 1) **Cathode Materials for Hydrogen Suppression.** Significant effort directed to the research and development of hydrogen-suppressing cathode materials based on metal Te will continue in FY 2004. During this time, researchers plan to synthesize a large number of compounds and alloys for Te to be tested in the conventional electrolysis cell. They will perform electrolysis with dilute sodium hydroxide solution to study cathode behavior for hydrogen suppression.
- 2) **Conventional Electrolysis of  $\text{NaBO}_2$  to  $\text{NaBH}_4$ .** Once researchers identify a promising candidate cathode material in Task 1, they will test the material in conventional electrolysis of  $\text{NaBO}_2$  for conversion to  $\text{NaBH}_4$ . Then, they will analyze the processed solution for evidence of  $\text{NaBH}_4$  formation.
- 3) **Plasma Electrolysis of  $\text{NaBO}_2$  to  $\text{NaBH}_4$ .** Once researchers identify a promising candidate cathode material in Task 1, they will also test the material in plasma electrolysis of  $\text{NaBO}_2$  for conversion to  $\text{NaBH}_4$ . They will compare process characteristics between conventional and plasma electrolysis. They will then analyze the processed solution for evidence of  $\text{NaBH}_4$  formation.
- 4) **Assessing Other Plasma Concepts.** During this project, researchers will also study other plasma technology concepts for sodium borate to sodium borohydride conversion. They will choose the most successful conversion technology concept, including conventional and plasma electrolysis, for the next phase of research, which will include economics evaluation and scaling feasibility studies.





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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Coupling of High-Temperature, Lead-Cooled, Closed Fuel Cycle Fast Reactors to Advanced Energy Converters

PI: James J. Sienicki, Argonne National Laboratory    Project Number: 02-065

Collaborators: Oregon State University

Project Start Date: September 2002

Project End Date: September 2005

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### Research Objectives

The objectives of the project are to develop a high-temperature, modular, nuclear plant concept that combines the benefits of lead-cooled fast reactors:

- Sustainability and closed fuel cycle benefits of a fast neutron spectrum core;
- Passive safety of molten lead primary coolant;
- Autonomous operation benefits of a fast spectrum core enhanced by lead coolant;
- Economic advantages of modular construction, factory fabrication, full-transportability, and simplification;
- Natural circulation heat transport at power levels in excess of 100 percent;

with the advantages of advanced power conversion including a gas turbine Brayton cycle secondary system that utilizes supercritical carbon dioxide as the working fluid:

- Significantly improved cycle efficiency (44 percent at 550°C turbine inlet temperature) relative to the Rankine water/steam cycle;
- Reduced plant footprint due to fewer, simpler, and smaller-sized secondary side components; and the
- Prospect of reduced capital and operating costs and reduced plant staffing requirements by radically simplifying the plant and eliminating costly Rankine cycle components.

A coupled, autonomous, lead-cooled fast reactors (LFR)-supercritical CO<sub>2</sub> Brayton cycle plant is well-suited for developing nations that do not have a nuclear infrastructure or a base of nuclear expertise. These nations will benefit from the deployment of low power, autonomous, passively safe, modular plants that reduce operator workload and requirements and long-term operation after which the entire core cartridge is removed for reprocessing. Domestic

power producers can also benefit from these plants as they require minimal electric grid modification, can be sited closer to cities, and provide capital and operating cost savings, greater efficiency, plant simplification, and reduced staffing.

### Research Progress

Researchers on this project studied the feasibility of coupling the 400-MWt Secure Transportable Autonomous Reactor-Liquid Metal (STAR-LM) natural circulation LFR to a supercritical carbon dioxide (S-CO<sub>2</sub>) Brayton cycle. It has been shown that such a coupling is indeed feasible and that the S-CO<sub>2</sub> temperatures achieved would result in a Brayton cycle efficiency of 44 percent as well as a compact plant footprint. To study the feasibility and to determine the efficiency, researchers developed an analysis computer code for the plant's conceptual design. This computer code models the steady state behavior of both the autonomous natural circulation LFR and the S-CO<sub>2</sub> Brayton cycle secondary side. With this code, researchers calculated temperatures, pressures, and velocities for the lead and S-CO<sub>2</sub> around the primary and secondary circuits. They also performed an analysis to determine optimal designs for the S-CO<sub>2</sub> turbine and compressor (i.e., number of stages and stage dimensions) that maximize the cycle efficiency.

The code was utilized to perform design trade studies and to produce an optimized coupled plant conceptual design. The key to achieving an effective coupling is the design of lead-to-S-CO<sub>2</sub> heat exchangers that can fit into the available volume within the reactor vessel and heat the S-CO<sub>2</sub> to high enough temperatures to provide the desired cycle efficiency. The code analyses showed that efficient in-reactor heat exchangers that meet the requirements are feasible with S-CO<sub>2</sub> flowing up inside tubes and lead flowing down over the tubes. Figure 1 shows the calculated reactor and Brayton cycle conditions.

It was demonstrated that the core clamping and re-strain approach can be designed such that the reactor power autonomously adjusts itself to changes in load demand with nearly unvarying core outlet temperature. As a consequence, the Brayton cycle efficiency remains approximately unchanged by load demand from the electrical grid. This project's researchers developed a control scheme for the S-CO<sub>2</sub> Brayton cycle secondary side for autonomous load following.

Researchers analyzed the consequences of a postulated heat exchanger tube rupture and blowdown of CO<sub>2</sub> into the lead coolant. The analysis showed that the transient growth of the bubble/void would be retarded by the heavy lead density such that the void breaks up into smaller bubbles that rise benignly to the lead upper/free surface without being transported to the core.

Researchers on this project developed new core designs with improved burnup and power peaking. They also developed a concept to enhance core radial expansion feedback. They performed computational fluid dynamics analyses of multidimensional temperatures and velocities in the core to quantify the effects of coolant crossflow and intermixing as well as entrance effects in the large hydraulic diameter, open-lattice core. The team investigated alternative corrosion control/coolant chemistry approaches to protect steel structures from lead attack.

In addition, researchers analyzed the stability of lead natural circulation. They identified candidate austenitic stainless steel and inconel materials for use in S-CO<sub>2</sub> Brayton cycle components. They used engineering mechanics calculations to determine turbine blade stress limitations upon turbine design and incorporated the resulting stress models into the conceptual design code. Researchers on this project completed an assessment of experiment data needs for the coupled plant covering both the LFR and the S-CO<sub>2</sub> Brayton cycle. They initiated an investigation into the feasibility of coupling STAR-LM to an alternative advanced energy converter that utilizes two-phase liquid metal magnetohydrodynamic (MHD) power conversion. Analyses and results from the first year of the project will be documented in nine, full-length papers in international conference proceedings.

### Planned Activities

Researchers on this project will analyze operational transients and postulated accidents for the coupled STAR-LM-S-CO<sub>2</sub> Brayton cycle plant and develop an approach for cooling and transporting the spent cartridge core. If researchers find that two-phase liquid metal MHD power conversion is assessed to be practical, they will develop and assess a conceptual design for a coupled STAR-LM-MHD plant and MHD-related experiment data needs. Research-

ers will perform stability analyses for two-phase liquid metal flow and evaluate mechanical design issues.

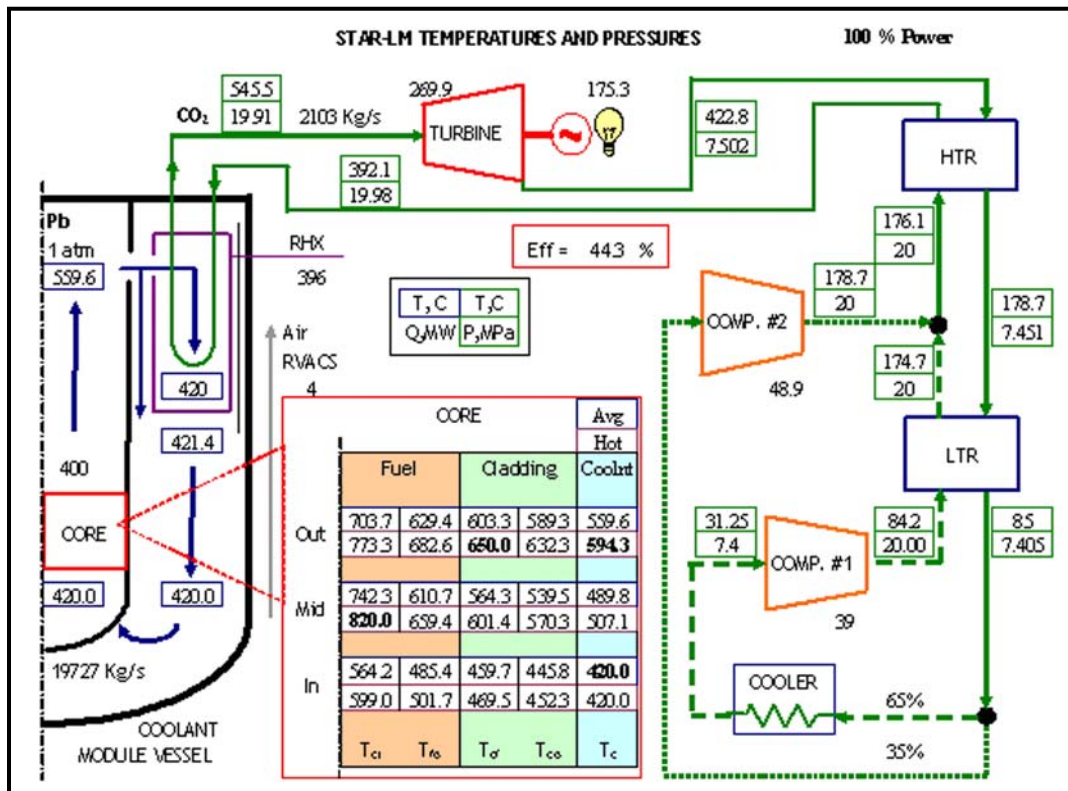


Figure 1. Nominal power operating conditions for STAR-LM coupled to supercritical CO<sub>2</sub> Brayton cycle.

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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Experimental Verification of Magnetic Insulation for Direct Energy Conversion Fission Reactors

PI: Donald King, Sandia National Laboratories

Project Number: 02-068

Collaborators: Texas A&M University, General Atomics

Project Start Date: September 2002

Project End Date: September 2005

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### Research Objectives

To operate successfully, a direct energy conversion (DEC) device must direct fission fragments and electrons to the appropriate device electrodes and withstand large internal voltage gradients created during the conversion process.

The objective of this project is to demonstrate that prototype, direct energy conversion devices can be designed and fabricated that can direct high energy, positively charged particles and electrons to different electrodes in the prototype and withstand voltage gradients of one-half to several million volts. When finished, the program will have fabricated and demonstrated the operation of two prototype direct energy conversion devices—the fission electric cell and the magnetic collimator. It will also have completed development of direct energy conversion theory development and established models and analytic tools.

In particular, this project will demonstrate that high-energy ions representing fission fragments and electrons can be reliably guided to the DEC collectors by the applied external magnetic field of the central solenoid. For the magnetic collimator, this project will demonstrate that electrons can be suppressed so that they do not reach the collector stages. It will also demonstrate that the scaled prototypes can withstand and be operated at high voltages required for high DEC efficiencies.

### Research Progress

Year 1 activities focused on preparing tests to demonstrate the successful operation of non-nuclear fission electric cell and magnetic collimator prototypes that will meet the objectives of the project. The test preparation activities included setting test goals, developing test data acquisition instrumentation, selecting the test facility, and designing the prototypes. Prototype design involved

selecting the source of high-energy ions and electrons, designing the physical layout of the emitter and collector structures for the fission electric cell and magnetic collimator, and modeling the electric and magnetic fields as well as the particle trajectories expected to occur in the prototypes.

Researchers on this project team selected the K500 Superconducting Cyclotron Facility at the Texas A&M University Cyclotron Institute as the site for studying the scaled prototype of fission fragment magnetic collimator reactor (FFMCR). The design characteristics of the full-scale FFMCR have been frozen and transformed to a scaled, non-fission, prototype system that is suitable for experimental studies. As a goal for the prototype experiments, the primary-stage voltage has been set at 1.5 MV. This primary-stage voltage is approximately 0.4 of that expected for the full-scale FFMCR. The reactor core as a source will be represented by ion beams scattered by a copper target. Electromagnetic components ( $\frac{1}{2}$  of the central solenoid system and collimator) will be represented by a single 7T superconducting solenoid.

In cooperation with the staff of the Texas A&M Cyclotron Institute, researchers on this team are currently developing a detailed experimental design. As part of this project, they plan to purchase a Ultra High Vacuum (UHV) target chamber with an extension that protrudes to the midpoint of the superconducting solenoid. A copper disk, located at the end of the extension, will provide a vacuum barrier between the UHV of the target chamber and the nominal vacuum of the beam line. An energetic helium ion beam, approximately 20 MeV/nucleon, will be transmitted through the copper disk and emerge with an average voltage/charge ratio of 1.5 MV/charge. The transmitted helium ion beam will be guided and collimated by the magnetic field of the superconducting solenoid to a collector plate. The collector plate will be charged to a voltage of 1.5 MV. Figure 1 illustrates this prototype.

The fission electric cell (FEC) will use two designs so researchers can study the electron beam control in high electric and magnetic fields. The first design will use a 150-KV power supply to generate electric fields up to 6 MV/cm between emitter and collector. The second design will use the energetic electron beam of the White Sands Missile Range LINAC to charge the FEC prototype up to 1 MV. The intense field created between emitter and collector will

generate electron emission. A 5 Tesla gyrotron solenoid magnet that surrounds the prototype will be used to prevent electron streaming from emitter to collector. Figure 2 illustrates the proposed prototype that uses a power supply.

### Planned Activities

Researchers will complete the fission electric cell and magnetic collimator designs by January 2004. A final design review will be held. The final designs will be used to fabricate the fission electric cell and magnetic collimator prototypes. Researchers will then test the prototypes to demonstrate their abilities to control high energy ions and electrons in high electric fields through the use of magnetic fields. They will complete the tests in Year 2. Based on test results, researchers on this project will redesign the prototypes to address any deficiencies encountered from the test results. They will perform a second test series to confirm the new designs. The design improvements and second test series will be completed at the end of Year 2 and during Year 3.

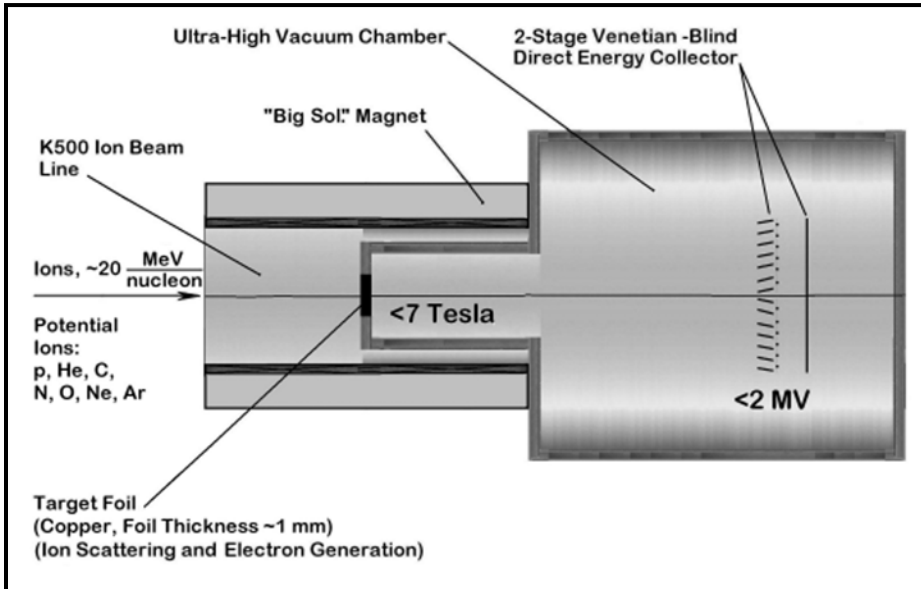


Figure 1. Scaled FFMC prototype.

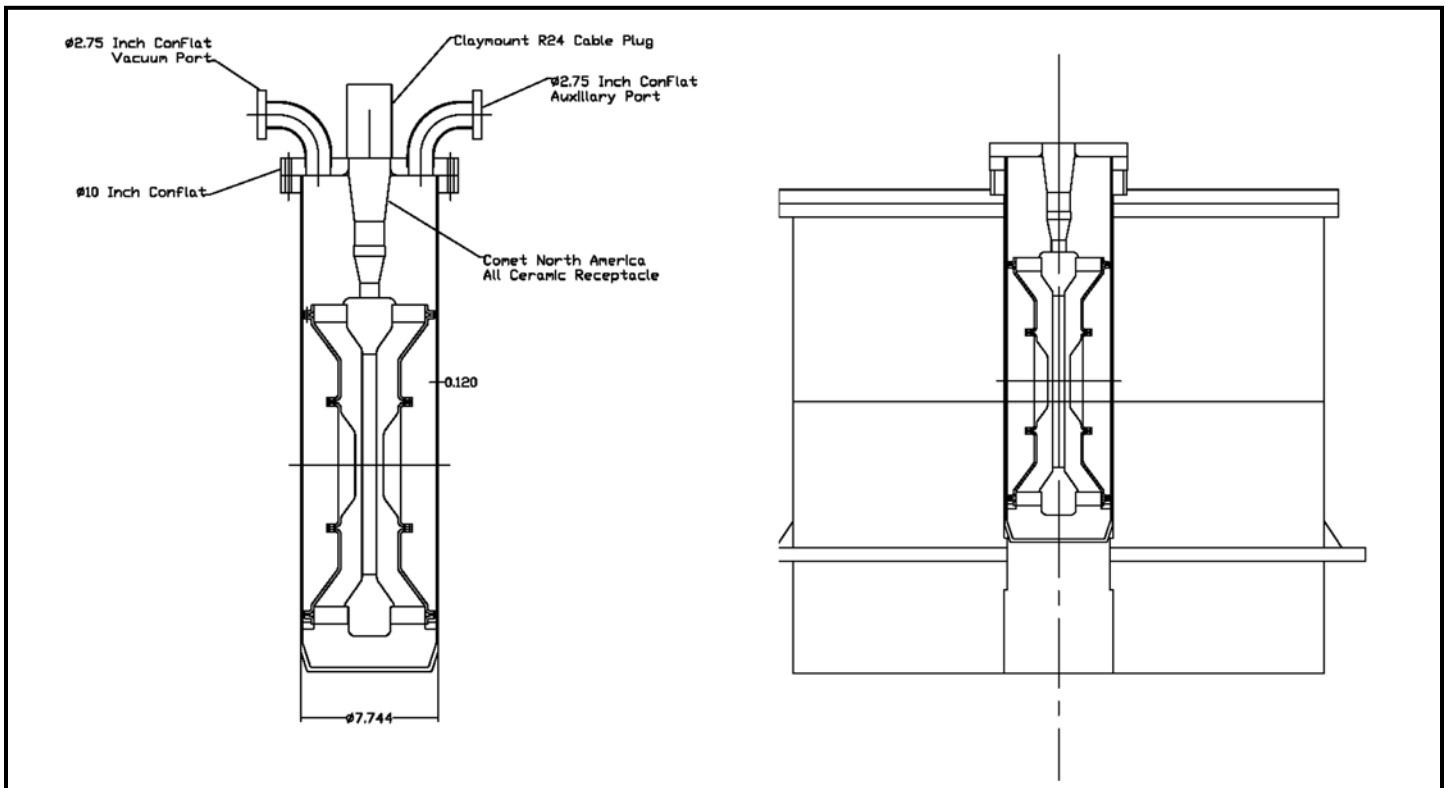


Figure 2. The prototype layout design for the voltage power supply driven diodes.

# NUCLEAR ENERGY RESEARCH INITIATIVE

## Innovative, Low-Cost Approaches to Automating QA/QC of Fuel Particle Production Using On-line Nondestructive Methods for Higher Reliability

PI: Ronald L. Hockey, Pacific Northwest National Laboratory

Project Number: 02-103

Collaborators: General Atomics, Iowa State University, and Oak Ridge National Laboratory

Project Start Date: September 2002

Project End Date: September 2005

### Research Objectives

Researchers are considering a fuel design for both near-term and Generation IV nuclear systems consisting of small spheres (about 1 millimeter in diameter) of uranium oxide which are uniformly coated to prevent release of fission products into the reactor. About 15 billion of these spheres would be used to fuel a single reactor. This project is exploring, adapting, developing, and demonstrating innovative nondestructive evaluation (NDE) methods to assure the quality of each of the fuel particles.

Replacing present quality assurance and quality control (QA/QC) methods, done manually and in many cases destructively, with nondestructive methods that are automated for higher speed will make fuel production and reactor operation more economical, considering the extremely large fuel particle throughput rates required. To achieve this objective, researchers must establish standard signatures for the most problematic types of defects as well as for acceptable particles using several nondestructive examination methods.

The technical scope of this project includes:

- Establishing a full-spectrum set of test standards representing "good" and characterized defective particles so that as a particle or group of particles pass a sensor, a multiple-attribute dependent signature will be measured and used for qualification or process control decisions.
- Evaluating, developing, and demonstrating NDE QC capability on unfueled and fueled-coated particles to reduce cost and improve reliability of manufacturing particle-based fuels.
- Developing and demonstrating a multiple-attribute "Quality Index."
- Specifying NDE design parameters using commercial equipment to build a large-scale fuel manufacturing inspection system.

### Research Progress

The project team has evaluated the specific requirements for on-process and in-line fuel particle fabrication QA/QC in terms of defect detection and process control at or near production throughput rates. The estimate for minimum particle fabrication throughput rates approaches 200 particles per second (pps), based on current Generation IV reactor designs, burn-up rates, and refueling requirements. TRISO (isotropic coatings of three materials) fuel particles have a fuel kernel in the center covered by three isotropic materials—a layer of silicon carbide sandwiched between pyrocarbon layers above a lower-density carbon buffer layer. Researchers rank-ordered the representative defect conditions, such as thin spots in the multi-layer coatings, cracks, and missing layers, according to their potential impact on fuel performance.

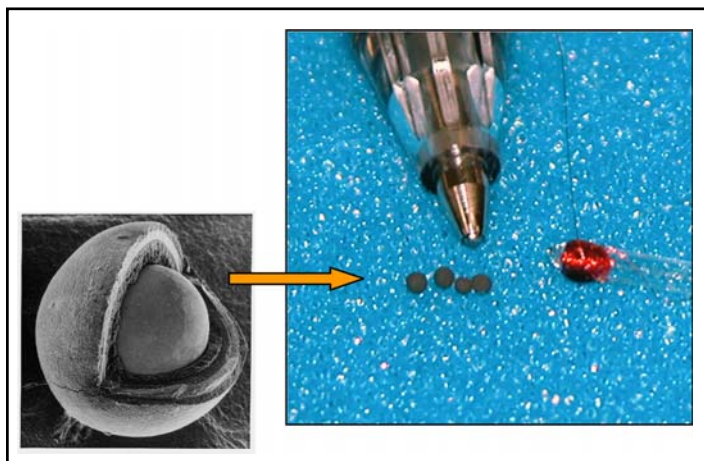


Figure 1. Surrogate TRISO fuel particles compared with a ballpoint pen and coil sensor.



Working from these requirements, the project team has evaluated in-line NDE methods that have the potential for detecting the various defects at a maximum inspection rate of about 200 pps. (This rate becomes smaller for multiple sensors working in parallel or for specific defects requiring inspection of only a fraction of the particles.) The in-line NDE methods evaluated include acoustic, electromagnetic, and optical, which are described below.

**Acoustic Method.** This method was evaluated for both in-line and on-process control. Work to date, using a model coater, is showing that acoustic/ultrasonic methods have the potential for monitoring the coating process to determine the particle fraction having a specified coating thickness. Higher frequency acoustic microscopy and resonant ultrasound techniques are showing promise for off line characterization of micro-structural material properties; but, without simplification, these methods require development beyond the scope of this project.

**Electromagnetic Method.** This method, commonly referred to as eddy current, is beginning to show promise for rapidly providing a signature of the combined coating properties in the TRISO particle. Researchers characterized several hundred TRISO particles known to have highly variable coating properties (layer thickness and particle shape) using radiography and Computed Tomography (CT) X-ray techniques. These same particles, placed in an induction coil, exhibit a strong correlation between their combined buffer and inner pyrocarbon (IPyC) layer thickness and sensor coil impedance, as shown Figure 2.

**Optical Method.** Researchers evaluated several existing high-speed optical characterization systems and found that each system was deficient in at least one important aspect of the surface characterization requirements. Therefore, an initial feasibility study is under way to determine if a digital, optical imaging technique can be developed to meet surface inspection requirements.

Evaluating the performance and development potential of each on-line or on-process measurement method requires characterized particles or standards. Researchers have developed digital radiography and CT X-ray techniques to successfully provide the geometric and the dimensional parameters to begin formulating a comprehensive library of defective and relatively good TRISO particle samples. The team refined particle-handling techniques to simultaneously scan 40 to 50 particles, allowing them to survey large particle batches for defects. Another important particle characterization development was improving data processing and dealing with the extremely large data set generated by high-resolution CT X-ray techniques.

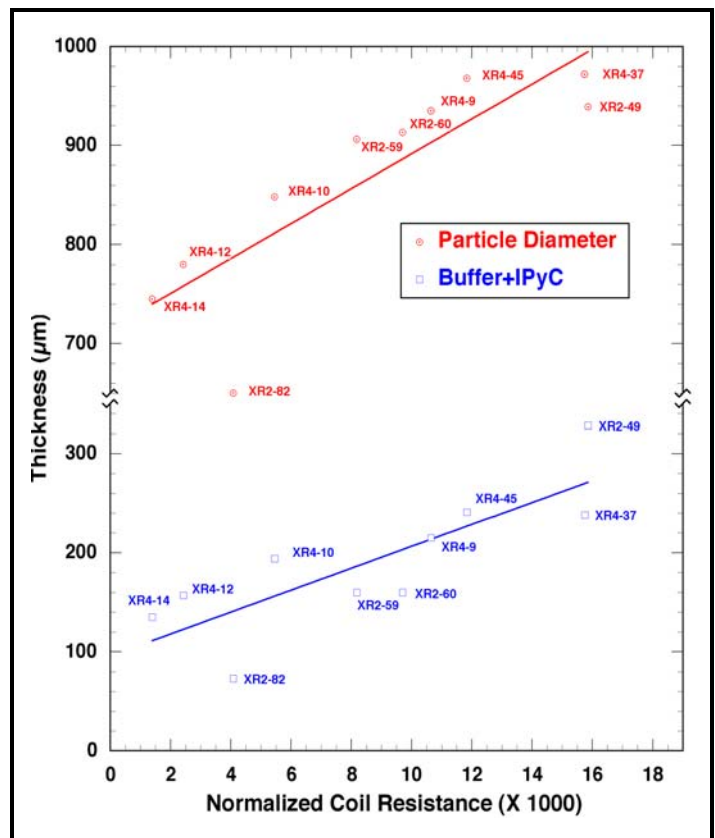


Figure 2. Thickness vs. Coil Resistance.

## Planned Activities

Remaining activities include:

- Populate a comprehensive library of particle defects and NDE methods signatures.
- Identify the best NDE method for a particular defect type and process control.
- Demonstrate maximum throughput speed for each NDE inspection method.
- Assess NDE method differences between surrogate and fueled TRISO particles.
- Show on-process NDE method process control capability.
- Implement a measurement quality index.
- Specify design parameters for the developed NDE inspection system.

The project will continue to accumulate and survey fully and partially coated surrogate fuel particles using the most promising NDE methods and will obtain a comprehensive library of defect conditions known to affect fuel performance. Researchers on the team plan to create defective particles by deliberately varying the coating processes that normally produce flawless particles. Researchers will use the resulting library of defective particles and the resulting

NDE signature from each defect type (such as thin or missing layers, atypical coating density, or crystalline anisotropy) to evaluate the NDE methods in the remaining portions of this project.

The NDE methods showing the greatest sensitivity to each defect class will be further refined for in-line, on-process, or off-line inspection at key stages in the fuel fabrication process. The evaluation of each NDE method

will encompass both motionless and maximum throughput particle speeds. Researchers are developing the NDE methods using surrogate particles. The effects that the fueled particles may have on these results will be accounted for in later activities to reduce costs and accelerate progress. Once implemented, a quality index currently under development will relate the NDE measurement data to acceptable process control parameters.





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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Model-Based Transient Control and Component Degradation Monitoring in Generation IV Nuclear Power Plants

PI: James Paul Holloway, University of Michigan

Project Number: 02-113

Collaborators: Westinghouse Electric Company  
LLC, Sandia National Laboratories

Project Start Date: September 2002

Project End Date: September 2005

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### Research Objectives

The overall objective of this research project is to develop and demonstrate advanced algorithms for the safe and efficient control of operational transients in nuclear power plants and for the continuous on-line monitoring of the system's status to warn of system degradations and incipient failures. These algorithms combine sensor measurements with physical models of key plant systems in order to predict and control the state of the plant. Additionally, because identifying the system's state is an important requirement for both of these activities, researchers on this project will seek an optimized approach for acquiring sensor data. This data can be used to extract information about the plant's state. Researchers will demonstrate these new, integrated, monitoring approaches within the context of advanced and Generation IV nuclear power plant designs.

This innovative project promises to provide an integrated approach to plant control and degradation monitoring. Many of the same signals and plant models that are used to define optimal control strategies will be used to simultaneously diagnose degradation of the controlled components. The methods for fusing sensor data with physical models of plant systems will be generally applicable to advanced nuclear power systems, but are being demonstrated for a next generation reactor concept of significant maturity, the International Reactor Innovative and Secure (IRIS).

The proposed research is developing two new capabilities for the nuclear engineering community:

- A method to develop robust, nonlinear control algorithms that combine plant sensor measurements with a predictive physical model of key plant systems to provide optimal, closed-loop performance of complex nonlinear systems.

- A method for monitoring plant system degradation based on comparing plant sensor readings with a physical model of key plant systems and exploiting component transition probabilities to provide probability distributions for degraded states.

The methods for fusing sensor data with physical models of plant systems will allow nuclear plant engineers to design optimal maintenance and control strategies into the new generation of nuclear plants. They will also provide nuclear plant operators with tools to operate their plant safely and efficiently within the complex energy market of the 21<sup>st</sup> century.

### Research Progress

During the first year, researchers on this project have identified key requirements for IRIS control systems. Simultaneously, they have identified and explored an approach to nonlinear, model-based predictive control that they will apply to IRIS during Year 2 of this project. Westinghouse is developing classical, proportional, control schemes, similar to controls used in existing plants, which will be compared with nonlinear, model-based, predicted control. For nonlinear, model-based control, researchers will focus on the IRIS pressure and level control, and the power, rod, feedwater flow, and steam pressure control systems.

The nonlinear, model-based, predictive, control method is based on first using a plant measurement to provide a model of the plant's state. This model can then predict plant trajectory as a function of specified (open loop) control actions. Researchers formulate a cost function to predict the cost of deviations of the plant from the desired state, and the cost of control. This cost function is a function of the anticipated control actions, and is minimized

over all feasible open-loop control actions. The initial part, and only the initial part, of the resulting optimal, open-loop control is applied to the real plant, which is then measured again and the process repeated. The closed-loop control for the plant is provided by extracting information from a sequence of optimal, open-loop controls. Researchers have successfully applied this method to abstract, nonlinear dynamic systems with chaotic dynamics, as well as nuclear reactor control. Figure 1 shows an example of this scheme, which is applied to the rapid startup of a reactor. The controller determines the velocity of the control elements, which is nonlinearly related to the inserted reactivity; the nonlinear system is well controlled without any linearization of the model.

A key element of this model-based, predictive control is the system model. The team has been developing a detailed model of the IRIS thermal-hydraulics. They will use this model to refine traditional proportional-integral-derivative (PID)-based control schemes and to help validate models to be used in the nonlinear predictive control of the same IRIS systems.

Researchers have also formulated a basic strategy for model-based, component degradation monitoring that uses all available plant state and component reliability data. The key elements of this method are determining the conditional probability of system state given a set of plant measurements, and solving a Chapman-Kolmogorov equation for the joint probability density of plant state and component state. Determining this latter probability density requires solving an integro-partial differential equation on a high-dimensional phase space. This is computationally challenging. A version of this equation for linear plant dynamics is currently solved by a Monte Carlo method. Although this process is very time consuming, it can provide excellent information on system faults.

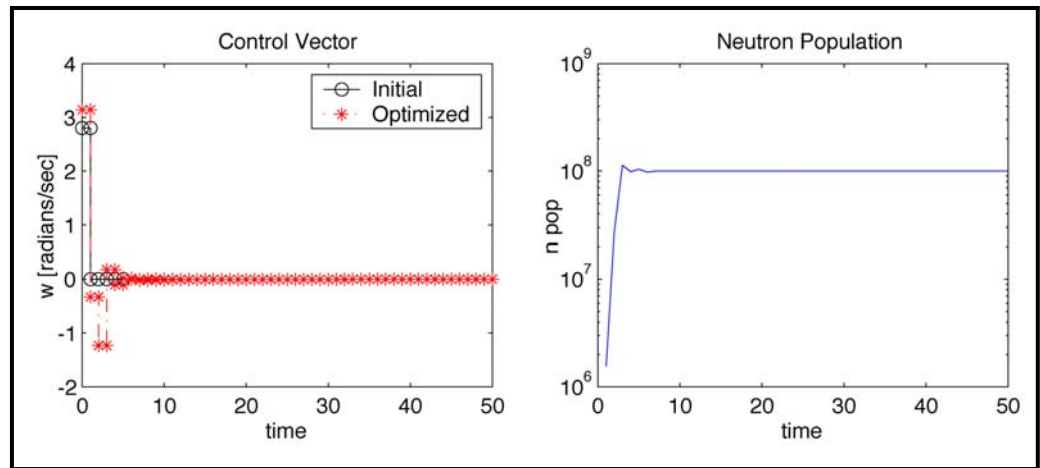


Figure 1. The velocity of control elements and the desired rapid increase in neutron population as a function of time in a reactor managed by a model-based predictive controller. The control eventually converges to zero because, as the steady state is reached, only very slow control element motions are needed.

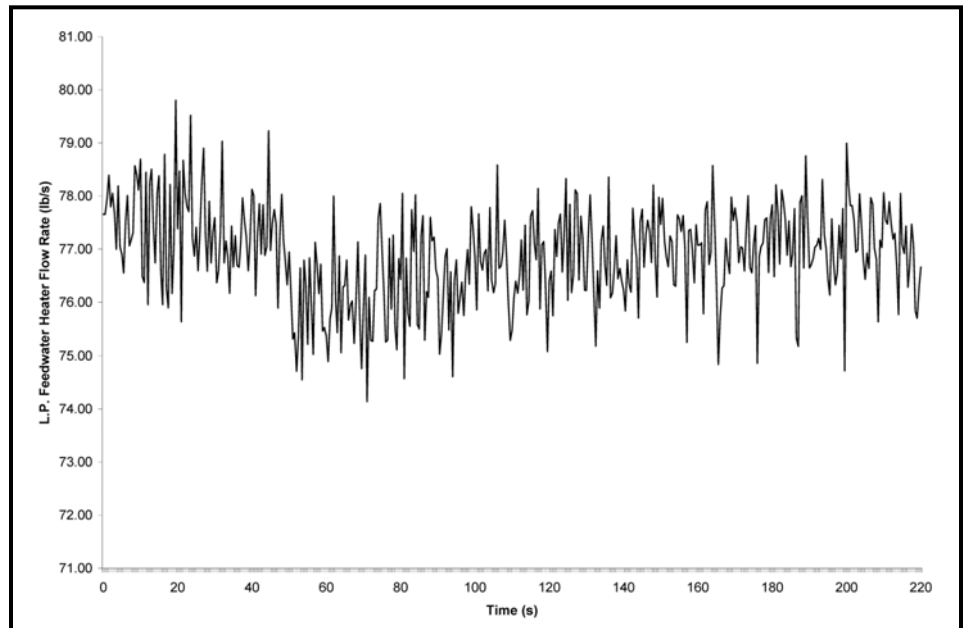


Figure 2. Feedwater heater flow rate through a degraded system, with the fault introduced at 50 seconds. The fault affects other process variables in even more subtle ways, so determining the nature of the fault from this subtle signature is difficult, but can be accomplished with the stochastic degradation monitor, which is under development.

Figure 2 shows a process variable (i.e., feedwater heater flow rate) in a nuclear plant model in which faults occur in two systems. It is difficult to notice the fault, starting at 50 seconds, in the noisy signal, let alone diagnose the cause. However, the stochastic degradation monitor correctly identifies the two independent faults that occurred, and provides probabilities for each possible set of component states that can explain the measured data.

The team has begun to identify models that they will study as the basis for degradation monitoring of the IRIS steam generators. They expect to use both degradations in heat and mass flow characteristics and changes in flow-induced acoustical signatures as the measurements that can drive the degradation monitor.

## Planned Activities

The IRIS pressurizer will be one of the first IRIS systems to which the team will apply a nonlinear, model-based, predictive control. The system is not tightly coupled to the rest of the plant, so it can be most easily studied in isolation. Westinghouse has developed a proportional control scheme from which the team can compare. The other major focus of control efforts will be a nonlinear, model-based, predictive controller for IRIS steam generator control. The once-through steam generators offer significant challenges to control, particularly at low power. Westinghouse is currently defining a traditional approach to control these systems. Researchers on this project will compare Westinghouse's traditional approach with model-based, predictive control. The nonlinear, model-based, predictive control algorithm requires solution of an optimi-

zation problem whose dimension is proportional to the number of control variables and the horizon used for control (effectively the time scale of the system). Researchers must study how this problem can be efficiently solved.

Solving the Chapman-Kolmogorov equation is central to the component degradation monitor, because it provides the probability density that brings information component reliability together with plant measurement. However, solving this equation presents significant computational challenges because of the dimensionality of the phase space. In order to solve this, researchers must further study the Monte Carlo approach. The team will investigate the thermal-hydraulic and fluid-induced vibration behavior of the helical-coil tube bundle in the IRIS steam generators as potential degradation monitors.



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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Centralized Hydrogen Production from Nuclear Power: Infrastructure Analysis and Test-Case Design Study

PI: William A. Summers, Westinghouse  
Savannah River Company

Project Number: 02-160

Collaborators: General Atomics; University of  
South Carolina; Entergy Nuclear, Inc.

Project Start Date: September 2002

Project End Date: September 2005

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### Research Objectives

Hydrogen production from nuclear power can provide a significant new source of energy for both the transportation and industrial sectors. Generation IV (Gen IV), high-temperature, nuclear reactors can be combined with thermochemical hydrogen production processes to dissociate water into hydrogen and oxygen through a series of thermally driven chemical reactions. Nuclear fuel and water are the only consumables, and the process generates no air pollutants or greenhouse gases. Hydrogen produced in this manner could provide a new source of fuel for hydrogen fuel cell vehicles, thus fulfilling the goals of the President's *FreedomCAR* Initiative, which seeks to develop a transportation system independent of petroleum.

The objectives of this project are to identify, characterize, and evaluate the critical technical and economic issues associated with nuclear hydrogen production, including the integration of the plant into an overall hydrogen infrastructure. This work complements other design studies related to nuclear hydrogen production by expanding their analyses to include factors beyond the production plant, including consideration of on-site hydrogen storage and handling, hydrogen transmission and distribution, integration with end-user processes, and overall energy system economics.

In phase A of this project, researchers will conduct a generalized study of nuclear hydrogen production systems. This work will be followed by Phase B: a test-case, pre-conceptual, design study for a site-specific nuclear hydrogen production plant based on a Gen IV reactor design and a thermochemical process connected to a regional hydrogen end-user.

### Research Progress

The first year of the project was devoted to work on Phase A, Plant and Infrastructure Analysis. The purposes of this task were to 1) identify and analyze the major requirements for nuclear hydrogen production, and 2) to define the physical characteristics and major considerations for the nuclear reactor, the thermochemical hydrogen production process, and the related hydrogen infrastructure. The nuclear reactor is based on the modular helium reactor (MHR) under development by General Atomics (GA). It is a passively safe, modular-sized, helium-cooled, graphite moderated gas reactor. The MHR operates at a thermal power level of 600 MW(t) with a core outlet helium temperature in the range 850-1,000°C. The possibility of a core meltdown is precluded through the use of refractory, coated-particle fuel, the use of nuclear-grade graphite fuel elements with high heat capacity and thermal conductivity, and operation at a relatively low power density with an annular-core arrangement. Heat is delivered to the thermochemical hydrogen production process through the use of a secondary helium cooling loop, which is heated to 925-975°C in an intermediate heat exchanger.

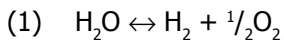
GA performed a study to investigate MHR core design options that would allow an increase in the average coolant outlet temperature from 850°C to 1,000°C, while maintaining fuel temperatures at acceptable levels. In general, researchers can determine the feasibility of operating at higher coolant outlet temperatures by performing detailed core physics and thermal hydraulic calculations, followed by detailed calculations of fuel performance and fission-product release. The scoping parametric studies performed should be viewed as the first step in the design process—the results should be used primarily to define which design options merit further consideration and more detailed analysis. The results of this preliminary analysis are encouraging. They indicate that it may be possible to

operate the MHR with a coolant outlet temperature as high as 1,000°C without making any substantive changes in the fuel or reactor vessel materials or design.

The baseline hydrogen production process used in the analysis was the sulfur-iodine thermochemical cycle. This process consists of a series of three chemical reactions that utilize high-level heat from the reactor to thermally dissociate water into hydrogen and oxygen. Heat and water are the only process inputs, and all the remaining chemical reactants are recycled. Researchers used the results of a recently completed NERI project<sup>1</sup> as a basis for designing the plant. They also used the results to evaluate the effect of process parameters on the overall infrastructure parameters of centralized hydrogen production from nuclear power.

The primary reactions in the sulfur-iodine cycle are:

- (2)  $H_2SO_4 \leftrightarrow SO_2 + H_2O + \frac{1}{2}O_2$  (850°C)
- (3)  $I_2 + SO_2 + 2H_2O \leftrightarrow 2HI + H_2SO_4$  (120°C)
- (4)  $2HI \leftrightarrow I_2 + H_2$  (300°C)



Researchers used process modeling based on the AspenPlus™ code to calculate the overall thermal efficiency for the nuclear hydrogen plant. They defined efficiency as the higher heating value (HHV) of hydrogen product divided by the thermal energy input from the nuclear heat source. The results indicated an efficiency range of 40-52 percent depending on the reactor's helium outlet temperature and the degree of optimization in the process design. Researchers continue to refine the process design and the efficiency estimates.

Researchers on this project also studied the hydrogen infrastructure requirements for integrating a nuclear hydrogen plant with hydrogen end-users. They analyzed various options for storing the hydrogen, including compressed hydrogen storage, liquid hydrogen storage, inclusion of a hydrogen liquefier at the nuclear hydrogen plant, and the use of pipelines for hydrogen storage. They compared various hydrogen transport options, including tube trailers, liquid hydrogen trucks, and pipelines (a more detailed pipeline analysis is in progress). They studied two main types of end-users: industrial users and hydrogen energy consumers (e.g., hydrogen vehicles, distributed

power, etc.). The industrial users are a current market, whereas the hydrogen energy users' market will evolve with the hydrogen economy. The large industrial users include oil refineries, ammonia plants, methanol plants, and other large-scale hydrogen users. These plants primarily produce and use their own hydrogen on-site, although the use of purchased merchant hydrogen is becoming an increasing option. Nuclear hydrogen plants could potentially replace the on-site hydrogen production at these plants, which in most cases means displacing the use of natural gas for steam reforming.

Researchers performed detailed energy and economic analyses for conventional hydrogen plants to determine the merits of this option. For example, they performed an economic analysis to compare the cost of nuclear hydrogen to the cost of using on-site natural gas steam reforming. The estimated cost of the nuclear hydrogen at the plant gate was \$1.42 per kilogram, as shown in Table 1.

Economic Parameters	Production Costs, \$/MW-hr <sub>H2</sub>
• 4x600 MW(th) H <sub>2</sub> -MHR	Fixed Charges = \$20.2
• S-I Process @ 52% efficiency	Fuel Cycle = \$ 6.8
• H <sub>2</sub> = 4x190 tonnes per day	Nuclear O&M = \$ 2.7
• Reg. Utility Financing	H <sub>2</sub> O&M = \$6.3
• Fixed Charge Rate = 10.5%	TOTAL = \$36.0
• Capacity Factor = 90%	
• MHR Capital Cost = \$880/kW <sub>H2</sub>	1 tonne H <sub>2</sub> = 39.4 MW-hr <sub>H2</sub> (HHV basis)
• S-I Plant Capital = \$638/kW <sub>H2</sub>	
• 3-year construction	<b>H<sub>2</sub> Cost at plant gate = \$1.42 per kg</b>

Table 1. Nuclear hydrogen production costs.

Then, they determined the infrastructure costs for delivering this hydrogen to a regional industrial hydrogen user:

Production Cost =	\$1.42/kg	MHR-SI plant
Onsite Storage =	\$0.16	24-hr LH <sub>2</sub> Backup
Transportation =	\$0.10	50-mile pipeline
Oxygen Credit =	(\$0.29)	\$36 per ton less delivery costs
H <sub>2</sub> Cost =	\$1.39/kg	Delivered to User's plant gate

Researchers calculated the projected cost of conventional hydrogen production using steam reforming of natural gas for several large industrial end-user applications, including: 1) an existing large ammonia plant with 400 tonnes per day (TPD) H<sub>2</sub> production, 2) a new ammonia plant with 200 TPD H<sub>2</sub> import, 3) a new large hydrogen plant with 200 TPD, 4) a new package hydrogen plant with 20 TPD, and 5) a new liquid hydrogen plant with 20 TPD. The results were compared with the cost of importing nuclear hydrogen, as shown in Figure 1.

The delivered hydrogen cost from the nuclear plant is competitive with hydrogen from reformed natural gas in the case of an average natural gas price of \$5 per million BTU

<sup>1</sup> L.C. Brown, et al., "High Efficiency Generation of Hydrogen Fuels Using Nuclear Power," Final Technical Report for the period August 1, 1999, through September 30, 2002. Prepared under Nuclear Energy Research Initiative (NERI) Program Grant No. DE-FG03-99SF21888 for the U.S. Department of Energy, June 2003.

and assuming a \$40 per ton CO<sub>2</sub> carbon credit. This carbon credit represents a mid-range cost estimate for CO<sub>2</sub> capture and sequestration based on the review of existing studies. Researchers will perform sensitivity analyses for various natural gas prices, carbon credits, and other financial variables. They also initiated an economic analysis comparing centralized nuclear hydrogen production with distributed electrolysis. Initial results indicate that both approaches to nuclear hydrogen may be viable, depending on the price of the electrolyzers and the cost of off-peak electric power. Further analysis will be performed next year.

## Planned Activities

During the next fiscal year, the team will complete Phase A and initiate Phase B of this project. Work remaining on Phase A includes finalizing the definition of the nuclear hydrogen plant and continued work on infrastructure analysis and economics. Researchers will conduct a detailed analysis of hydrogen transport using pipelines, and they will assess the impact of hydrogen refueling stations on the end users. Researchers will refine the economics by performing sensitivity analyses and further comparing distributed electrolysis. They will continue process modeling to determine overall plant efficiency. During

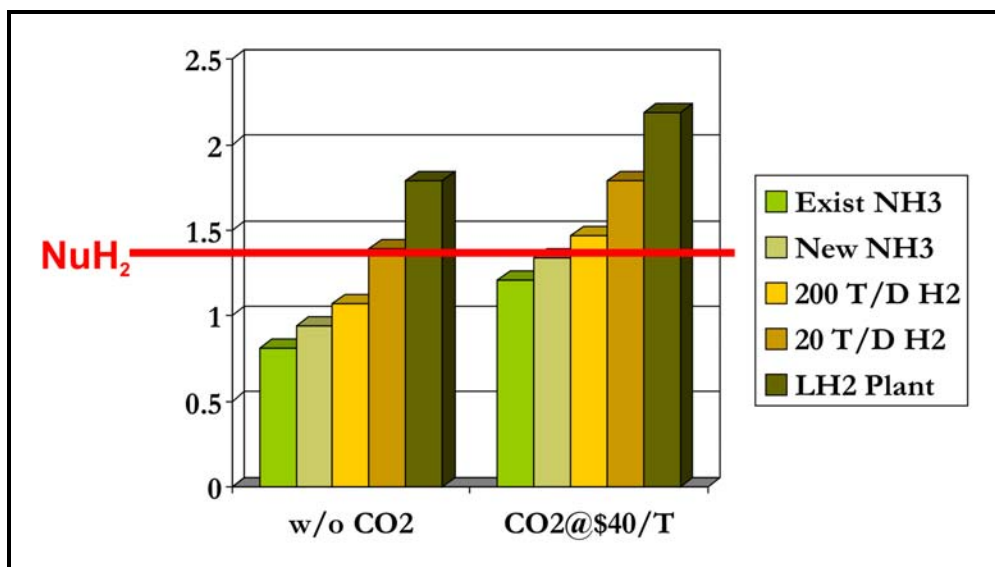


Figure 1. Hydrogen production costs w/ \$5 per MMBtu natural gas.

Phase B, researchers will initiate work on the pre-conceptual design of a nuclear hydrogen plant and its associated infrastructure, which will be designed to supply hydrogen to a large industrial hydrogen user. Goals at the end of the project include:

- Defining the physical characteristics, infrastructure requirements, and economics for a centralized, thermochemical, hydrogen production plant driven by a helium-cooled modular nuclear reactor.
- Preparing a pre-conceptual design for a test-case plant that exports hydrogen to a local chemical plant hydrogen user.
- Identifying needs and a path forward for commercializing the nuclear hydrogen option.





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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Near-Core and In-Core Neutron Radiation Monitors for Real-Time Neutron Flux Monitoring and Reactor Power Level Measurements

PI: Douglas McGregor, Kansas State University

Project Number: 02-174

Collaborators: None

Project Start Date: September 2002

Project End Date: September 2005

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### Research Objectives

There is a need for neutron radiation detectors capable of withstanding intense radiation fields, capable of performing "near-core" reactor measurements, capable of pulse-mode and current-mode operation, capable of discriminating neutron signals from background gamma ray signals, and tiny enough to be inserted directly into a nuclear reactor without significantly perturbing the neutron flux. A device that can address the above list is the subject of the present NERI research project, in which miniaturized fission chambers are being developed and deployed in a TRIGA (Training, Research, Isotopes, General Atomics) research reactor. The unique miniaturized neutron detectors are to be used for three specific purposes: 1) as reactor power level monitors, 2) as power transient monitors, and 3) for real-time monitoring of the thermal neutron flux profile in a core. The third application has the unique benefit of providing information that, with mathematical inversion techniques, can be used to infer the three-dimensional distribution of fission neutron production in the core. The project has two specific tasks: 1) detector development, characterization, and deployment, and 2) data reduction and computer code development for determining real-time reactor core power levels.

Detector development involves the design, construction, and deployment of the radiation hard, thermally resistant, inexpensive gas-filled fission chambers. Electronics attached to the devices will allow for both pulse-mode and current-mode read-out. Further, each detector pack consists of a triad of devices: a  $^{233}\text{Th}$ -based fast neutron detector, a  $^{235}\text{U}$ -based thermal neutron detector, and an uncoated device for gamma ray background. Seventy-five (75) triads, amounting to a total of 225 detectors, will be distributed through a plane in the Kansas State University's (KSU's) TRIGA reactor core. Researchers are developing a

back-projection algorithm that uses detection information extracted from the detector triad arrays to determine the power density within the fuel elements of the nuclear core.

### Research Progress

The design of a micro-pocket fission detector (MPFD) is shown in Figures 1 and 2. The device consists of a point anode and a cathode conductive plate separated by a gas volume that is lined by a neutron reactive material such as  $^{235}\text{U}$  or  $^{232}\text{Th}$ . The micro-pocket is made out of an insulating ceramic that can withstand the high-radiation and high-temperature environments in a nuclear reactor core. Figure 2 shows how three simple pieces of temperature- and radiation-resistant ceramic are formed together to make the MPFD. A conductive metal is used to form the cathode plate and anode point with connections from the chamber through micro-drilled holes. A sealant is used to hold the ceramics together and trap a fill gas in the cavity. Either argon or P-10 (10 percent methane/90 percent argon) is used as the charge-detecting medium. The cavity width ranges from 500 microns to 3 mm, depending on the design. Such small devices can be treated as point detectors, thereby greatly simplifying the back-projection calculations.

Argon-filled chambers have an inherently low probability of gamma ray interactions, allowing for natural discrimination of gamma-ray background noise. In addition, being gas-filled, there is no detecting medium that radiation can actually destroy, a clear advantage over liquid or solid detectors. Being a small chamber, less voltage is needed to sweep the electrons and ions across the chamber, thus lowering the power requirement. This will also limit the potential of detecting non-neutron-induced events and will prolong the life of the gas. The neutron reactive coating can also be tailored for detection of specific neutron

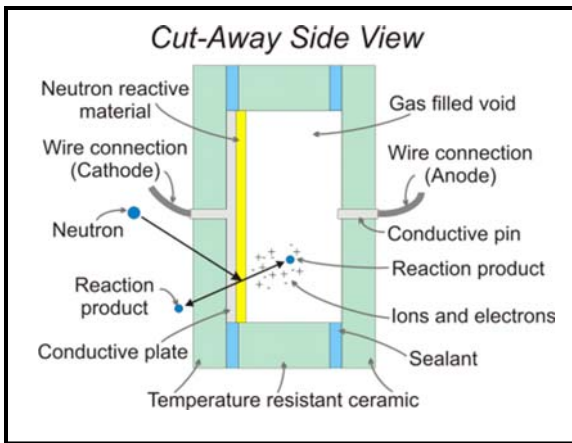


Figure 1. Cut-away side view of an MPFD chamber.

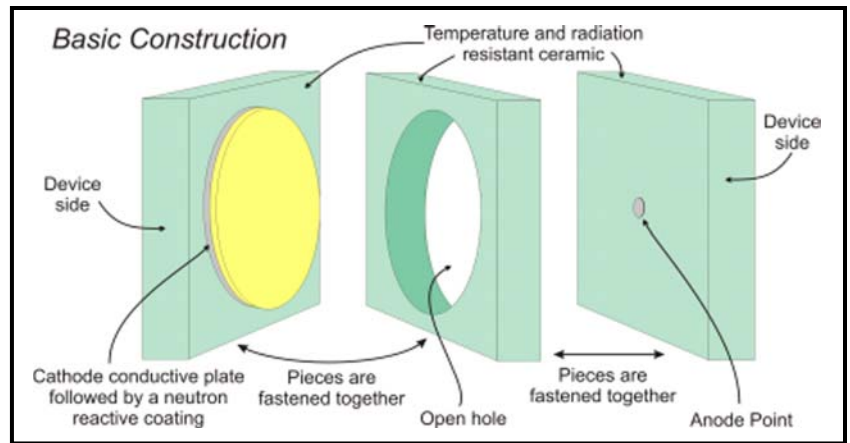


Figure 2. Basic construction of an MPFD chamber.

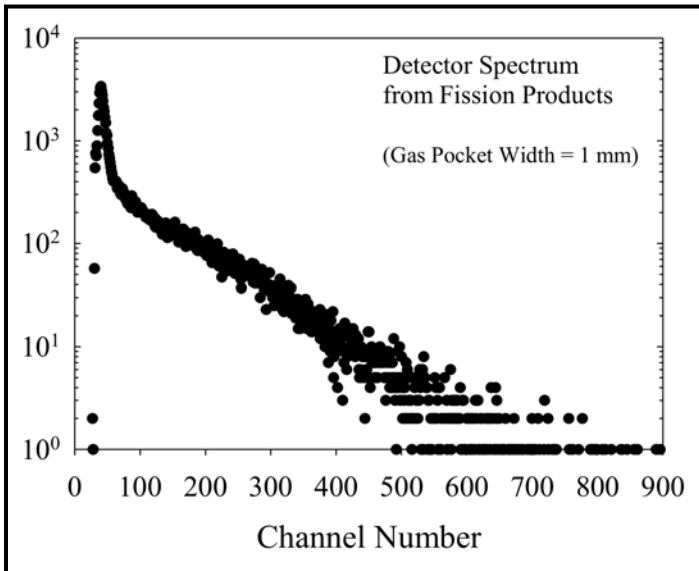


Figure 3. Spectrum from natural uranium-coated fission detector placed in a neutron beam with a large gamma background.

energies and for specific efficiencies.

Prototype MPFDs that were uranium coated and manufactured with aluminum oxide substrates yielded spectacular results. Figure 3 shows a fission product spectrum that was collected by an MPFD chamber in a neutron beam of approximately  $10^6 \text{ cm}^{-2} \text{ s}^{-1}$  neutrons and  $10^2 \text{ R/h}$  gamma rays. This spectrum correlated well with modeled results. Researchers measured the gamma ray background with the neutron beam blocked by a 2-mm-thick sheet of cadmium. Absolutely no radiation counts were registered from the gamma rays, thereby proving that the devices are truly insensitive to gamma ray background.

Researchers on this project have constructed a device for testing detectors and their electronics in the central thimble of KSU's TRIGA Mk-II Nuclear Reactor. The central thimble is the highest neutron and gamma ray flux region of the reactor. The device has a 1-inch diameter dry

chamber that extends vertically through the reactor volume. A box is located three feet above the core for housing preamp electronics. Detector wiring is drawn through a bent dry tube extending from the box up to the pool surface. The bend in the tube eliminates beam-port effects and minimizes personnel radiation exposure on the observation deck. The entire device is made of aluminum; therefore, any activation will decay within hours of high-power operations. Researchers are presently inserting MPFDs into KSU's TRIGA reactor for radiation damage tests and sensitivity tests.

Researchers can connect the data from the MPFD array into a power density map of the reactor core. They are currently working on producing the mathematical models that can relate the power density profiles in a reactor's fuel rods to the flux densities at the detector locations. Key to this formulation is constructing an appropriate response function that gives the flux at any position in the core to the fast neutrons born at an arbitrary axial depth in any of the core fuel rods. Researchers have response functions that are used to illustrate these analysis methods.

Using the measured fluxes at various locations through the core, the general model for the unknown power density profiles in the fuel rods solution requires that an ill-posed Fredholm integral equation be inverted. Using numerical quadrature, this integral equation can be converted into an under-determined set of algebraic equations for the power densities at various axial positions in the fuel rods. To solve this set of under-determined equations, researchers have employed the linear regularization method.

Some results using several MPFD fast fission (thorium) detectors intermixed with fuel rods are shown in Figure 4. The solid lines in the figure represent the actual fuel rod power densities; the points represent the back projected

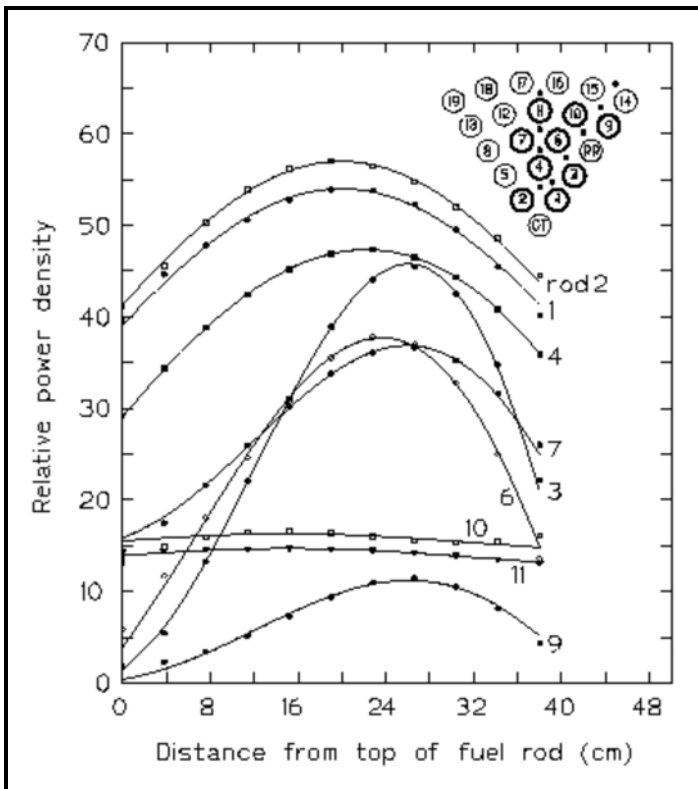


Figure 4. Power density profiles (lines) and unfolded results (solid circles) for nine fuel rods and nine fast-flux strings with 5 detectors each.

power density as determined from detector data sets. The close match is unmistakable. Geometry of the MPFD placement is proving critical in evaluating simulated flux profiles. As the source of fast neutrons (fuel) is located further from the detectors, the back calculation breaks down. This happens because the neutrons have little chance of reaching the detectors; thus, there is little data to formulate a proper reconstruction of their power profile. The results indicate that the detector array strings must be placed near the fuel rod or bundle that is to be monitored. Researchers are now using MCNP models of the full core and detectors in order to gain a better understanding of developed theoretical models.

## Planned Activities

During the second research year, researchers on this project will deploy arrays of MPFDs (which have  $^{232}\text{Th}$  and  $^{235}\text{U}$  inside) into the flux probe holes of the KSU TRIGA Mark II nuclear reactor to observe real-time neutron flux measurements. These array assemblies will form a "sheet" of detectors across the core. Researchers will extract the signals in both pulse and current modes and they will use the information to calculate the power density in the fuel. Real-time core mapping will be performed. Data acquired from the MPFDs will be used for inverse power density distribution calculations.

Researchers will also explore silicon dioxide ( $\text{SiO}_2$ )-based MPFDs.  $\text{SiO}_2$  can withstand high temperatures and has a low total neutron interaction cross-section. An inductively coupled plasma etcher, recently acquired by KSU, can be used to etch holes through thin silicon wafers. A small stack of these wafers can be placed together to form an MPFD array. Oxidation will produce a thin silicon dioxide layer that is non-conductive and can be used to further fuse the stack of wafers together. While these detectors have yet to be manufactured and tested,  $\text{SiO}_2$  can withstand temperatures exceeding  $1,100^\circ\text{C}$ ; hence, it is attractive as a detector material.

The completion of the second year goals will demonstrate that miniaturized gas pocket detectors can be used to simultaneously give information on the nuclear reactor power levels at various locations inside the reactor core.



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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Development of a Supercritical Carbon Dioxide Brayton Cycle: Improving Pebble Bed Reactors (PBR) Efficiency and Testing Material Compatibility

PI: Chang Oh, Idaho National Engineering and Environmental Laboratory

Project Number: 02-190

Collaborators: None

Project Start Date: September 2002

Project End Date: September 2003

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### Research Objectives

Generation IV reactors will need to be intrinsically safe, have a proliferation-resistant fuel cycle, and other advantages relative to existing light water reactors (LWR). Generation IV reactors must overcome certain technical issues and the cost barrier before they can be built in the U.S. Nuclear power would need to cost 3.3 cents/kWh in order to compete with fossil combined-cycle, gas turbine power generation. This goal requires a 30-percent reduction in power cost for state-of-the-art nuclear plants. It has been demonstrated that this large cost differential can be overcome only by technology improvements that lead to a combination of better efficiency and more compatible reactor materials.

The objectives of this research are 1) to develop a supercritical carbon dioxide Brayton cycle in the secondary power conversion side that can be applied to high-temperature gas-cooled reactors (HTGR) such as the fast gas-cooled reactor (FGR) and the very-high-temperature gas-cooled reactor (VHTR), 2) to improve the plant net efficiency by using the carbon dioxide Brayton cycle, and 3) to test material compatibility at high temperatures and pressures. The reduced volumetric flow rate of carbon dioxide due to higher density compared to helium will reduce compression work, which eventually will increase turbine work and enhance the plant's net efficiency.

### Research Progress

This project consists of three major tasks with a number of subtasks under the major ones. The primary activities and key accomplishments for each task are summarized below.

**Task 1. Development of CO<sub>2</sub> Brayton Cycle.** This task consists of five subtasks. The proposed supercritical Brayton cycle deals with high pressure and temperatures.

At these conditions, an ideal gas law, isentropic compression and isentropic expansion, cannot be applied because of real gas effects in carbon dioxide associated with compressibility. As part of this task, researchers developed analytical equations for polytropic expansion through a turbine and polytropic compression through a sequence of compressors. They are using these equations for a parametric study aimed at investigating the effect of the overall plant efficiency. For the detailed computation of the balance-of-plant (BOP) efficiency calculations, a CO<sub>2</sub> database is required to make accurate calculations. Researchers checked various equations of state with several CO<sub>2</sub> databases. They found that the National Institute of Science Technology (NIST) CO<sub>2</sub> database is the most accurate and the properties are consistent with those referenced in *Perry's Handbook*.

In order to compare the plant efficiency depending on turbine shaft configurations, researchers used a pebble bed reference design, which was developed by Massachusetts Institute of Technology (MIT) as shown in Figure 1. Then, researchers used two process optimization codes, ASPEN PLUS and HYSYS, which are widely used in the chemical and refinery industry for the optimization of their process balance of plant. The objective was to determine if the results calculated using these codes would match the design parameters that were established in the reference design shown above. Both codes agree very well with those defined in the reference design, with a less than 0.5 percent deviation. Researchers selected HYSYS code for this project because HYSYS has more capabilities than those of ASPEN PLUS. The capability of polytropic expansion and compression would give them more accurate results when there is a need to increase the system pressure up to 20 MPa range. Researchers also used a Visual-Basic computer-language-based, steady-state, numerical model that was originally developed by MIT and revised by

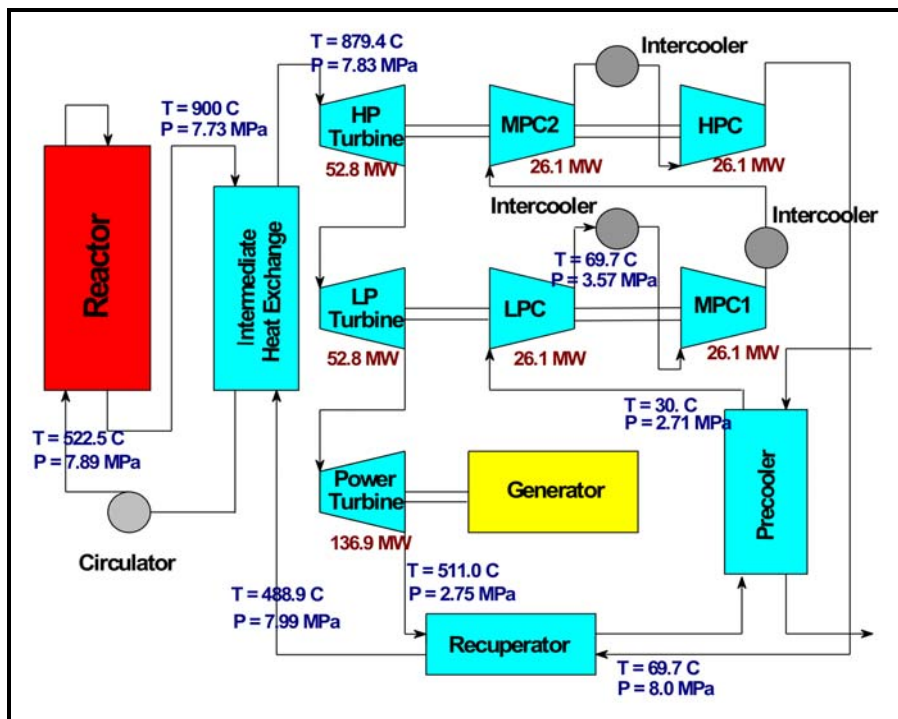


Figure 1. PBER reference design.

the Idaho National Engineering and Environmental Laboratory by coupling the NIST CO<sub>2</sub> database to the numerical model. The results from HYSYS were compared with those from Visual-Basic model. They agree very well for the 3-shaft baseline case. In order to make initial calculations for the CO<sub>2</sub> Brayton cycle, researchers used the baseline layout. They established energy and material balance to make certain that each flow stream has a positive pressure drop, single phase CO<sub>2</sub>, and no temperature crossover in the heat exchanger and recuperator. The initial CO<sub>2</sub> Brayton cycle gives 53-percent plant efficiency, which is an improvement over 47 percent for the helium Brayton cycle using the same layout. The improvement is attributed to the reduced volumetric flow of CO<sub>2</sub> over that of helium, which results in less compression work and an increase in the plant's efficiency. Simulations on one-shaft vs. multiple-shaft (up to four) were made using a helium Brayton cycle. Researchers will select the best shaft configuration based on the plant efficiency and cost, which they will investigate in the next two years.

### Task 2: Improvement of HTGR Net Efficiency.

The inlet temperature to the high-pressure turbine is very important on the plant's efficiency. For a given power conversion unit with a fixed intermediate heat exchanger (IHX) effectiveness, the turbine inlet temperature is solely dependent on the primary reactor outlet temperature.

By holding the reactor core outlet temperature constant and varying the reactor core inlet temperature, researchers can obtain a variable IHX primary outlet temperature. By plotting the cycle efficiency and cycle pressure ratio as a function of the IHX primary outlet temperature, researchers observed that there was a maximum cycle efficiency for a given core exit temperature. They also observed that the cycle pressure ratio increases as the core outlet temperature is increased but decreases as the IHX primary outlet temperature is increased. Maximum cycle efficiency coincides with an optimum pressure ratio. The parametric study will continue until the end of the second quarter of FY04.

### Task 3: Material Compatibility.

Material testing is a very important part of this research because of the high temperatures and pressures involved. Researchers evaluated the corrosion resistance and creep resistance in order to determine the suitability of this alloy for long-term applications in the supercritical CO<sub>2</sub> Brayton cycle. Mechanical property and microstructural analyses as well as the creep rate determination are addressed under Task 3-1, Characterization of Creep Deformation of MA 754. The corrosion analysis is addressed under Task 3-2, Thermogravimetric Analyses.

Highlights of the annual activities are summarized below:

- Researchers completed Task 1 (development of CO<sub>2</sub> Brayton cycle) along with five subtasks:
  - 1-1) Development of the efficiency equation of turbine and compressor for real gas.
  - 1-2) Check of supercritical CO<sub>2</sub> properties with equations of state.
  - 1-3) Selection of the optimization computer code.
  - 1-4) Layout of CO<sub>2</sub> thermal cycle and initial calculations.
  - 1-5) Performance of baseline calculations.
- Researchers have begun Task 2 (parametric study due to the improvement of HTGR efficiency).
- Researchers determined mechanical properties of MA 754 at temperatures ranging from room temperature to 1,000°C.

- Researchers completed creep testing between 800-900°C using MA 754 (up to 1,400 hrs) on both the transverse and longitudinal directions of the as-received material.
- Researchers completed construction of the supercritical CO<sub>2</sub> test loop and corrosion testing is in progress.
- Researchers will link the Visual-Basic based module to an optimization scheme and then obtain the optimized efficiency and the estimated cost.
- For material research, researchers will complete the characterization of creep behavior of MA 754 in the optimized heat-treated condition (large grain size) during FY04. They will also explore creep testing of MA 754 in conditions other than the optimum heat treatment (thermo-mechanically processed—fine grain size). During the same year, researchers will also complete corrosion testing of MA 754 (both fine and large grain size conditions) in supercritical CO<sub>2</sub>.

## Planned Activities

The following activities are planned for the upcoming year:

- Researchers will continue studying the improvement of HTGR net efficiency by performing parametric investigation on the overall efficiency.





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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Hydrogen Production Plant Using the Modular Helium Reactor

PI: Arkal Shenoy, General Atomics

Project Number: 02-196

Collaborators: Idaho National Engineering and Environmental Laboratory, Texas A&M University

Project Start Date: September 2002

Project End Date: September 2005

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### Research Objectives

The primary objectives of this project are 1) to develop a conceptual design of an H<sub>2</sub>-modular helium reactor (MHR), which consists of a hydrogen production plant coupled to a MHR and 2) to provide DOE, utilities, and energy-policy planners the information needed to make decisions regarding additional research and development for producing hydrogen using nuclear energy. To achieve these objectives, the work will be structured to satisfy five major goals:

- Goal 1: Using a Systems Engineering Approach, Develop Functions and Requirements for an H<sub>2</sub> Production Plant Using the MHR
- Goal 2: Develop a Conceptual MHR System Design for Supplying Process Heat and/or Electricity to an H<sub>2</sub> Production System
- Goal 3: Develop a Conceptual Design for a Thermochemical H<sub>2</sub> Production System that Receives Process Heat from an MHR
- Goal 4: Develop a Conceptual Design for an H<sub>2</sub> Production Plant that Integrates the Reactor and H<sub>2</sub> Production Systems
- Goal 5: Complete Assessments of the Plant Design with Respect to Performance, Safety, Economics, and Licensing

### Research Progress

The overall goal of this project is to complete a conceptual design for an H<sub>2</sub>-MHR plant and perform the engineering analyses to support the design. The MHR portion of the design is based on the gas-turbine modular helium reactor (GT-MHR). During Year 1 of this project, work was initiated in the following tasks: 1) development of plant functions and requirements, 2) intermediate heat exchanger (IHx)

design and operating envelopes, 3) fuel element thermal design and impacts on fuel performance, 4) assessment of tritium transport, 5) facility layout, and 6) RELAP5-3D/ATHENA model development.

#### Task 1: Plant Functions and Requirements.

For this conceptual design effort, researchers are performing functional analyses at the plant and major systems levels. They prepared a report titled *H<sub>2</sub>-MHR Functions and Requirements*, which included a separate section on environmental, safety, and health considerations for nuclear hydrogen production. They performed functional analysis using a systems-engineering approach, which included development of a function flow block diagram to define the flow from higher-level functions to lower-level functions. Each function is supported by one or more performance requirements, which provide the quantitative measures that the design must satisfy. This report also included a preliminary set of plant-level design requirements organized into 16 separate areas. In general, researchers used accepted industry codes and standards as the basis for the plant-level design requirements.

#### Task 2: IHx Design and Operating Envelopes.

Researchers evaluated an IHx concept based on the printed circuit heat exchanger (PCHE) designs being developed by HEATRIC. These heat exchangers consist of metal plates that are diffusion bonded. Fluid-flow channels are chemically milled into the plates using a technique that is similar to that used for etching printed electrical circuits. With this technique, the PCHE design can be optimized for specific applications. HEATRIC has developed designs with thermal effectiveness greater than 98 percent. For the H<sub>2</sub>-MHR, researchers developed a concept that consists of 120 HEATRIC-type modules manufactured from Alloy 800H material. The modules are housed in an IHx vessel with a diameter of 6.9 meters and active heat-transfer height of 8 meters (similar in size to that of the MHR reactor vessel).

The modules are arranged in an annular configuration with 4 axial layers (30 modules per layer). The total heat-transfer area for this concept is 5,230 m<sup>2</sup> and the pressure drop on the primary side is 5.9 psid.

**Task 3: Fuel Element Thermal Design and Impacts on Fuel Performance.**

Researchers performed several analyses in this area, including investigating H<sub>2</sub>-MHR core design options that would allow an increase in the average coolant outlet temperature, from 850°C to 1,000°C, while maintaining fuel temperatures at acceptable levels. One of these options is to use fixed orifices in the upper reflector, lower reflector, or both locations to control the flow distribution. To assess the effects of using orifices to control the flow distribution, researchers ran the POKE code in a mode where it calculates orifice coefficients and distributes the flow to virtually eliminate coolant hot/cold streaks. They ran two cases using optimized flow distributions: 1) the inlet coolant temperature was set at 641°C and the coolant flow rate was maintained at 320 kg/s, and 2) the inlet coolant temperature was lowered to the GT-MHR reference value of 491°C and the coolant flow rate was lowered to 226 kg/s so that the average coolant exit temperature would be maintained at 1,000°C. Using the conditions for the latter case, researchers ran a third case with a set of discrete, specified loss coefficients for the orifices (since it is recognized that an optimized flow distribution cannot be achieved with fixed orifices). These specified loss coefficients were based on the values that POKE calculated for the cases with optimized flow distributions. If the coolant inlet temperature is maintained at 641°C (corresponding to a flow rate of 320 kg/s), optimizing the flow distribution reduces the peak fuel temperature by approximately 100°C, but the addition of the orifices increases the core pressure drop by about 4.5 psid. If the coolant inlet temperature is dropped to 491°C (corresponding to a flow rate of 226 kg/s), there is only a modest increase in maximum fuel temperature (from 1,204°C to 1,239°C)

and, because of the lower flow rate, the core pressure drop is lowered by more than a factor of two to 6.9 psid. For the case with specified orifice coefficients, the maximum fuel temperature was only somewhat higher than the optimized flow case (1,276°C vs. 1,239°C). Based on these results, researchers will further evaluate using fixed orifices.

**Task 4: Assessment of Tritium Transport.** In order to assess the potential for tritium contamination in the hydrogen product gas, researchers assessed tritium permeation through the IHX, based on the HEATRIC-type design described above. Using these assumptions, they calculated the tritium permeation rate to the secondary side to be approximately 29.5 μCi/s. If the tritium is assumed to be in the hydrogen-tritium molecular form, the mass permeation rate is approximately  $4 \times 10^{-12}$  kg/s. Using this source term to the secondary helium side, researchers will assess product gas contamination when the interfaces between the secondary helium and the hydrogen production plant are better defined. They will use these assessments to determine if coolant purification is required on the secondary loop in order to reduce the tritium concentration in the product hydrogen gas to acceptable levels.

**Task 5: Facility Layout.** When developing the layout of the H<sub>2</sub>-MHR facility, it is important to ensure that hypothetical accidents in the hydrogen production plant do not impact the passive safety features of the MHR. The impact of explosions and/or chemical spills in the hydrogen plant

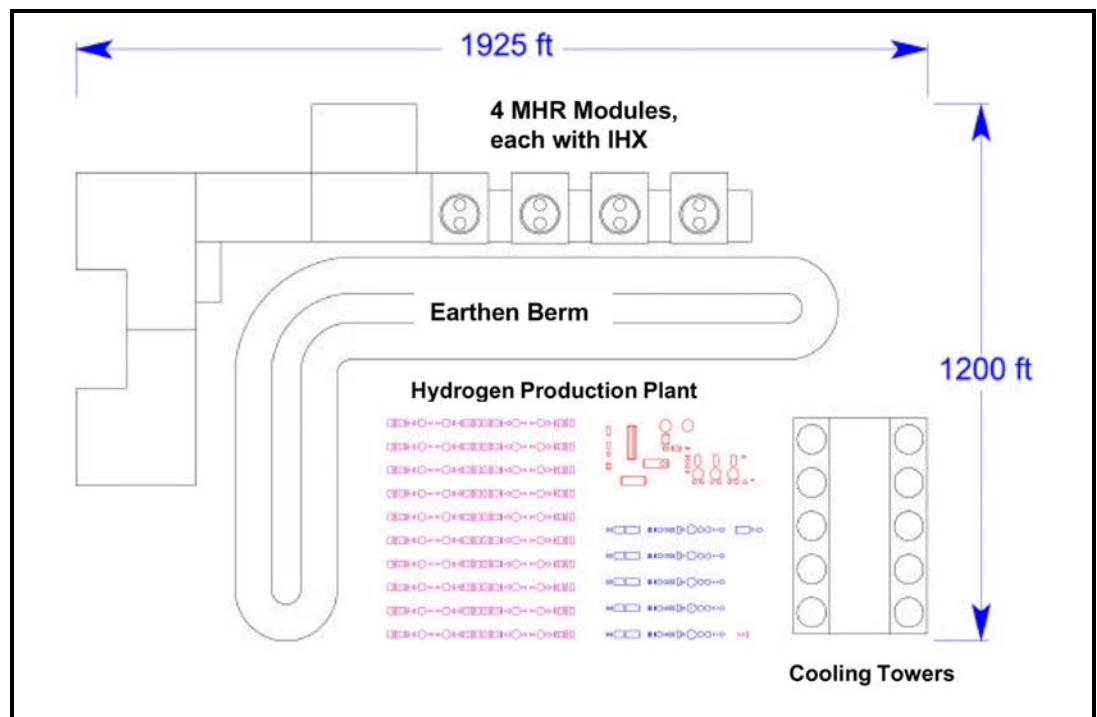


Figure 1. Conceptual layout of SI-based H<sub>2</sub>-MHR.

on reactor safety can be mitigated by physically separating the MHR from the hydrogen plant. One concept being evaluated is to use an earthen berm to provide protection while also minimizing the separation distance (and lengths of piping runs) between the MHR and the hydrogen plant. If a chemical spill occurred, additional protection would be provided by the ventilation system for the MHR control room. Figure 1 shows a conceptual layout of an H<sub>2</sub>-MHR plant consisting of four MHR modules.

**Task 6. RELAP5-3D/ATHENA Model Development.**

Researchers developed an initial RELAP5-3D/ATHENA model of the H<sub>2</sub>-MHR (reactor vessel, primary system, and intermediate loop) used to provide heat for hydrogen production. The models of the reactor vessel and the reactor cavity cooling system (RCCS) are based on recent models developed to support the design of the Next Generation Nuclear Plant, which are based on the General Atomics GT-MHR design. As part of this project, researchers developed models of the IHX and the secondary coolant system. The sulfur-iodine (S-I) hydrogen production system was modeled with boundary conditions applied to the heat exchangers representing the sulfuric acid and hydrogen-iodine decomposers. Researchers used this model to calculate steady-state point design parameters, assuming a coolant outlet temperature of 900°C. They will also use this model for transient and accident analyses.

## Planned Activities

Work will continue with the H<sub>2</sub>-MHR conceptual design, in the areas defined by the work breakdown structure for the project. Specific tasks planned for Year 2 include additional work to optimize the reactor physics and thermal hydraulic design for higher-temperature operation, development of a reliability model for the hydrogen production plant, additional flow sheet analysis for operating the S-I process at higher temperatures, and additional development of RELAP5-3D/ATHENA and other analytical tools. Also planned for Year 2 is an evaluation of coupling the MHR to high-temperature electrolysis as an alternative method for hydrogen production.



# NUCLEAR ENERGY RESEARCH INITIATIVE

## Nuclear Reactor Power Monitoring Using Silicon Carbide Semiconductor Radiation Detectors

PI: Don W. Miller and Thomas E. Blue,  
The Ohio State University

Project Number: 02-207

Project Start Date: October 2002

Collaborators: Westinghouse Science and  
Technology Center, General Atomics

Project End Date: September 2005

### Research Objectives

The objective of this research program is to investigate the use of SiC-based sensor arrays as ex-core neutron monitors in the International Reactor Innovative and Secure (IRIS) Reactor and in the prismatic-core, gas turbine modular helium-cooled reactor (GT-MHR). This investigation has two primary tasks:

1. Researchers will analytically define the ideal location for SiC-based sensor arrays in the IRIS and GT-MHR nuclear power plants and use the predicted neutron flux levels and environmental conditions at these locations to estimate the performance of the SiC sensor arrays, and
2. Researchers will design, construct, and evaluate a high-speed pulse counting system, which will be used in the SiC neutron sensor channels to optimize their performance in a power monitoring system.

### Research Progress

**Task 1.** The initial task required to define the ideal location of SiC neutron sensor arrays used in power monitoring systems is to calculate the thermal neutron flux in the regions adjacent to the reactors in the IRIS and GT-MHR plant systems. Researchers completed this task through an MCNP analysis of those regions. Selected results for the IRIS and GT-MHR systems are presented in the next two sections.

**Task 1.1 Neutron Flux Profile in the IRIS.** Figure 1 is the neutron flux radial distribution for three energy groups, as well as for

the total neutron flux. The results in Figure 1 were calculated without shielding plates in the down comer region.

As shown in Figure 1, the thermal neutron flux changes from up to  $7.81 \times 10^{12}$  at the edge of the core to  $6.39 \times 10^1$  at the reactor pressure vessel (RPV). The flux exhibits a local minimum in the middle of the reflector, decreases exponentially within the down comer region, and then exhibits a second local minimum in the RPV. It is almost flat in the cavity except for a  $1/r$  geometrical decrease.

*Neutron Flux Comparison With and Without Shielding Plates.* Researchers performed another calculation with two shielding plates placed at 220-230 cm and 240-250 cm. By introducing these two, 10-cm-thick, low-carbon, steel shielding plates, the thermal neutron flux at the RPV is reduced by a factor of two to five and the thermal neutron flux at the biological shielding is reduced by a factor of five to ten.

*Without Instrumentation Tubes.* The instrumentation tubes that are used to introduce detectors and cables into

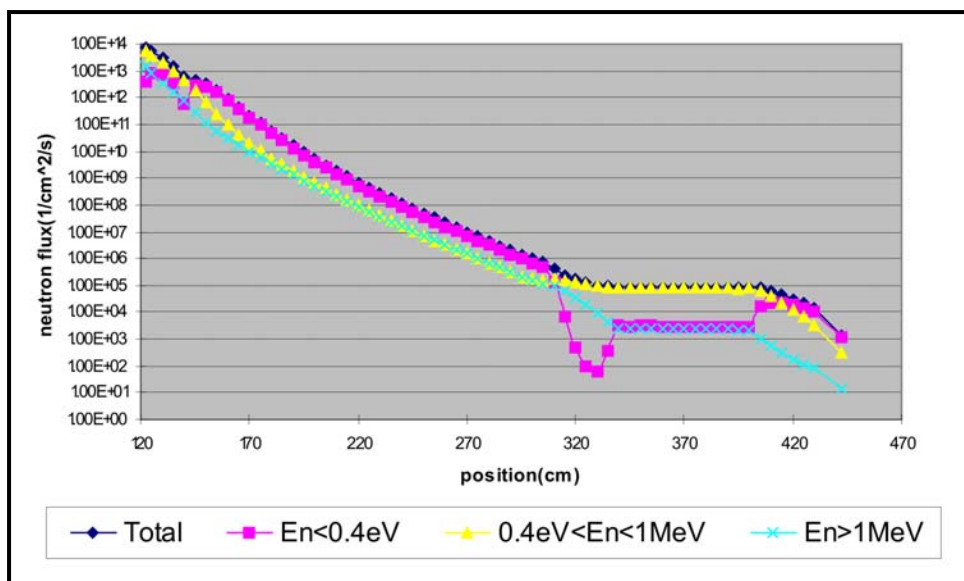


Figure 1. Neutron flux radial distribution.

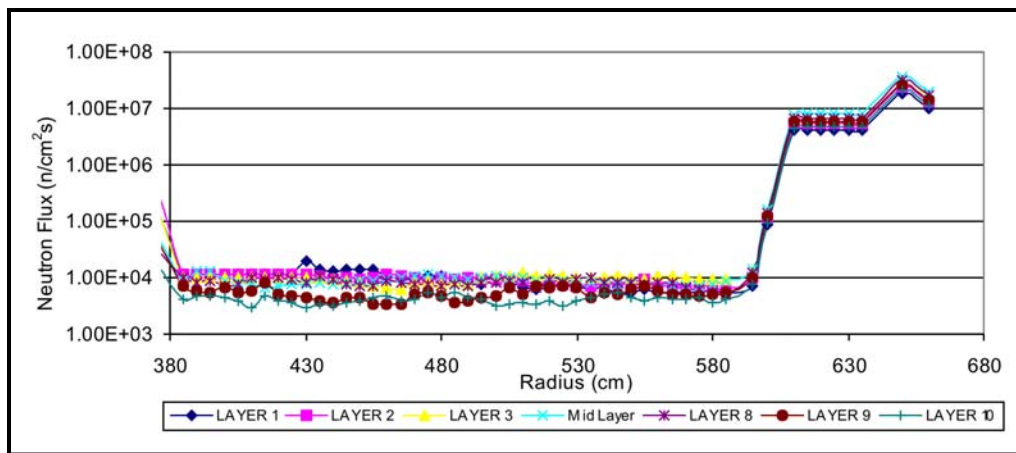


Figure 2. Total neutron flux radial distribution for normal operation.

the reactor have an effect on the thermal neutron flux inside the tube. Therefore, researchers performed one calculation to estimate how great this effect is. For this calculation, researchers place one stainless steel instrumentation tube with a 4-cm inner radius and an 8-cm outer radius at 155 cm from the center of the core. The result of the calculation shows that the thermal flux inside the tube is five times less than the thermal flux at that location without the instrumentation tube.

**Conclusions.** Researchers have calculated the neutron flux distributions using MCNP for two internal shielding configurations. Moreover, they have evaluated the effects of design or modeling modifications and the differential contribution of the various radial zones of the core to the response of the detector. Researchers will use these distributions to adjust the design of the detectors and their placement to achieve the required monitoring and safety functions.

**Task 1.2 Radial neutron flux results for normal operation in the GT-MHR.** Figure 2 presents the total neutron flux radial distribution in seven vertical positions. As can be seen in this figure, the total flux decreases by five orders of magnitudes from the edge of the core to the reactor cavity. This sharp decrease is due to thermal neutron absorption in the boron carbide pins. Consequently, the total neutron flux at potential detector locations in the case of normal operation is from  $10^8$  to  $10^9$  neutrons/cm<sup>2</sup>s. The thermal neutron flux inside the reactor cavity has a value between  $10^3$  and  $10^5$  neutrons/cm<sup>2</sup>s and, in the reactor cavity cooling system (RCCS) between  $10^6$  to  $10^7$  neutrons/cm<sup>2</sup>s. Its value is very important because the detector is sensitive to thermal neutrons.

**Task 2. Design, Fabrication, and Evaluation of a High-Speed SiC Neutron Monitoring Channel.** This task is directed to the design, fabrication, and evaluation of

a high-speed SiC neutron monitoring channel for use as an ex-vessel power monitor for the IRIS and the GT-MHR Generation IV nuclear power plants. The researchers at Westinghouse have developed designs for the SiC diode detectors that are to be used in the neutron monitoring channel. Researchers at Ohio State have simulated a four-layer configuration of a diode detector, consisting of LiF, Al, Au, and SiC, with

the TRIM computer code to find the response of the SiC detector to incoming particles from the reactor core. Specifically, they have used TRIM output files to calculate the energy deposited in the detector active volume by the charged particles that are produced when thermal neutrons interact with Li, in the LiF radiator. The TRIM results have been used to develop a Matlab simulation model of the detector output current signals.

## Planned Activities

In the next 12 months, researchers will develop a model of the remainder of the detector channel. Pulses, which are created in the same manner as those in developing the detector model, will be propagated through the detector channel in order to optimize its characteristics with respect to speed and resolution for application to the IRIS and the GT-MHR. Based on the results of the detector modeling, researchers have selected components for the channel and will assemble them into an operational channel. The channel performance will initially be evaluated using an ultra-high-speed pulse generator with adjustable rise and fall times of less than one nanosecond to simulate the detector signal. Researchers will compare the results of this evaluation to the detector channel model and, if necessary, they will modify the channel design.

In the next nine to twelve months, Westinghouse will deliver the first SiC detectors. Researchers will incorporate the SiC detectors into the channel and begin performance measurements. They will also link the detector channel model to models of the detector locations in the IRIS and the GT-MHR in order to assess the performance of SiC neutron monitoring in these plants.

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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## 7. Advanced Nuclear Fuels/Fuel Cycles

This element of the program includes 8 NERI research projects of which 1 was awarded in FY 2000, 1 in FY 2001, and 6 in FY 2002. It includes research and development to provide measurable improvements in the understanding and performance of nuclear fuel and fuel cycles with respect to safety, waste production, proliferation-resistance, and economics, in order to enhance the long-term viability of nuclear energy systems. This effort includes enhanced performance of fuels for advanced systems, development of fuels capable of withstanding the conditions in the supercritical LWR regime, and development of advanced proliferation-resistant fuels capable of high burn-up such as those needed in support of the Generation IV concepts.

The scope of this long-term R&D encompasses a variety of thermal and fast spectrum power reactor fuel forms, including ceramic, metal, hybrid (e.g., cermet or cercet), and liquid, as well as fuel types such as oxides, nitrides, carbides, and metallics. Enabling technologies such as advanced cladding, water chemistry, and alternative moderators and coolants are also considered. The fuel

cycle research includes consideration of advanced enrichment technologies for fuel and burnable absorbers and considers the impact of fuel cycle options on the proliferation of nuclear weapons materials. R&D topics also include development of higher density low-enriched uranium (LEU) (<20 percent U-235) fuels for research and development reactors.

Currently selected projects include innovative concepts for the following:

- Material preparation and production of nuclear fuels.
- Inherently safe fuel designs and core response.
- Study of life-limiting phenomena for high burn-up or long-life fuels.
- High-temperature fuel and material performance.
- Critical safety data and reactor physics data for advanced fuel compositions and enrichments above 5 percent.
- Innovation in fuel design, composition, or other attributes that maximize energy production, optimize fissile material utilization, or reduce production costs.

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# NUCLEAR ENERGY RESEARCH INITIATIVE

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# NUCLEAR ENERGY RESEARCH INITIATIVE

## Optimization of Heterogeneous Schemes for the Utilization of Thorium in PWRs to Enhance Proliferation Resistance and Reduce Waste

PI: Michael Todosow, Brookhaven National Laboratory

Project Number: 00-014

Project Start Date: September 2000

Project End Date: September 2003

**Collaborators:** Massachusetts Institute of Technology; Ben-Gurion University of the Negev, Israel; the Russian Research Center-Kurchatov Institute; Commissariat a l'Energie Atomique, France; Korea Atomic Energy Institute; Kyung Hee University, Korea; Korea Advanced Institute of Science and Technology

### Research Objectives

The objective of this work was twofold: 1) to examine heterogeneous core design options for the implementation of the Th-<sup>233</sup>U fuel cycle in pressurized water reactors (PWRs) and 2) to identify the core design and fuel management strategies that would maximize the benefits of including thorium in the fuel. The assessment concentrated on key measures of performance in several important areas including proliferation characteristics of the spent fuel, reliability, safety, cost, environmental impact, and licensing issues. The focus was on once-through fuel cycles that do not involve reprocessing of the spent fuel. Researchers used a 193-assembly Westinghouse reactor that utilized 17x17 fuel as the model core.

Design optimizations involved heterogeneous core options that aggregated the thorium in subassembly units or whole typical PWR assembly units. Researchers compared the case of all-uranium fuel (the current fuel cycle and its future extrapolations), as well as the case of Th-U fuel mixtures within individual fuel pins (in both homogeneous and micro-heterogeneous embodiments). Researchers have performed optimization of the homogeneous fuel cycles under separate projects.

In this project, researchers explored and expanded on two heterogeneous thorium implementation options: 1) the seed-blanket unit (SBU, also known as the Radkowsky Thorium Fuel [RTF] concept), which employs a seed-blanket unit that is a one-for-one replacement for a conventional PWR fuel assembly, and 2) the whole assembly seed and blanket (WASB), where the seed and blanket units

each occupy one full-size PWR assembly and the assemblies are arranged in the core in a modified checkerboard array (as shown in Figure 1). The studies for both approaches 1) identified the core design and fuel management strategies that would maximize the benefits from inclusion of thorium in the fuel and 2) extended the analyses to validate the results over a range of possible operating conditions.

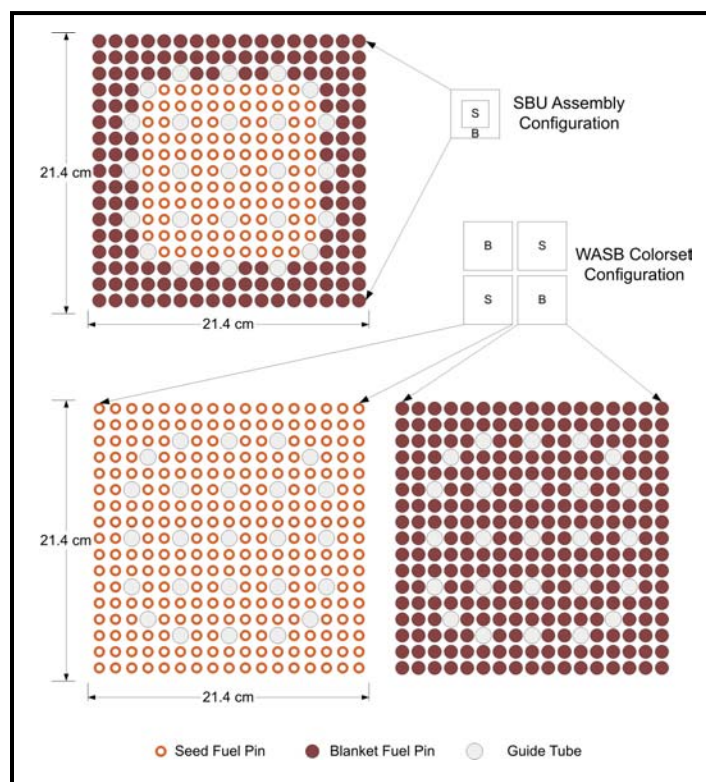


Figure 1. SBU and WASB fuel assembly design.

## Research Progress

Researchers have developed designs for both the SBU and WASB approaches, which significantly improve the intrinsic proliferation resistance and waste characteristics of the fuel while achieving 18-month cycles. The total production of plutonium was reduced by a factor of approximately three relative to a present commercial PWR operating on the uranium cycle. Furthermore, the plutonium produced was of inferior quality for potential utilization in weapons: it had a higher heat generation from increased Pu-238, and a stronger neutron source from increased Pu-238, Pu-240, and Pu-242. In addition, the fuel cycle costs were comparable and competitive. Significantly, both approaches utilized assembly designs based on a Westinghouse 17x17 assembly where the sole modification was in the details of the fuel rods. Therefore, in principle, they are retrofittable into existing PWRs with little or no modification.

Specific achievements for each approach are summarized below.

**The Seed Blanket Unit Approach.** Brookhaven National Laboratory (BNL) (with support from Ben Gurion University) examined the heterogeneous thorium implementation scheme based on the seed-blanket unit (SBU). The project was closely related to an ongoing project under the DOE Initiatives for Proliferation Prevention (IPP) program and private funding which is focused on Research Development and Demonstrations (RD&D) activities in Russia and the West. The initial reference point for the optimization studies was based on the results for the PWR from that IPP study.

Following is a summary of the progress achieved on this approach over the past three years:

- Researchers have defined a reference "improved" SBU design based on neutronic and thermal-hydraulic sensitivity studies, which included varying seed fuel and burnable poison compositions, and rod parameters within the constraints of a Westinghouse 17x17 assembly design (rod pitch, guide-tube locations). The design assumes annular uranium dioxide pellets with a central burnable poison annulus for the seed, and solid thorium/uranium dioxide pellets for the blanket. The resistance of the grid spacers and the rod outer diameters were profiled to enhance coolant flow into the high-power seed region, resulting in a minimum departure from nucleate boiling ratio (MDNBR) of approximately 1.3 at 118 percent power.
- Researchers have adopted a reference mechanical design for the SBU which allowed insertion and removal

of seed rods into an SBU. The selected approach removed and inserted rods, one-by-one, using a machine based on one designed to replace failed fuel rods. The virtue of this approach is that the basic mechanical design of the assembly (e.g., grid-spacers, upper and lower end-fittings) can be identical to that currently employed.

- Researchers performed a series of sub-channel analyses using the COBRA-EN code to study the thermal design of the SBU core. Analyses were done with two geometric models, a  $1/8$  hot assembly model (individual seed and blanket rods) and a  $1/8$  core model ( $1/8$  hot assembly plus several lumped assemblies representing the rest of the  $1/8$  core). Out of the six fuel cycles analyzed, researchers found that the first cycle had the lowest MDNBR. Based on the W-3 CHF correlation, the  $1/8$  core nominal power case (3,400 MWT) with uniform grid loss coefficients, had a MDNBR of 1.588, while the  $1/8$  assembly nominal power case has a MDNBR of 1.585. This showed that the effect of the surrounding assemblies on the hot channel was minimal.
- Researchers performed the accident analysis of the SBU core with the RELAP5 code. They executed the large break loss of coolant accident (LBLOCA) input deck from the Massachusetts Institute of Technology (MIT) for the standard PWR design with RELAP5-3D (the DOE version of the code). The results were quite different from those obtained at MIT using the MARS code. A study was performed to understand the cause of the differences. A parallel effort has been initiated to modify the WASB LBLOCA input to replace the WASB core components with the corresponding SBU components. This effort will enable a comparison between the accident analysis of the SBU design and the reference PWR.

### **The Whole Assembly Seed and Blanket Approach.**

The WASB design assumes that each type of fuel (seed and blanket) occupies a whole PWR assembly. MIT was largely responsible for developing and assessing this option.

Following is a summary of the progress achieved on this approach over the past three years:

- After investigating a number of core designs, the MIT researchers recommend a design consisting of 84 seed assemblies with 20 percent enriched  $U^{235}$  in  $UO_2$  and 109 blanket assemblies with 87 percent  $ThO_2$  and 10 percent enriched  $U^{235}$  in the remaining  $UO_2$ . Both the seed and blanket assemblies used the same 17x17 rod

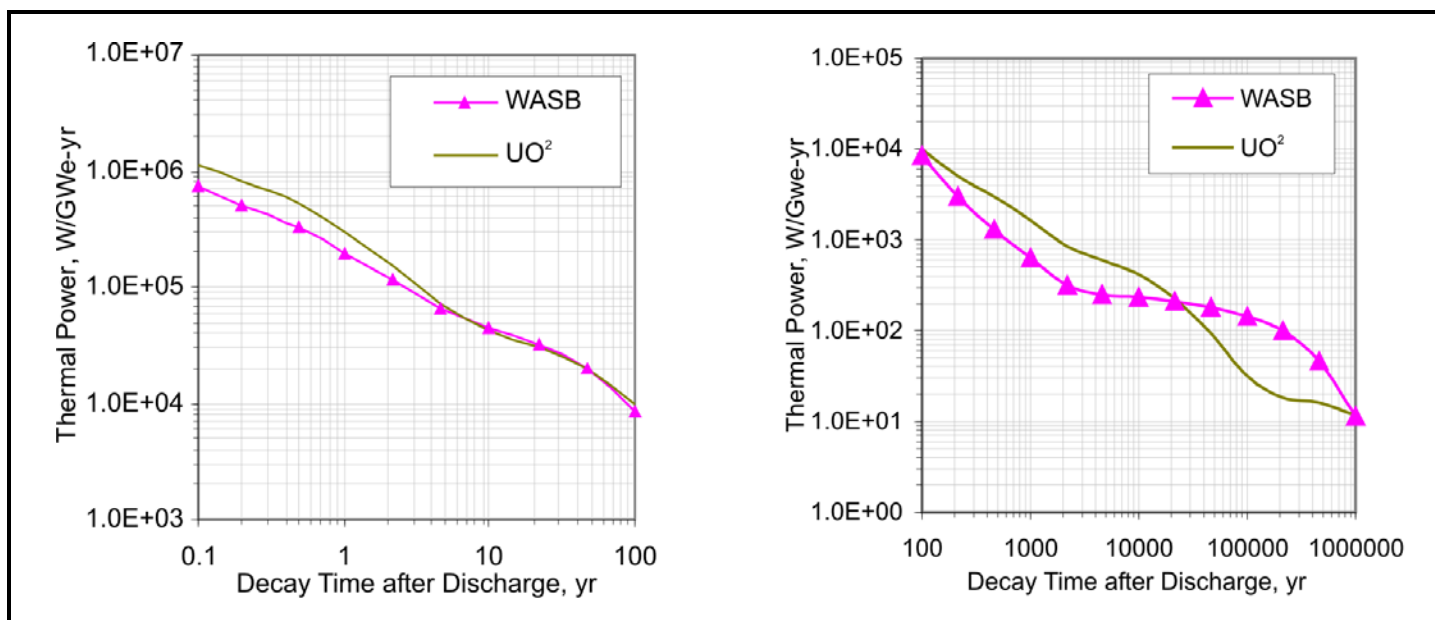


Figure 2. Decay heat of the WASB spent fuel per electrical energy generation.

- array as used in typical Westinghouse PWR. Researchers recommended using smaller diameter seed rods with internal void, but larger diameter solid blanket rods. Researchers adjusted grid or spacer resistances in order to enhance flow in the higher power seed assemblies and reduce flow in the lower power blanket assemblies. With this, they have attained acceptable DNB margins under overpower conditions. Researchers employed typical three-batch fuel management with 18-month cycle for the seeds, achieving a discharge burn-up of about 145 MWD/kgU. The 109 blanket assemblies were loaded and discharged together, spending nine cycles in the core and achieving a discharge burn-up of about 90 MWD/kgHM.
- Assessment of spent fuel characteristic indicated that the WASB design discharged about 40 percent fewer assemblies per GWe-yr than a typical 18-month cycle PWR. Researchers also found that the discharged mass of heavy metal for WASB was about half of that for a similar PWR. WASB spent fuel produced less radioactivity and less decay heat than the conventional all-UO<sub>2</sub> fuel in the short term (up to about five years after discharge), and a comparable amount in the near term (up to about 10,000 years). After that, there was a local peak due to the decay products of U<sup>233</sup> in the blanket, but by that time both the radioactivity and the decay heat were at relatively low levels. Figure 2 shows the comparison of decay heats after discharge for the WASB and typical all-UO<sub>2</sub> PWR designs.
  - Researchers calculated the annual rate of plutonium production for the WASB design and found it to be only about 40 percent of that of a conventional PWR. Moreover, the total heat generated by the WASB plutonium is much higher than that produced by the typical PWR grade plutonium, making the former unsuitable for weapons development. Finally, the blanket uranium proliferation index was kept within the accepted upper limit of 12 percent.
  - Using a particular version of RELAP5, called MARS, available at MIT, researchers analyzed three accidents/transients, namely, LBLOCA, complete loss of primary flow (LOPF) and loss of off-site power (LOSP), for both the WASB and the conventional PWR designs. For LBLOCA, the peak cladding temperature (at the hottest rod in the hottest seed assembly) for the WASB design was calculated to be about 250°C higher than that for the conventional PWR design. However, this higher peak cladding temperature for the WASB design was still about 200°C lower than the present regulatory limit of 1,204°C. For the LOPF and LOSP transients, the results of the WASB and the typical PWR designs were very similar—no post-DNB type rapid cladding temperature rise was calculated. Although these results indicate adequate safety margin for the WASB design, researchers should analyze other accidents and transients before a more definitive conclusion is drawn.
  - High burn-ups of both seed and blanket fuel led to high fission gas release and consequently high internal pressure in the seed rods, and excessive oxide growth

on the surface of the blanket rods. Further analyses showed that the internal pressure can be reduced if a longer plenum is used for the seed rods, and the oxide growth can be contained if improved material such as M5 is used for the blanket cladding material.

## **Planned Activities**

This NERI project has been completed.

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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## High-Performance Fuel Design for Next Generation PWRs (Annular Fuel Project)

PI: Mujid S. Kazimi, Massachusetts Institute of Technology

Project Number: 01-005

Collaborators: Gamma Engineering Corporation, Westinghouse Electric Corporation, Duke Engineering & Services (now Framatome ANP), Atomic Energy of Canada Limited

Project Start Date: August 2001

Project End Date: September 2004

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### Research Objectives

The overall objective of this NERI project is to examine the potential for a high-performance advanced fuel for pressurized water reactors (PWRs), which would accommodate a substantial increase of core power density while simultaneously providing comparable or larger thermal margins than current PWRs. This advanced fuel will have annular geometry that allows internal and external coolant flow and heat removal. Following are the detailed tasks of this project:

1. Identify the most promising fuel assembly arrangement of the internally and externally cooled annular fuel for PWRs to achieve a significant increase of power density (by at least 30 percent).
2. Optimize the fuel for superior thermal hydraulic and safety performance. Examine and optimize the flow distribution, core pressure drop, departure from nucleate boiling ratio (DNBR), and resistance against parallel channel instabilities. Perform safety analyses, such as loss of coolant accident (LOCA) analyses, to confirm safety benefits expected for the new fuel.
3. Evaluate the neutronic fuel design to achieve high reactivity-limited burn-up and reasonably long refueling cycle to attain good economic features. Confirm the acceptability of the coefficients for reactivity feedbacks and reactivity control.
4. Select fabrication processes to produce annular fuel elements with the required product characteristics, including fissile loading and high integrity cladding, which are capable of eventual scale-up into a low-cost, efficient production process for economic and reliable fuel element performance.

5. Evaluate the performance of  $\text{UO}_2$  fuel forms obtained by production technologies different from current U.S. practices (e.g., vibropacked fuel), and operating under new conditions (especially low-peak fuel temperature) on fission gas release, and fuel dimensional properties during burnup. Develop models for assessing fuel performance as well as for scoping irradiation tests performed at the Massachusetts Institute of Technology (MIT) reactor.
6. Estimate the electricity cost in cases of using the annular fuel for uprating current Generation II PWRs or in new advanced PWRs.

### Research Progress

The progress will be summarized according to tasks.

**Task 1: Thermal Hydraulic and Mechanical Design and Safety Analysis.** A whole-core VIPRE model for the DNBR analyses of annular fuel rods was developed and used for thermal hydraulic optimization studies. Using this whole core model, researchers explored various array sizes (11x11 to 15x15) that fit in the fixed dimensions of a fuel assembly. They found that the most promising options, based on DNBR considerations, were the 13x13 and 12x12 arrays. Because thermal expansion and swelling of fuel pellets during operation are expected to be towards the outer cladding and the 13x13 array accommodates higher heat flux to the outer channel, the 13x13 array (see Figure 1) was selected as the most promising design. The 13x13 design allows a 50 percent power uprate, in terms of DNBR limit. This is a significant power uprate, raising the extracted power from the same core size to support increasing the plant output from the current 1,150 MWe to 1,750 MWe. At this high power, the peak fuel temperature is still about 1,300°C lower than the solid fuel in today's PWRs.

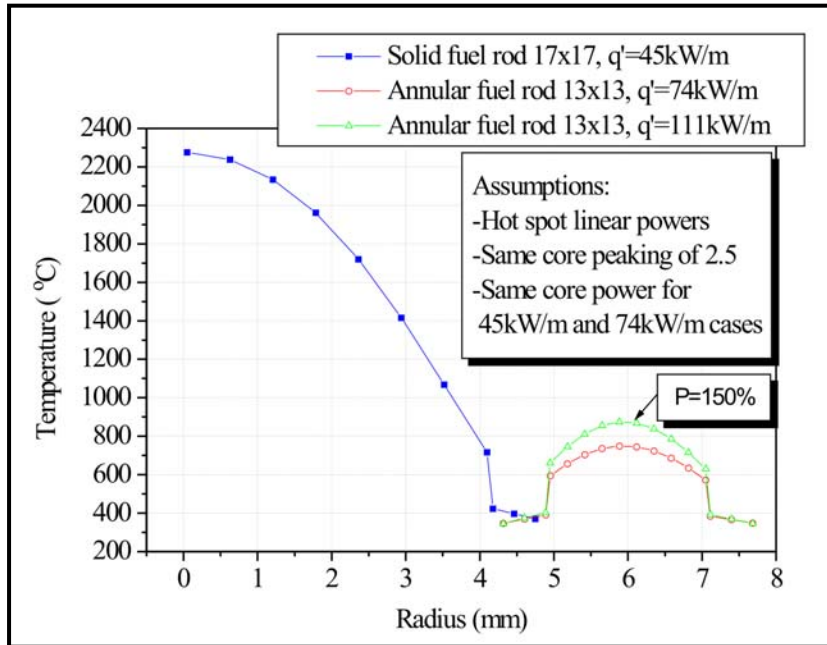
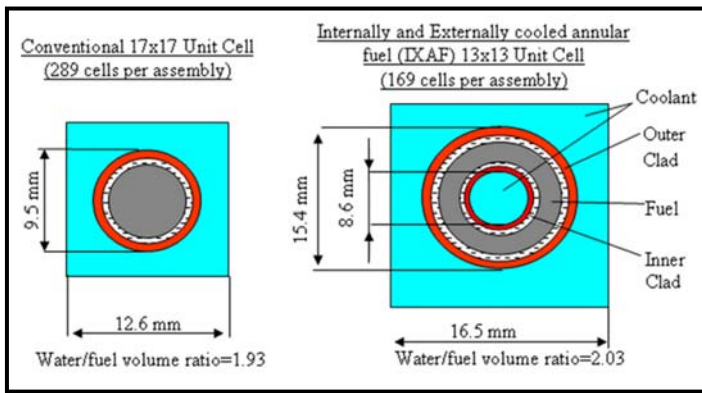


Figure 1. The graphic compares performance of solid and annular fuel.

Such a high power uprate requires a proportional increase of core flow rate resulting in larger pressure drop and velocity, which in turn raises vibration and fuel assembly lift-off concerns. However, vibration analyses showed that annular fuel even at 150 percent flowrates is, due to its high rigidity, more resistant to various modes of vibration than solid fuel. Annular fuel was also found to be resistant to both excursive (Ledinegg) instability and density wave instability. However, hydraulic lift-off forces are several times higher than for the reference fuel and will require design modifications of the fuel assembly and fuel rod holding mechanisms.

Researchers developed and used a RELAP5/MOD3.2 model of a Westinghouse 4-loop plant for a Large Break LOCA (LBLOCA) analysis. Researchers compared peak cladding temperature for solid and annular fuel. These comparisons showed that for 100 percent power for both cases, the blowdown peak is eliminated for the annular fuel due to the small stored energy. In fact, the cladding

temperature decreases during this accident phase. Lower cladding temperature prior to the core heat-up phase and larger heat transfer surface area results in significantly lower reflood peak temperature and earlier quenching.

**Task 2: Reactor Core Physics and Fuel**

**Management.** Benchmarking calculations of CASMO4 against the MCNP based burn-up code MCODE (developed at MIT) showed a significant discrepancy in the calculated eigenvalue because CASMO4 does not account for the higher resonance captures in U238 near the internal interface with the moderator. This deficiency has been circumvented by adjusting the CASMO4 U238 content to match the main spectral indices and reactivity burn-up curve to the results of MCODE. A 30 percent artificial increase in U238 number density was found to match the MCODE results for the case with burnable poison pins, while only a 20-percent increase in U238 was needed for poison-free cases. These fictitiously increased U238 number densities were used in the CASMO4/SIMULATE system to model the PWR core when fueled with the 13x13 annular fuel assemblies.

The poison-free results show that annular fuels have similar peaking factors, slightly smaller burnup, and 13-percent smaller cycle length compared to solid fuel. The smaller cycle length was the consequence of 10-percent smaller initial heavy metal loading and additional cladding volume. To achieve more realistic

power peaking and maintain a reasonable level of critical boron concentration, researchers developed a whole core model having burnable poison pins (gadolinium oxide mixed homogeneously with fuel). At 100-percent power, the peaking factors are very close to those for the solid fuel, but the effective full power cycle length is 13 percent smaller for the annular fuel mainly due to less fuel loading in the core. At 150 percent power density, an enrichment increase of 5 percent is necessary to maintain cycle length comparable to current utility practice and achieve higher burn-up of about 85 MWD/kgHM. Researchers on this project initiated a study using 8 percent enriched fuel.

**Task 3: Fuel Fabrication Studies.**

This task focused on two major fuel fabrication routes: the traditional pellet sintering route and the vibration packing (Vipac) route. Based on the annular fuel design, researchers developed preliminary specifications of key components. An evaluation showed that existing commercial manufacturing technology could produce the cladding tubes required by



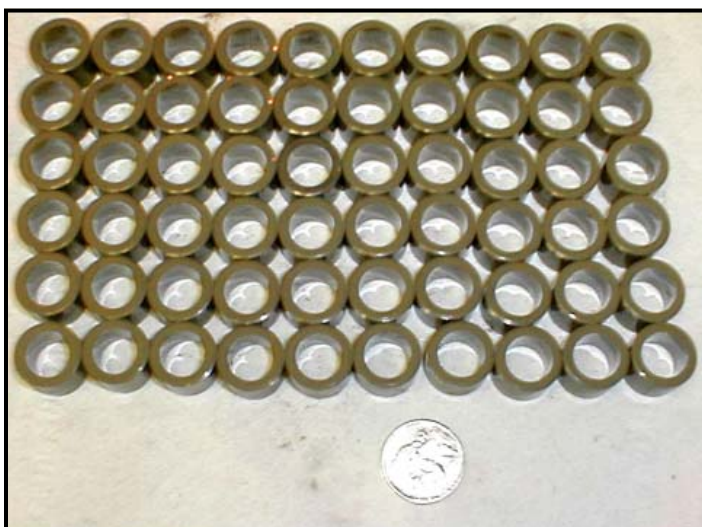


Figure 2. Sintered annular pellets manufactured at Westinghouse.

the annular fuel without prohibitively higher costs. Using Vipac fuel fabrication technology, Atomic Energy of Canada Limited (AECL) produced six annular fuel test specimens for irradiation testing at MIT. The AECL work provided valuable insight into Vipac fabrication techniques and product characteristics. The Vipac fuel fabrication route remains an attractive approach for manufacturing the annular fuel. Potential advancement of the Vipac technology will be evaluated in the third year. With respect to the traditional press and sinter fabrication route, Westinghouse Nuclear Fuel Company in Columbia, South Carolina, successfully completed a demonstration of pellet fabrication of the 13x13 annular fuels. The pellets are shown in Figure 2. This showed that the press-and-sinter fabrication route appears to be a very promising technology for commercially manufacturing the annular fuel. Further work on this process will get high priority in the third year. Researchers evaluated reaming (expanding) of the inner cladding of an assembled annular fuel element to reduce the internal gap between the fuel and cladding. They also evaluated alternative pellet fuel and cladding design dimensions to improve the heat split between the outer and the inner cladding surfaces. In addition, researchers assessed slurry extrusion and cold isostatic pressing (CIP) technologies for fabricating green annular pellets.

#### Task 4: Economic Analyses and Optimization.

In this task, researchers identified the manufacturing issues encountered when a central tube is introduced in the annulus of a fuel rod for both Vipac and pellet fuels. The baseline constraints and assumptions they used reflect the current permitting and operational constraints at the Westinghouse Nuclear Fuels Plant in Columbia, South Carolina. For pellet annular fuels, the pellets are first loaded into the outer tube, as is currently done. This

approach is used because the outside of the pellets can be ground to a very close tolerance. The inside tube is then inserted with a pre-welded bottom closure already attached. The addition of the second tube requires only a minor modification of the current assembly station. Minor increases in manufacturing costs are expected for two new welding stations. The only major capital investment is for doubling the sintering furnace capacity due to the larger volume of the pellets. However, no significant increase in the final cost of fuel is expected. For the Vipac fuel, significant issues have been identified including low production rates during fuel rod loading; low final fuel density; maintenance of uniform density during handling, shipping, and use; and increased dust loads during manufacture. However, no significant increases in costs are expected.

Researchers evaluated the economic benefits of the higher power density achieved using annular fuel using the European Organization for Economic Cooperation and Development (OECD) methodology. Three options using annular fuel were compared to two options using standard pellet fuel. The discounted rates of returns for the various options (listed best to worst) were:

1. 500 MWe uprate to an existing Generation II PWR; annular fuel (Option 2) – 10.0 percent.
2. 1,500 MWe Generation III new PWR; annular fuel (Option 3) – 4.7 percent.
3. 1,500 MWe Generation III new PWR; standard fuel (Option 4) – 4.3 percent.
4. 1,000 MWe Generation III new PWR; annular fuel (Option 5) – 1.8 percent.
5. 1,000 MWe Generation III new PWR; standard fuel (Option 1) – 1.5 percent.

The use of annular fuel always improves the rate of return on invested capital. For a new power plant, the use of annular fuel can be used to either get more capacity from the same sized nuclear island or to reduce the size of the nuclear island. For the currently operating Generation II power plants, annular fuel provides a means to significantly upgrade the power output (50 percent or more) using the same nuclear island with new reactor internals, steam generators and circulation pumps, and a new incremental balance-of-plant to handle the increased power production. Since the balance-of-plant is built while the power plant remains operational, the Generation II PWR is only out of service for the time it takes to replace the reactor internals, steam generators, and circulation pumps. Based on current steam generator replacement times of about 90 days, the downtime is estimated to be about six months.

**Task 5: Fuel Performance Evaluation.** Part of this task is to design the fuel irradiation experiment and develop a fuel performance model. MIT received six sample fuel segments produced by AECL using Vipac methods. A Safety Evaluation Report was presented to the MIT Research Reactor II (MITR-II) Safeguards Committee and a revised version has been accepted by the designated subcommittee pending resolution of the issue of ultimate disposal of the irradiated fuel elements. The U.S. Nuclear Regulatory Commission approved the license amendment required to permit irradiation of sample fuel in the MITR-II. To raise the fuel temperature to prototypic conditions, a thermal bath of liquid lead will separate the cladding from an outer aluminum jacket that is cooled by the reactor coolant. Researchers completed the thermal testing of the liquid metal heat transfer medium for the in-core sample capsules and calculated the final dimensions for the capsules based on this test data and the as-received parameters for the fuel samples. Researchers have completed initial core flow experiments and manufacturing of capsules for fuel specimens is in the final stage. Irradiation of Vipac fuel specimens is planned in the third year.

For the fuel performance modeling, FRAPCON-3 code has been modified and applied for pellet annular fuel. The results confirmed expectations of very low fission gas release from the annular fuel due to small fuel temperature, which makes it possible to achieve high burnups. The cladding strain and oxide thickness were within the design limit even at high burnup and at high power density. On the other hand, the model predicts an imbalance between the inner and outer gap conductances, which negatively affects the minimum DNBR in the outer channels. The use of different inner and outer initial gap sizes or application of metallic bonds are recommended to circumvent the problem.

## Planned Activities

Future activities will focus on:

Task 1: Sensitivity studies to assess the various ways to overcome the fuel-cladding gap asymmetry using results from Task 3 on achievable fabrication tolerances; whole-core VIPRE model for Vipac fuel to investigate the benefits of higher fuel-cladding contact conductances, and thus smaller conductance asymmetries on DNBR margin; safety analyses of LOCA; rod ejection and main steam line break and the established final optimum design, based on feedbacks from other tasks.

Task 2: Establishment of core design and fuel management for 150 percent power density core at minimum enrichment and power peaking while achieving 18-month cycle length.

Task 3: Demonstration testing(s) of the most promising fuel fabrication technology identified during the first 2 years—the fabrication of long annular fuel rods by the press-and-sinter pellet fuel route and the fabrication of long annular fuel rods by Vipac fuel route.

Task 4: Economic analyses have been completed. Thus, the funds allotted for this task in FY04 will be used for manufacturing annular fuel pellets at Westinghouse, which will be used under Task 3 to demonstrate the fabrication of long annular fuel rods by the press-and-sinter pellet fuel route and to identify minimum achievable tolerances.

Task 5: Irradiation of four fuel samples for 4-6 months, post-irradiation examination on two samples from first irradiation (fission gas release, burnup confirmation, gamma scan) and analysis of results, development of FRAPCON-ANNULAR code for modeling of Vipac fuel, and evaluation of Vipac annular fuel performance.



# NUCLEAR ENERGY RESEARCH INITIATIVE

## An Innovative Transport Theory Method for Efficient Design, Analysis, and Monitoring of Generation IV Reactor Cores

PI: Farzad Rahnema, Georgia Institute of Technology

Project Number: 02-081

Collaborators: Idaho National Engineering and Environmental Laboratory, Penn State University

Project Start Date: September 2002

Project End Date: September 2005

### Research Objectives

The objective of this research project is to develop a next-generation, high-order variational transport method for core-level neutronics calculations in advanced and Generation IV light water reactors (LWRs) and pebble bed reactors (PBRs). Researchers will implement the method in computer code and apply realistic models of large-scale reactor cores in order to demonstrate the practical feasibility of the method. The research team expects that the new approach will achieve a significantly higher degree of accuracy than current state-of-the-art methods, especially for heterogeneous reactors and smaller Generation IV designs. The products of the project will be:

- A computer code system based on the new transport method for the following advanced reactor types and geometries:

Reactor Type(s)	Geometry	Abbreviation
LWR and PBR	1-D Slab	1-D( $z$ )
LWR	2-D Cartesian	2-D( $x, y$ )
PBR	2-D Cylindrical	2-D( $r, z$ )

- A computer code system for automated calculations of 1-D( $z$ ) and 2-D( $r, z$ ) PBR models in the asymptotic fuel loading pattern, developed by integrating the transport method into the Idaho National Engineering and Environmental Laboratory (INEEL) PBR fuel cycle code PEBBED.
- A theoretical method for 3-D Cartesian geometry advanced and Generation IV LWR models.
- A suite of benchmark problems for the PBR and heterogeneous LWR cores with detailed reference transport results.

### Research Progress

The main focus of the first-year effort was to develop and implement the transport method for 1-D( $z$ ) applications, and to construct realistic, one-dimensional benchmark problems for testing the new method. Toward the end of the year, work was initiated on 2-D( $x, y$ ) geometry applications.

The development of the theoretical transport method proceeded well ahead of what had been anticipated in the first year's schedule. The team's approach was to characterize coarse meshes (e.g., fuel assemblies in reactor calculations) using a set of response functions (RFs) instead of using homogenized cross sections, as is done with current core neutronics methods. The advantage is that the RFs are invariant quantities, whereas the exact homogenized cross sections (e.g., from generalized equivalence theory) are problem-dependent. In addition, using RFs allows researchers to accurately and consistently treat the heterogeneous nature of the coarse meshes (i.e., between the fine and coarse mesh calculations) as opposed to current methods that rely on *ad hoc* heterogeneous flux reconstruction schemes. A fundamental challenge faced in this work is that the number of response functions needed to exactly characterize the intra-nodal (i.e., within the coarse mesh) flux shape becomes extremely large in two- and three-dimensional geometries. Researchers developed a technique during the first year of this project to reduce the number of RFs needed to accurately characterize a coarse mesh for 1-D( $z$ ) applications. Table 1 summarizes the eigenvalue and rod-wise fission density (FD) relative errors (REs) in three seven-assembly, two-group 1-D( $z$ ) core problems. For these problems, the number of RFs was reduced from  $N$  down to four per coarse mesh type, where  $N$  is the discrete ordinates quadrature order of the problem.

The extension of the transport method to 2-D( $x, y$ ) geometry for light water reactor applications is seemingly straightforward. Researchers recently completed a modification to the DORT code to support the computation and storage of 2-D( $x, y$ ) response functions.

The team developed two new sets of PBR and heterogeneous LWR 1-D( $z$ ) benchmark problems, along with reference fine-mesh results. In addition, researchers on this project generated a reference solution to the NEA 2-D PWR Mixed Oxide (MOX) benchmark problem using the DORT code. This problem is a quarter core LWR model consisting of four fuel assemblies surrounded by a thick reflector, as

$N$	Problem 1		Problem 2		Problem 3	
	$k$ RE	Max. Rod FD RE	$k$ RE	Max. Rod FD RE	$k$ RE	Max. Rod FD RE
16	0.003%	0.274%	0.002%	0.151%	0.001%	0.588%
32	0.005%	0.280%	0.001%	0.176%	0.002%	0.549%
64	0.009%	0.273%	0.013%	0.181%	0.002%	0.534%
128	0.006%	0.278%	0.004%	0.207%	0.005%	0.539%

Table 1. Summary of the eigenvalue and rod-wise fission density relative errors in three seven-assembly, two-group 1-D(2) core problems.

shown in the Figure 1. Researchers studied variations in the quadrature order and spatial fine-mesh distribution in order to assure that a high-quality reference solution was obtained. This benchmark problem will be used to evaluate the new transport method in 2-D( $x, y$ ) geometry, to be developed in the second year.

The first-year accomplishments of this project are listed below:

- Researchers wrote and tested a preliminary version of a computer code system for 1-D( $z$ ) advanced and Generation IV LWR and PBR models using the new method.
- They developed a new technique for greatly reducing the number of response functions required to achieve highly accurate results for heterogeneous 1-D( $z$ ) core problems.
- They developed a set of 1-D( $z$ ) PBR benchmark problems with reference transport results.
- They developed a preliminary version of a specialized fine-mesh code for 2-D( $x, y$ ) fine mesh calculations to be used by the coarse mesh method.
- They wrote one journal paper and one conference paper on the transport method.

D. Ilas and F. Rahnema, "A Heterogeneous Coarse-Mesh Transport Method," *Transport Theory and Statistical Physics*, 32, 441-467 (2003).

S. W. Mosher and F. Rahnema, "An Intra-Nodal Flux Expansion for a Heterogeneous Coarse Mesh Discrete Ordinates Method," *Proceedings of ANS Nuclear Mathematical Methods Sciences: A Century in Review, A Century Anew*, April 6-10, Gatlinburg, Tennessee (2003).

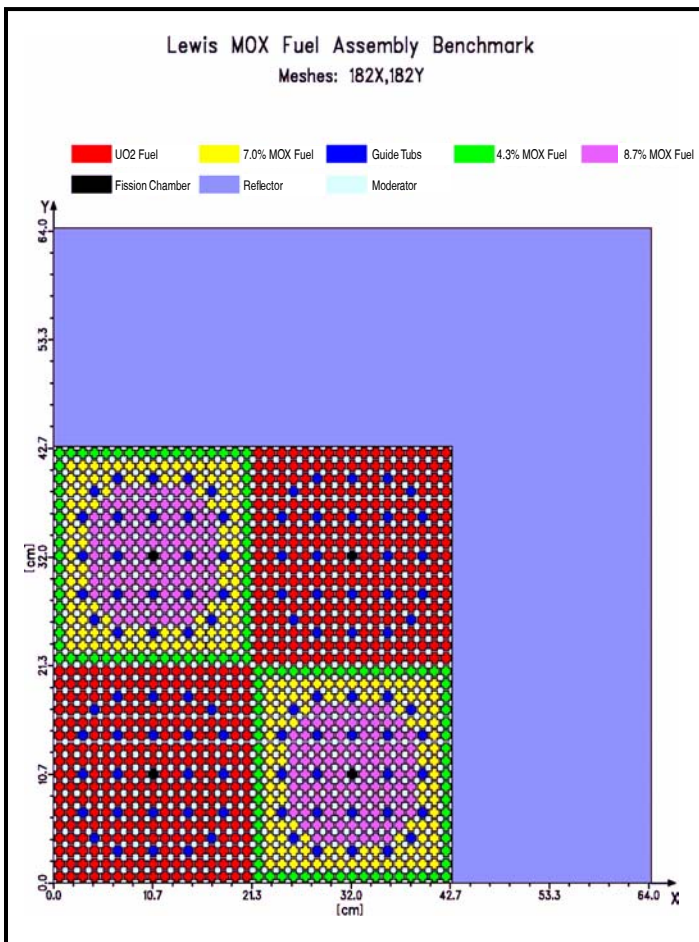


Figure 1. A quarter core LWR model consisting of four fuel assemblies surrounded by a thick reflector.

## Planned Activities

The main focus of the second year is extending and implementing the transport method to two-dimensional Cartesian geometry. The challenge is to continue to produce efficient and highly accurate coarse mesh solutions in problems with two additional degrees of freedom (i.e., an additional spatial and angular variable). Additional second-year activities include:

- Incorporating the 1-D( $z$ ) coarse mesh code into the pebble transport code PEBBED and testing the coupled code on the PBR benchmark problems that were developed during Year 1.

- Developing 2-D( $r, z$ ) PBR benchmark problems to be utilized in year three.
- Developing a specialized 2-D( $r, z$ ) geometry fine mesh capability to support the application of the transport method to 2-D PBR problems in the third year.

Project Year 3 involves developing the 2-D( $r, z$ ) transport code and incorporating it into PEBBED. In addition, researchers will develop a theoretical 3-D Cartesian geometry transport method; however, this will not be implemented as part of this project.



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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Advanced Extraction Methods for Actinide/Lanthanide Separations

PI: Michael Scott, University of Florida

Project Number: 02-098

Collaborators: Argonne National Laboratory

Project Start Date: September 2002

Project End Date: September 2005

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### Research Objectives

Separation chemistry has always played a crucial role in preparing reactor fuels for both nuclear energy and nuclear weapons production. It is now assuming a central position in strategies for cleaning up decommissioned nuclear facilities and disposing high-level radioactive waste. Although the United States does not currently allow spent fuel to be recycled, as it is practiced around the world, it has taken an active role in developing nuclear waste reprocessing technologies.

Nuclear fuel reprocessing is based on the dissolution of irradiated material in a nitric acid solution. The reprocessing operations produce high-and-medium level liquid wastes (HLLW and MLLW, respectively) containing different radioactive elements as  $\beta/\gamma$  emitters and  $\alpha$  emitters. In order to simplify the conditioning of such wastes, it would be highly desirable to separate the different radioactive components with respect to their lifetime. Their separation would decrease the volume of waste disposed in deep geological repositories, such as Yucca Mountain, and instead utilize subsurface repositories, which are easier to manage. Furthermore, these nuclides, once isolated, could be turned into short-lived or non-radioactive elements, thereby eliminating the radiological hazards and waste disposal problems.

The separation of Am (III) ions from chemically similar Ln (III) ions is perhaps one of the most difficult problems encountered during the processing of nuclear waste. In the 3+ oxidation states, the metal ions have an identical charge and roughly the same ionic radius. They differ strictly in the relative energies of their f- and d-orbitals, and to separate these metal ions, ligands will need to be developed that take advantage of this small but important distinction. During the project performance period, the binding attributes of various ligand systems developed at the University of Florida will be tested with Am (III) in addition to several other actinides including Pu (IV) and

U (III) at Argonne. The information gained from these studies will be used to develop new, more sophisticated ligands. Further refinement should afford ligands that are adept at selectively sequestering actinide ions from acidic nuclear waste streams.

### Research Progress

The extraction of uranium and plutonium from nitric acid solution can be performed quantitatively by the extraction with the monofunctional organophosphorous compound TBP. Commercially, this process has found wide use in the PUREX (plutonium uranium extraction) reprocessing method. The TRUEX (transuranium extraction) process is further used to coextract the trivalent lanthanides and actinides ions from HLLW generated during PUREX extraction. This method uses CMPO [*N,N*-diisobutylcarbamoymethyl) octylphenylphosphineoxide] (compound 1) intermixed with TBP (tributyl phosphate) as a synergistic agent. However, the final separation of trivalent actinides from trivalent lanthanides still remains a challenging task.

In TRUEX nitric acid solution, the Am (III) ion is coordinated by three CMPO molecules and three nitrate anions. Taking inspiration from this data and previous work with calix [ligand 4] arene systems (compounds 2 and 3), researchers on this project have developed a  $C_3$ -symmetric tris-CMPO ligand system 4 using a triphenoxymethane platform as a base. The triphenoxymethane ligand systems have many advantages for the preparation of complex ligand systems. The compounds are very easy to prepare. The steric and solubility properties can be tuned through an extreme range by including different alkoxy and alkyl groups such as methoxy, ethoxy, *t*-butoxy, methyl, octyl, *t*-pentyl, or even *t*-pentyl at the *ortho*- and *para*-positions of the aryl rings. The new extractants also exhibit much higher selectivity for the actinide thorium over all of the lanthanides in comparison to other multi-CMPO ligands as

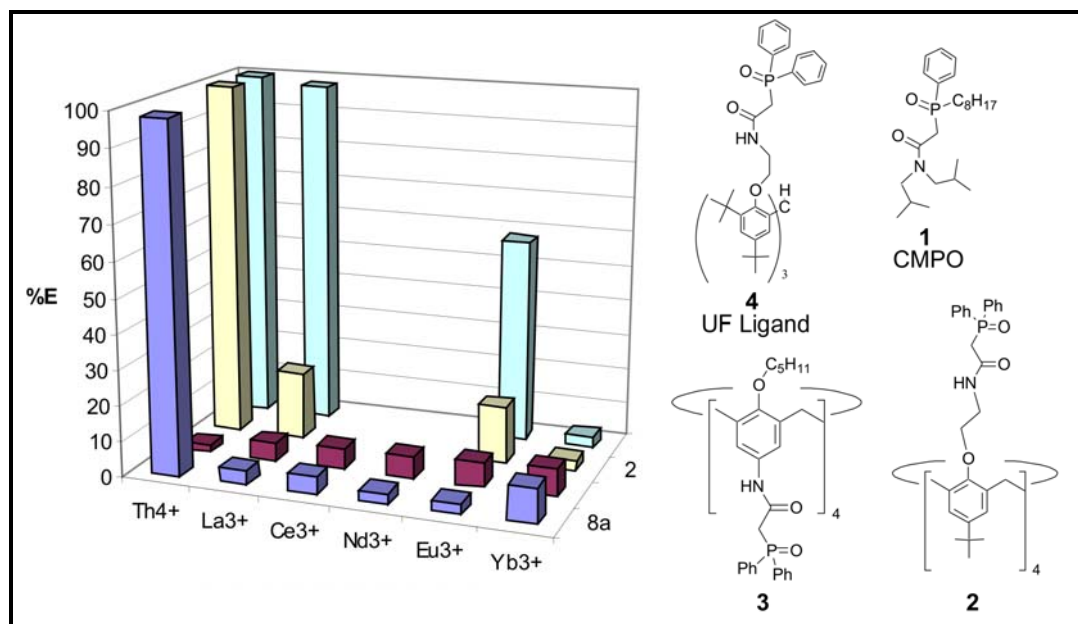


Figure 1. Percentage of metal ions extracted from nitric acid by ligands 1 (CMPO), 2, 3, and the UF compound 4.

well as CMPO itself. It shows considerable promise as improved extractants for actinide recoveries from high-level liquid waste and for general clean-up operations. The design and synthesis of that tris-CMPO ligand system has focused on combining high distribution coefficients for the selected metal ions, high ion selectivity, and great stability toward hydrolysis in acidic media.

The separation of the light actinides (Th, U, Pu, and Np) can be achieved by exploiting the oxidation states of these 5f elements. Since results of the extraction experiments have proven the ability of ligand 4 to take advantage of differences in oxidation states of tetravalent thorium and a series of trivalent lanthanides, researchers on this team were prompted to study the extraction of radioactive metal ions. The Pu (IV) extraction experiment was performed at Argonne National Laboratory to verify the ability of the tri-CMPO scaffold to preferentially extract other tetravalent light actinides. Ligand 4 was found to be very effective in extracting Pu (IV) at the earlier presented conditions—significantly more effective than a commercially used mixture of mono-CMPO and (TBP) in TRUEX process. In fact, much lower concentrations of ligand 4 were required to achieve approximately the same distribution ratio ( $D$ ) of Pu (IV) that the mono-CMPO extractant (with synergistic

agent) can attain. After 24 hours of extraction, the 97.76 percent ( $D = 43.60$ ) of Pu (IV) was removed from aqueous phase by ligand 4 at extractant concentrations as low as  $10^{-3}M$ . To reach similar  $D$  value, the concentration of CMPO molecule 1 in organic phase needs to be *two hundred* times higher than ligand 4. In addition, the CMPO system requires copious amounts of coextractant (1.0M TBP). Thus, derivatives of ligand 4 may have great utility for the removal of An (IV)

atoms since the binding ability is significantly enhanced and efforts to refine the ligands for this purpose are underway.

Quantum mechanics calculations have predicted that the degree of covalency in the Am-S sulfur bonds in the Cyanex-metal complex is higher than the corresponding Eu-S bonds. This subtle difference allows for a partitioning of the two metal ions. Unfortunately, Cyanex cannot be used at very low pH; hence, the ligand is not ideal to extract actinides from acidic solutions. Researchers have designed procedures to replace the P=O donors with P=S donors, as depicted in Figure 2. During the fourth quarter, researchers examined the properties of this ligand in Gainesville. Upon complex formation with Am (III), the increased interactions with the *three* sulfur donor should significantly enhance the ability of the ligand to discriminate between Am (III) and Ln (III) ions in acidic solutions. Researchers have isolated in high yield, and are undertaking an initial examination of the binding properties.

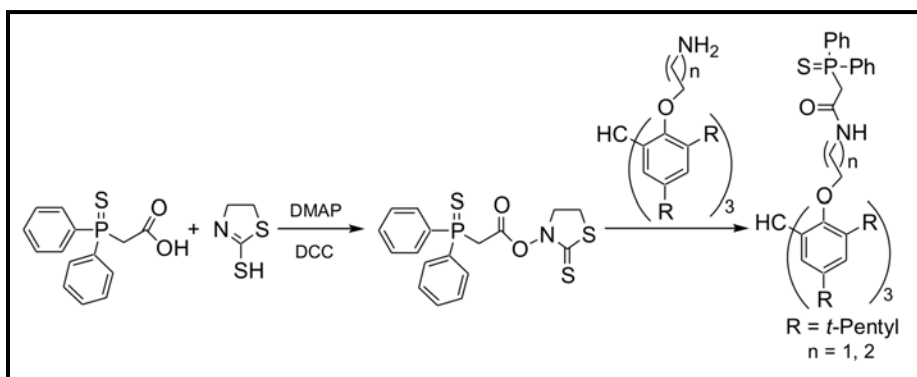


Figure 2. Procedure for the preparation of C3-symmetric CMPS derivatives.

Researchers have taken efforts to substitute the N-H groups with a simple methyl group, since this change in ligand 4 should greatly enhance the solubility of the ligand. In addition, the alkylation will increase the hardness of the carbonyl oxygen donor and enhance the binding affinity for actinides. Researchers found that an unusual synthetic pathway was an effective method to prepare the new ligand in reasonable yield. As predicted, the compound is much more soluble in non-polar solvents in comparison to ligand 4. During the next quarter, researchers will prepare the complex in large scale and delineate the binding properties.

### **Planned Activities**

The tris-CMPO ligand system developed at the University of Florida shows promise as an improved extractant for both tetravalent and trivalent actinide recoveries from high-level liquid wastes and as a general actinide clean-up procedure. The selectivity of the standard extractant for tetravalent actinides, CMPO, was markedly improved by the attachment of three CMPO-like functions onto a

triphenoxymethane platform. The results clearly demonstrate a cooperative action of these three ligating groups within a single molecule, confirmed by composition and structure of the extracted complexes. The use of such an extractant permits the extraction of the metal ions highly acidic environments through the ability of the compound to buffer the effect of high acid concentration. Stability toward hydrolysis and ease of synthesis and purification are additional favorable properties. The tris-CMPO and tris-CMPS ligands are not only easily available in large quantities but also amenable to nearly unlimited chemical modifications. Ligand refinement and testing is constantly pursued at the University of Florida, while the Am (III) binding properties are studied at Argonne National Laboratory. Based on the results from the experiments at Argonne, the Florida group refines the ligands to enhance the binding properties. The continued cooperation between the two organizations should produce an advanced extraction process for separating the chemical similar actinides and lanthanides found in acidic nitrate nuclear waste streams.





# NUCLEAR ENERGY RESEARCH INITIATIVE

## Improving the Integrity of Coated Fuel Particles: Measurement of Constituent Properties of SiC and ZrC, Effects of Irradiation, and Modeling

PI: Lance L. Snead, Oak Ridge National Laboratory

Project Number: 02-131

Collaborators: Idaho National Engineering & Environmental Laboratory

Project Start Date: September 2002

Project End Date: September 2005

### Research Objectives

The main goal of this project is to develop the techniques for evaluating the physical properties of all constituents of the fuel and using these data in a realistic, complex stress model using finite element techniques. Additionally, this project will generate fundamental data on the effects of irradiation on the thermo-mechanical properties of ZrC, which will allow researchers to directly compare the SiC and ZrC systems using updated modeling techniques. It is anticipated that the understanding gained from this experimental and modeling work will lead to the development of a more robust fuel pebble.

### Research Progress

Researchers on this project have made considerable progress in developing techniques for measuring mechanical properties of coated fuel components. The team has established all theoretical bases, experimental setups, and data analysis (statistical analysis) methods for two evaluation techniques for miniature tubular and ring specimens. The first technique is an internal pressurization method, in which tubular specimens are internally pressurized by the axial compression of incompressible plastic inserts (polyurethane rod). The second method is the ring crush test, in which ring specimens, or short tubes, are compressed by a dia-

metrical load. Researchers investigated the size effects in the tensile hoop strength of alumina using the developed testing and evaluation techniques and Weibull statistical theory, as shown in Table 1. They analytically calculated stress distributions for the two loading methods, which were used to evaluate the failure strength from measured failure load and to evaluate effective volume and effective area for each specimen type. The failure strength displayed significant size effect; the mean strength of the smallest specimens was about 70 percent higher than that of the largest specimens, as shown in Figure 1. Using Weibull analysis, researchers also predicted similar size effect when the effective area-based method was applied.

Researchers are fabricating a batch of surrogate fuel in the High-Temperature Materials Laboratory using the hemispherical pressurization techniques. This fuel is for irradiation and mechanical testing. Researchers have

Series Name	Loading Method	Specimen Dimensions, mm			# of Specimens
		I.D.	O.D.	L	
0.51L	Internal pressurization	0.51	0.787	2.361	24
0.51E	Internal pressurization	0.51	0.787	3.148	25
0.51F	Internal pressurization	0.51	0.787	4.722	22
1.02SM	Internal pressurization	1.016	1.981	1.981	21
1.02M	Internal pressurization	1.016	1.981	3.962	24
1.02LM	Internal pressurization	1.016	1.981	5.943	21
2.39SM	Internal pressurization	2.388	3.175	3.175	21
2.39MM	Internal pressurization	2.388	3.175	6.35	27
2.39LMM	Internal pressurization	2.388	3.175	9.525	15
2.39LM	Internal pressurization	2.388	3.175	9.525	22
6.35SM	Internal pressurization	6.35	9.5	9.5	21
6.35MM	Internal pressurization	6.35	9.5	19	18
6.35LM	Internal pressurization	6.35	9.5	28.5	16
1.02S*	Diametral loading	1.016	1.981	1.981	21
2.39S*	Diametral loading	2.388	3.175	3.175	21
6.35S*	Diametral loading	6.35	9.5	9.5	18

Table 1. Specimen dimensions and loading method.

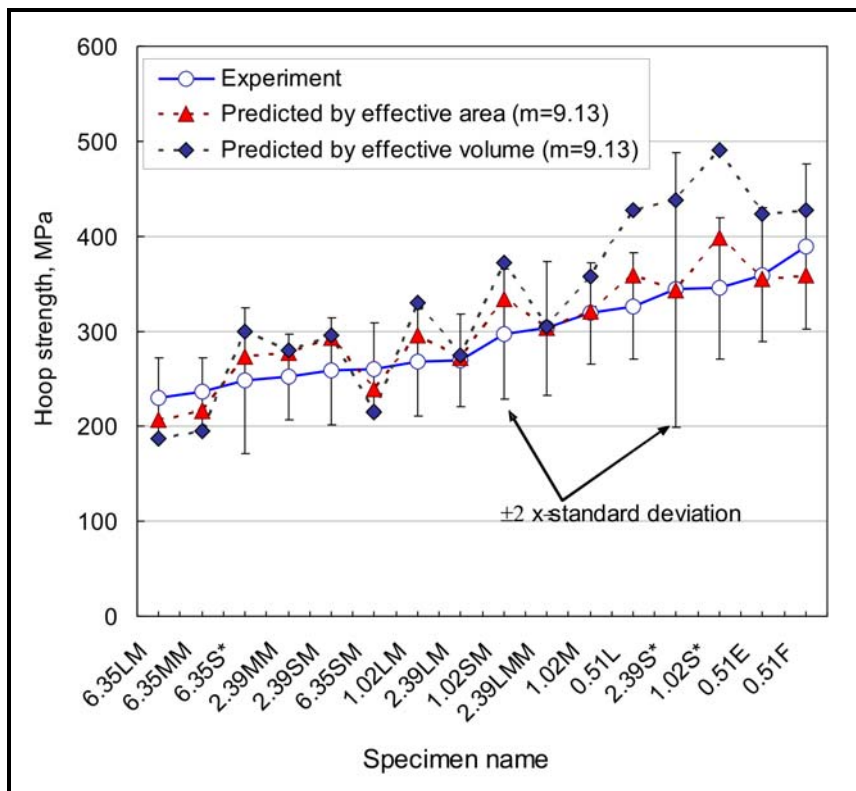


Figure 1. Size effects in the failure hoop strength of alumina specimens.

carried out metallography to ensure high-quality, crack-free coatings and to determine if the grain size is uniform. They are also fabricating tubular SiC specimens using graphite cores of various diameters suspended in the fluidized bed. The team successfully produced hemispherical SiC shell specimens from the surrogate fuel particles by grinding the fuel particles to hemispheres and burning out carbon layers by annealing at 950°C for an hour.

Finally, researchers have carried out an extensive review of the irradiation-effects database for Chemically Vapor Deposited (CVD) SiC to identify the data-needs (i.e., holes) in support of the handbook effort. Many of the data deficiencies in the Combustion Engineering-General Atomics (CEGA) report can be adequately addressed either by data recently (over the past several years) published in the open literature or by further testing of material already irradiated. Specifically, by the end of this project, researchers should completely map density, thermal conductivity, elastic modulus, and strength information for stoichiometric bulk CVD SiC.

## Planned Activities

In search of a method to measure more direct strength data from the pieces of SiC layer from tri-coated isotropic (TRISO) fuel particles, researchers have pursued an internal pressurization technique for hemispherical shell specimens. The team expects to complete development work for the pressurization technique in 2004.

Researchers will prepare specimens from surrogate fuel for baseline tests; some of these will be carried into an irradiation program. The irradiation capsules will be high flux isotope reactor (HFIR) rabbit capsules, which will be irradiated in the 0.1-10 dpa range in a range of temperatures from 600-1,300°C. Moreover, monolithic SiC, SiC shells, and zone-refined ZrC specimens will be irradiated separately in the mapping elevated temperature swelling (METS) core capsules. The METS capsules are made up of three HFIR in-core vehicles, which will be irradiated up to 10 dpa at 600-1,500°C.

Researchers will examine the irradiated samples to determine density, elastic modulus, brittle-ring and internal pressurization strength, and irradiation creep properties.

Finally, the research project team will perform a finite-element structural analysis using the PARFUME integrated fuel performance model and the newly generated non-irradiated and irradiated materials data. These data will also be compiled and published in a Materials Property Handbook.

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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Enhanced Thermal Conductivity Oxide Fuels

PI: Alvin Solomon, Purdue University

Project Number: 02-180

Collaborators: Framatome ANP

Project Start Date: September 2002

Project End Date: September 2005

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### Research Objectives

The objective of this project is to develop a processing methodology to enhance the conductivity of light water reactor (LWR) oxide fuels by incorporating a high-conductivity solid phase that is stable and compatible with  $\text{UO}_2$  and Zircaloy, that does not impose significant neutronic penalties, and that is commercially realizable. The approach selected is to produce sintered  $\text{UO}_2$  fuel with open interconnected porosity, and to impregnate this fuel with a ceramic precursor using a process called polymer impregnation and pyrolysis (PIP) to form a stable, interconnected, high-conductivity phase. The thermal properties of the improved fuel will be measured by thermal diffusivity coupled with specific heat determination. The research is bolstered by theoretical and experimental studies of structural/chemical stability of the two-phase structure, thermal property correlations, and finite element heat transfer codes to optimize the microstructure (fraction of high-conductivity phase, spacing, scale, and pore structure), and to obtain thermal responses of the optimized structures to steady-state and transient reactor conditions.

### Research Progress

The results of the team's analytical thermodynamic studies show that the reactions between SiC and  $\text{UO}_2$  at temperatures approaching  $1,400^\circ\text{C}$  and above depend on the release of gaseous species CO and SiO. The research group performed equilibration experiments with  $\beta$ -SiC and sintered high-density  $\text{UO}_2$  to verify these reactions and characterize the reaction products and degree of the reaction for various times. The reaction product under these conditions was a uranium silicon phase, probably  $\text{USi}_{1.67}$ , previously reported in the literature. Scanning Electron Microscopy (SEM) examination after processing PIP specimens at temperatures above  $1,400^\circ\text{C}$  showed only interdiffusion of carbon into the  $\text{UO}_2$  to form a uranium oxycarbide and a uranium carbide phase, leaving a Si-rich species behind.

Published experiments show stability between SiC and  $\text{UO}_2$  to temperatures at least in excess of  $1,800^\circ\text{C}$  in sealed containers. Therefore, researchers on this project fabricated a special set of nested  $\text{Y}_2\text{O}_3$  crucibles to allow evacuation around the specimens, but to restrict the escape of SiO and CO. However, compatibility experiments using the nested crucibles did not completely eliminate reactions. Therefore, the team is restricting processing temperatures to below  $1,350^\circ\text{C}$  until better containment conditions are obtained using capsules or barrier methods. As a backup effort, they are considering the alternative of BeO as the conductive phase, which is stable in contact with  $\text{UO}_2$  to approximately  $2,100^\circ\text{C}$ , and the same thermal conductivity as SiC. Researchers have obtained Be and BeO powders to investigate several methods of producing the interconnected high-conductivity phase. Organic precursors do not exist with sufficiently high Be concentration to make this approach feasible. Initial experiments using Be have shown some promise in forming a conductive phase of BeO.

Researchers used ANSYS, a finite element code, to study the fuel pin steady-state and transient thermal behavior to determine the maximum centerline temperatures and times for transient conditions for various assumed microstructures, SiC conductivity, and interfacial barriers. They will also use the code for sensitivity and optimization studies. They are beginning to develop indices of performance, like the temperature difference across the pin, for various structures.

The PIP processing activity has advanced on several fronts. Using a special apparatus and methodology, researchers on this project have determined the necessary evacuation times for specimens of various porosities or in various stages of infiltration. Also, they have measured the impregnation times for specimens in various stages of pore filling. As a corollary, they measured the viscosity of the precursor as a function of temperature, both before and after degassing. The viscosity agrees with the data supplied by the vendor at room temperature, but there are

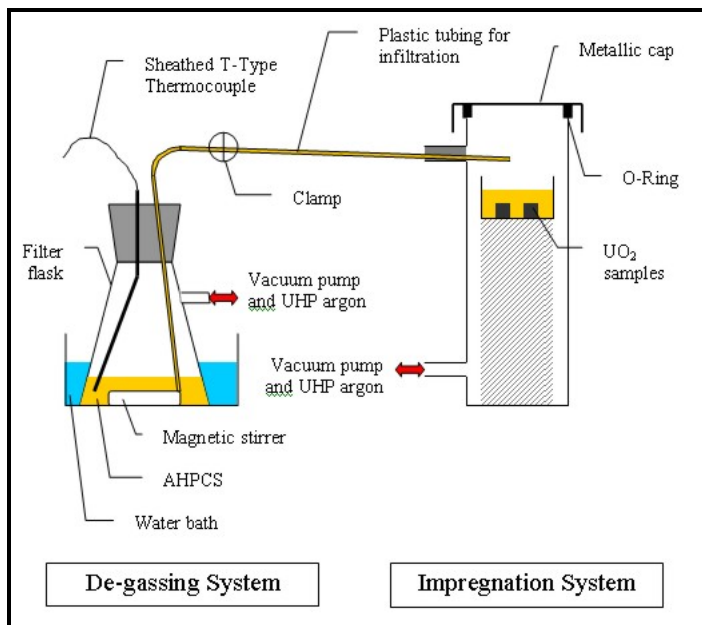


Figure 1. Degassing/impregnation system for porous  $UO_2$  pellets.

important reductions at the degassing temperature that the team uses to improve impregnation.

Researchers have constructed a new evacuation/impregnation system, shown in Figure 1, that is able to achieve a much greater vacuum than previous systems (15 millitorr), and is able to handle specimens of various geometries. Using this new system, they have performed impregnations, pyrolysis, and up-to-the-second crystallization. They have determined that, in general, each impregnation/pyrolysis cycle fills approximately 30 percent of the available porosity. With their previous impregnation system, they found mercury intrusion porosimetry, that the porosity is "closed" after six PIP cycles. The number of cycles may be reduced with the new system. They also found that dispersions of  $\beta$ -SiC of 1  $\mu m$  do not appear to penetrate the specimens—even during the first infiltration. For this method to be effective, finer particles are needed.

Researchers used optical and scanning electron microscopy to characterize the impregnated samples. This showed there is excellent penetration of the precursor into the porosity of  $UO_2$ . Researchers on this project are concerned about possible thermal barriers between the  $UO_2$  and the SiC. Experiments are in progress to quantify the possible thermal barriers. Thermal conductivity measurements will, of course, be definitive. The researchers are still waiting for their initial specimens to be measured at Cadarache, but they are starting to fabricate specimens for thermal diffusivity and specific heat measurements at Purdue's Thermophysical Properties Research Laboratory (TPRL).

Two patent applications have been filed on the PIP processing methodology applied to fuels, and abstracts have been submitted to two U.S. meetings (American Ceramic Society and LWR Fuel Performance Meeting).

## Planned Activities

The finite element modeling of the two-phase fuel has shown that the ANSYS model yields good agreement with closed form solutions for simple series and parallel heat paths. Researchers used the model to perform sensitivity analyses for various SiC densities, which showed modest improvements in thermal conductivity. However, radiation improved the situation. On the negative side, the question of thermal contact barriers between the two phases needs to be addressed. Researchers are experimentally planning to examine this by creating a SiC thin layer between  $UO_2$  pellets. Another issue for SiC as the conductive phase, are possible reactions during safety-related transients. If the temperatures remain above approximately 1,400°C for long periods, reaction is expected in an "open" system. That is why other investigators are attempting to enclose  $UO_2$  in a SiC-sealed container. Researchers on this project are examining whether the same can be easily achieved with the PIP process. They plan to examine the kinetics of the reactions at the higher temperatures compared to the time/temperature histories for loss-of-coolant accidents.

In the processing area, the researchers plan to continue fabricating and characterizing PIP samples ceramographically, with Hg porosimetry, and with thermal property measurements. They will characterize the thermal conductivity of the matrix phase by producing specimens with only matrix phase using SiC powders as the "framework" for the precursor, i.e., by impregnating SiC powders. They will use a thermogravimetric analysis system at Argonne National Laboratory to examine the decomposition of the precursor with temperature. They need to better identify the actual reaction products between SiC and  $UO_2$  using x-ray diffraction, energy dispersive analysis, and/or electron microprobe. Efforts will be made to produce better encapsulation for higher temperature crystallization. The researchers have ordered closed-ended SiC tubes that will be sealed in a tight-fitting hole in graphite. They are examining sealing methods using PIP processing, and evaluating whether PIP SiC coatings can be effective barriers to the  $UO_2$ /Zircaloy reaction, so that higher fuel ratings are possible.

Work will progress in the neutronics area at Framatome ANP to offset the loss in  $UO_2$  volume with enrichment. If some success is obtained with BeO processing, the research team will include this in its neutronics calculations.

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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Use of Solid Hydride Fuel for Improved Long-Life LWR Core Designs

PI: Ehud Greenspan, University of California-Berkeley

Project Number: 02-189

Collaborators: Massachusetts Institute of Technology, Westinghouse, University of Tokyo (at no charge to DOE)

Project Start Date: September 2002

Project End Date: September 2005

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### Research Objectives

The general objective of this project is to assess the feasibility of improving the performance of the light water reactor (LWR) by using solid hydrides as one of the core constituents. Following is a list of potential improvements:

- Increasing the core life, discharge burnup, total energy generated per fuel load, and the capacity factor of LWR. Expected outcomes are reducing the fuel cycle cost and cost of electricity (COE), increasing fuel utilization, reducing the amount and toxicity of high-level waste, and improving proliferation resistance.
- Reducing the volume of the core and pressure vessel for a given power LWR, or increasing the power level of a given volume core, thus reducing the COE.
- Increasing the capability of LWR to recycle commercial plutonium and to dispose of military plutonium.
- Increasing the capability of LWR to utilize thorium.
- Improving the safety of LWR, due to the inherent negative temperature reactivity effect of hydride fuel, and improving the safety of the boiling water reactor (BWR), by reducing of the negative void reactivity coefficient.
- Reducing the heterogeneity of BWR cores and the negative void coefficient of these cores to simplify the fuel assembly design and the reactor control system, thereby improving the BWR economics.

### Research Progress

In this project, researchers performed neutronic and thermal-hydraulic parametric studies of pressurized water reactor (PWR) unit cells using U-ZrH<sub>1.6</sub> hydride fuel—like the fuel used in TRIGA research reactors. The independent design variables of the parametric studies include fuel rod diameter, lattice pitch-to-diameter (p/d) ratio, uranium enrichment, and coolant mass flow rate.

Following is a list of the constraints imposed in the study:

- There is a fuel peak steady-state temperature limit of 700°C for ZrH<sub>1.6</sub> based fuel.
- The coolant inlet and exit enthalpy are the same as for the reference PWR.
- The maximum coolant velocity will not exceed 8 meter per second and the core pressure drop will not exceed 4.14 bars.
- The minimum departure from nucleate boiling ratio (MDNBR) is comparable to that for the UO<sub>2</sub> fueled reference PWR.
- The core height and diameter are fixed.

Among the assumptions are the following:

- Liquid metal bonding is used to reduce the fuel-clad gap thermal resistance, accommodate fuel swelling, and provide a barrier against free hydrogen inside the fuel rod from interacting with the Zircaloy clad used in the reference PWR; the gap and the clad thickness scale linearly with the fuel diameter.
- The axial and radial core power distributions are the same as in the reference PWR.

Figure 1 shows a sample of burnup dependant infinite-multiplication-factor ( $k_{\infty}$ ) results obtained from the neutronic parametric study for fuel using 10 percent enriched uranium. Similar results were generated for 5 percent and 7.5 percent enrichment. Researchers observed that the p/d dependence of the hydride fuel  $k_{\infty}$  is significantly flatter than that of the reference oxide fuel. They also observed that the hydride fuel lattice  $k_{\infty}$  peaks at lower values of p/d and that the discharge burnup of hydride fuel corresponding to its peak  $k_{\infty}$  (at p/d of approximately 1.2) is comparable to that of the reference oxide fuel lattice (corresponding to p/d = 1.33 denoted by the dashed vertical line).



Regarding reactivity coefficients, the coolant temperature coefficient of reactivity of the hydride fuel lattice at a p/d of approximately 1.2 is significantly less negative than that of the reference oxide fuel lattice. However, the extra prompt negative temperature coefficient of hydride fuel, due to the temperature increase of the hydrogen in the fuel, more than compensates for the reduced coolant temperature coefficient. With erbium burnable poison, the magnitude of the fuel hydrogen temperature coefficient is comparable to the doppler effect of the reference oxide fuel lattice.

The number of fuel rods of a given diameter that can be packed into a given core volume with a lattice p/d of 1.2 is approximately 20 percent higher than with the reference p/d = 1.33 lattice for the same fuel diameter. Thermal-hydraulic analysis shows that the peak hydride fuel temperature in a PWR core designed to operate at 120 percent of the reference oxide fuel power is 580°C—well below the temperature limit.

Researchers performed a parametric study to determine the optimum combination of lattice pitch, rod diameter, and channel shape—further referred to as geometry—for maximizing power in existing pressurized water reactors loaded with U-ZrH<sub>1.6</sub> fuel subjected to four constraints: MDNBR, core pressure drop, flow velocity, and maximum fuel temperature. It was found that square and triangular channels of equivalent rod diameter and hydrogen-to-heavy metal ratio performed similarly.

Figure 2 gives the maximum achievable power as a function of the hydrogen-to-heavy metal (H/HM) atom ratio and of the fuel rod diameter. The geometry providing the highest power was found to have a H/HM ratio of 13.7, a pitch of 9.5 mm for a square array of 10.2 mm for a triangular array, and a rod diameter of 7 mm. Within the confines of an existing PWR core, U-ZrH<sub>1.6</sub> fuel arranged in this geometry can safely operate at nearly 150 percent of the existing PWR power level.

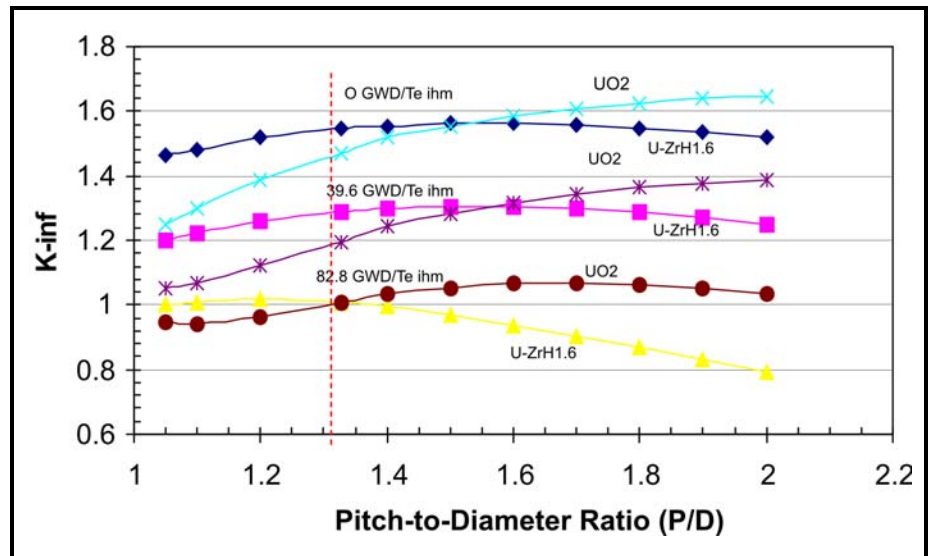


Figure 1. Comparison of  $k_{\infty}$  of hydride fuel versus oxide fuel at selected burnup levels as a function of the square lattice p/d. Uranium is enriched to 10% <sup>235</sup>U.

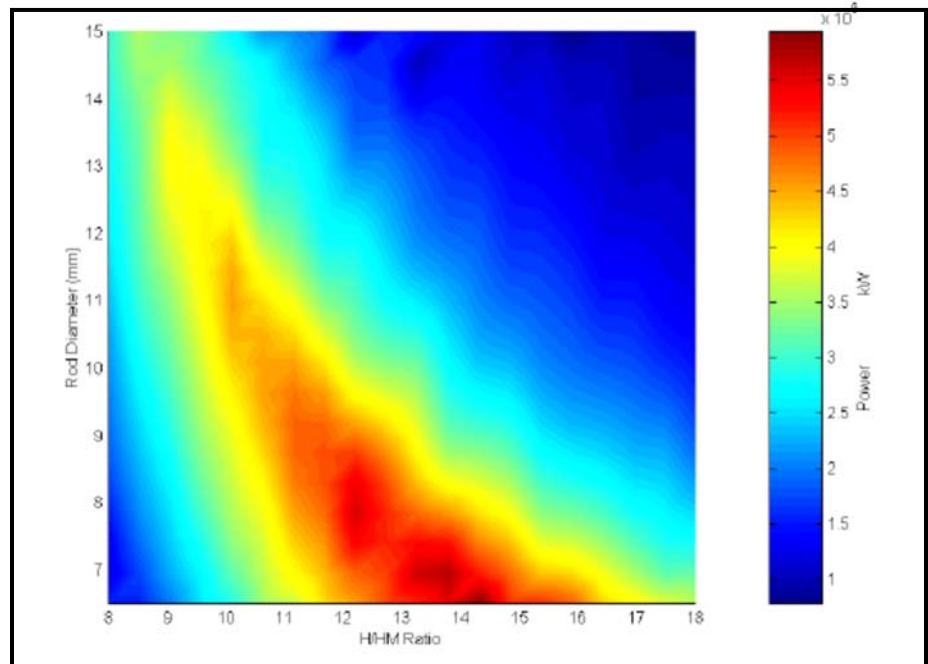


Figure 2. Maximum power attainable from a PWR core of given dimensions subjected to the thermal-hydraulic constraints. Reference core power is 3,800 MW<sub>e</sub>.

## Planned Activities

Subsequent work will narrow the acceptable technical performance domain of fuel rod diameter and lattice pitch by imposing additional constraints introduced by safety considerations (notably, negative coolant temperature reactivity coefficient) and by fuel integrity considerations. Researchers will use the FRAPCON code to determine maximum fuel rod life derived from internal pressure buildup, clad creep down, and thickness of external clad corrosion layer. Team members will also carry out a detailed vibration analysis to set a limit on the acceptable coolant

flow velocity as a function of the fuel rod diameter and lattice pitch. They will then perform an economic analysis to identify the core design within the acceptable technical performance domain that offers the lowest COE when capital, operation, maintenance, and fuel cycle costs are considered simultaneously. Researchers will compare the COE of hydride fuel PWR with the COE of oxide fuel PWR in order to evaluate the possible benefits of transferring from oxide into hydride fuel. Researchers will also compare the performance of the optimal hydride with that of the optimal oxide fuel PWR core.

They will perform similar analyses for PWR fueled with other types of hydride fuels, including U-ThH<sub>2</sub>, Pu-ZrH<sub>1.6</sub>, and Pu-ThH<sub>2</sub>. This will be followed by analysis of possible benefits from use of hydride fuel in BWR.





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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Development of Advanced Methods for Pebble-Bed Reactor Neutronics: Design, Analysis, and Fuel Cycle Optimization

PI: Abderrafi M. Ougouag, Idaho National Engineering and Environmental Laboratory

Project Number: 02-195

Collaborators: Georgia Institute of Technology, Pennsylvania State University, PBMR (Pty.) Ltd., and University of Arizona

Project Start Date: October 2002

Project End Date: September 2005

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### Research Objectives

This project is a comprehensive effort to develop analysis methods for pebble-bed reactors (PBRs). These methods are based on modern analytical nodal methods for solving neutron diffusion equation. They are also based on efficient techniques for node homogenization, which are incorporated into (or tightly interfaced with) the Idaho National Engineering and Environmental Laboratory's (INEEL) PEBBED code for pebble bed reactor (PBR) neutronics and fuel cycle analysis. The most novel aspect of this effort is that researchers are developing these analytical nodal methods for three-dimensional cylindrical geometry—a development that had not previously been accomplished because of mathematical obstacles encountered in the traditional approach. In prior work, the investigators found a way around these obstacles. The principal objective of this project is to implement that advance.

Researchers can apply the analytical nodal solutions of the diffusion equation either directly or in the framework of an existing finite-difference code in the coarse-mesh finite-difference (CMFD) approach. In the CMFD approach, researchers modified the seven-point difference equation for the node-averaged neutron fluxes in the original finite-difference code using correction coefficients to force the fluxes to contain the required nodal information. Researchers further modified the original code to incorporate the equations required for computing these correction coefficients.

The tasks in this project include an assessment of whether to apply the CMFD approach or to apply the nodal solution directly. PEBBED will also be provided with additional enhancements, such as a genetic algorithm to

facilitate design optimization. The techniques for node homogenization that will be implemented in the PEBBED system are based on recent advances at the Georgia Institute of Technology, one of the collaborators in this project. Furthermore, techniques developed at the Pennsylvania State University (Penn State), another collaborator, to account for the dependency of reaction cross sections on thermohydraulic feedback will also be implemented in PEBBED.

### Research Progress

In earlier work, researchers at INEEL developed the PEBBED code. As originally written, the code applied traditional finite-difference techniques to solve the neutron diffusion equation; but, it was organized in a modular form. This modular form allows researchers to incorporate upgrades in any physics area in which improvements become available. It was always intended that the finite-difference diffusion solver would be replaced or augmented by the new nodal method developed at INEEL.

Early in the project, researchers decided to apply the nodal solution through the CMFD approach, which uses the existing finite-difference framework as explained above. The first step in this approach was to derive the modified difference equation with correction coefficients and to obtain the solution for the correction coefficients from the nodal expressions for the fluxes and currents. This step has been accomplished. Next, researchers coded these mathematical constructions into PEBBED. Currently, the modified code is undergoing debugging and quality assurance.

In a parallel effort, researchers are implementing the nodal approach in a stand-alone code that does not couple the flux solution to the motion of fuel in a pebble-bed reactor. This code, called CYNOD, will be a general-purpose nodal diffusion solver in cylindrical geometry for reactor problems that do not involve the complication of moving fuel. CYNOD is adapted from PEBBED by removing portions of PEBBED that pertain to moving fuel. Researchers have completed this adaptation except for the nodal diffusion solver itself. For CYNOD, researchers decided to implement the nodal solution directly instead of through the CMFD approach. Furthermore, they discovered a new approach to the solution for the azimuthal variable, which was chosen for the direct nodal implementation. This approach was sought because the original solution involves the computation of a series of hyperbolic Bessel functions, which requires excessive computer time. If this direct approach is successful, it will also be used in PEBBED.

For optimization of PBRs, researchers must compare various core dimensions, pebble types, and pebble recirculation patterns. The PBR fuel management problem is different than in light water reactors (LWRs) because the fuel moves, the fuel elements are small, and fueling is essentially continuous. Little work had been performed previously in this area.

Genetic Algorithms (GAs) are a stochastic method recently applied to LWR fuel cycle optimization. As the name implies, GAs mimic the biological process in which traits coded as genes are passed on to future generations. A "net" is cast over the domain of parameter variations, and an objective function is evaluated at points in the net. Points that yield the highest values of this function have attributes re-combined and passed to the next generation of trials. After each generation, the net is reduced about the subdomain showing evidence of a global maximum.

Genetic algorithms are naturally applied to optimizations involving discrete variables. In LWR fuel management, there are finite numbers of locations and orientations for each fuel assembly. Given the steady refueling in the PBR, it would be better to use an algorithm for continuous variables. Under this NERI project, researchers are developing such an optimization feature and adding it to PEBBED to perform design studies. Researchers have developed and implemented a preliminary version of this capability. They tested this feature by applying it to studies of the PBR version of the next generation nuclear plant (NGNP), a

very-high-temperature reactor proposed for siting at the INEEL. Application of the algorithm facilitated the design of passively safe PBR cores of much higher power output than previously thought possible (i.e., up to 700 megawatts of thermal power).

When generating PBR cross-section libraries, it is very important to model the spectrum dependence. The assumption made in the LWR cross-section generation and modeling methodology that the neutron spectrum within a fuel assembly is dominated by the material composition and burnup of the assembly is not valid for the small PBR fuel spheres and the graphite moderation environment. The spectrum within a PBR fuel sphere is mostly determined by the material compositions and burnup of surrounding spheres. The first consequence of this is that the cross sections have to be generated using a reactor model or a color-set calculation rather than single assembly calculations (as traditionally done in the PWR case). The second consequence is that the cross sections should be represented as a function of some spectral parameter such as the leakage or buckling. Penn State has developed an approach that will be provided to the INEEL in two software packages:

- a) The first package automatically generates a microscopic cross-section library for a given PBR core model using an available PBR cross-section generation code. This library contains sets of microscopic 4-D cross-section tables for each composition. Users can specify the ranges of the feedback parameters as well as the number of reference points and the reference points themselves. Once this information is selected, it is stored at the beginning of the cross-section library. The information is read by PEBBED together with the reference cross section values. The library contains tables for transport, absorption, fission, production, and scattering cross sections.
- b) The second software package reads the tables and interpolates within them to obtain microscopic cross-section values for each spectral zone (core region) and for each broad energy group. This package interacts with the PEBBED code in the following way: first, the cross-section library is read once at the beginning of the calculation and stored in the PEBBED arrays. During the calculation process for each spatial mesh (node) of the PEBBED core model, four parameters

representative of this node are passed to the feedback module. Using these values, researchers then interpolate the four-dimensional tables for the appropriate microscopic cross section values. The updated microscopic cross sections are passed back to PEBBED to determine the new macroscopic cross sections and perform core calculations. The interpolation process is schematically illustrated in Figure 1.

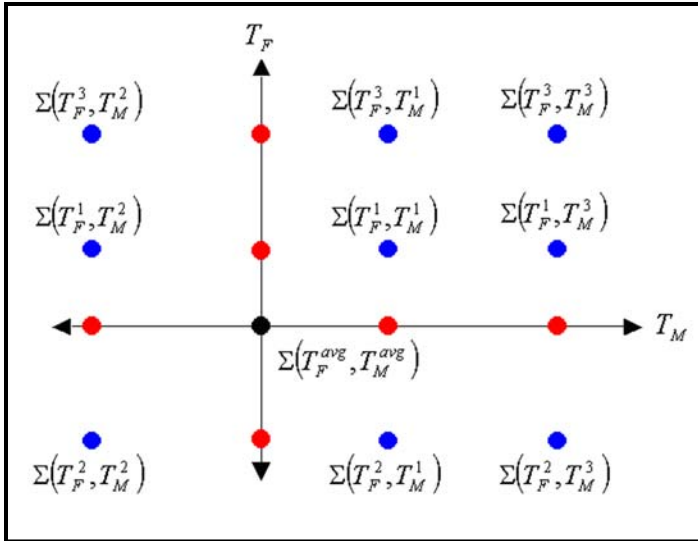


Figure 1. Multi-dimensional table cross-section representation.

## Planned Activities

In the remaining two years of the project, three principal tasks will be pursued. The first is to complete the coding, verification, and validation of the cylindrical geometry nodal solvers (both CMFD and stand-alone traditional nodal method). The second is to develop a nodal depletion capability in cylindrical geometry and incorporate it into the PEBBED code. The third is to finalize the development of the genetic algorithm optimization capability, including completion of testing and quality assurance. In parallel, supporting developments at Georgia Institute of Technology (Georgia Tech) and Penn State will continue. At Georgia Tech, research will focus on developing methods (and codes) to incorporate the depletion history effects into the PEBBED code. These effects will include spectral corrections. At Penn State, research will continue improving parametrization of the various feedback effects, with an emphasis on thermohydraulic applications and on more advanced mathematical methods. The new methods will be benchmarked against the latest design of the South African Pebble-Bed Modular Reactor (PBMR), and then they will be applied to two optimization problems: fuel cycle planning and nonproliferation.



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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## 8. Fundamental Nuclear Sciences

This element includes 12 NERI projects of which 1 was awarded in FY 2000, 5 in FY 2001, and 6 in FY 2002. It addresses the long-term R&D goals of developing new technologies for nuclear energy applications, of educating young scientists and engineers and training a technical workforce, and of contributing to the broader scientific and technological enterprise.

Today's U.S. reactors, which are based largely on technology from the 1970s, operate under close supervision in a conservative regulatory environment. Although the knowledge base is adequate for these purposes, improvements in the Nation's knowledge base and reduction of the inherent uncertainties concerning nuclear reactors could bring cost savings to current reactor operations and reduce the costs of future reactors. They could also enable innovative designs that reduce the need for excessively conservative and costly safety and reliability factors, and significantly extend safe operating lifetimes. Future reactor technologies are likely to involve higher operating temperatures, advanced fuels, higher fuel burn-up, longer plant lifetimes, better materials for cladding and containment vessels, and alternative coolants. To implement such features, substantial research must be carried out in fundamental science and engineering to supplement applied research on individual promising design concepts. Such fundamental research need not and should not be

directed to any specific design. Although motivated in part by the need for new nuclear reactor system designs, the research would also have a far-reaching impact elsewhere in engineering and technology.

The five broad topics identified in the Nuclear Energy Research Advisory Committee (NERAC) *Long-Term Nuclear Technology R&D Plan* related to fundamental nuclear sciences include the following:

- Environmental effects on materials, in particular the effects of the radiation, chemical, and thermal environments, and aging.
- Thermal fluids, including multiphase fluid dynamics and fluid structure interactions.
- The mechanical behavior of materials, including fracture mechanics, creep, and fatigue.
- Advanced material processes and diagnostics.
- Reactor physics.

Projects currently selected under this element include R&D in fundamental science in the fields of material science, chemical science, computational science, nuclear physics, or other applicable basic research fields. Selected research subjects include irradiation, chemistry, and corrosion effects on nuclear plant materials; advanced new materials research; innovative computational models; and the investigation of nuclear isomers that could prove beneficial in civilian applications.

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# NUCLEAR ENERGY RESEARCH INITIATIVE

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# NUCLEAR ENERGY RESEARCH INITIATIVE

## Isomer Research: Energy Release Validation, Production, and Applications

PI: John A. Becker, Lawrence Livermore National Laboratory

Project Number: 00-123

Collaborators: Los Alamos Scientific Laboratory

Project Start Date: September 2000

Project End Date: February 2004

### Research Objectives

The overall goal of this applied nuclear isomer research program is the search for, discovery of, and practical application of a new type of high energy density material (HEDM). Nuclear isomers could yield an energy source with a specific energy as much as a hundred thousand times as great as that of chemical fuels. The researchers on this project are working in 4 focus areas: x-ray induced decay of the  $^{178m}\text{Hf}$  isomer in the low-energy range (8–20 keV) of incident x-ray energy, a measure of the atomic-nuclear mixing matrix element in  $^{189}\text{Os}$ , the development of Superradiance and Stimulated Emission in crystals rich in isomeric nuclei, and an investigation of the  $^{229}\text{Th}$  doublet. Researchers have initiated a feasibility study of an experiment to validate the existence of the low-lying ground-state doublet in  $^{229}\text{Th}$  (3.5 eV), beginning with more precise determination of the doublet energy. The 3.5 eV level is isomeric, with a lifetime that depends on the chemical environment. The exceptionally low energy of this nuclear state offers the possibility of pumping a nuclear state with a laser beam in the laboratory.

The team formed a collaboration comprised of staff from DOE National Laboratories and, as required, obtained beam time and carried out experiments at DOE National Laboratories to fulfill these objectives. These experiments required the unique resources available at the National Laboratories.

### Research Progress

#### Task A: Isomer Energy Release on Demand.

Researchers completed two experiments to verify the reported X-ray-induced decay of the 31-yr Hf-178 isomer. The first experiment focused on the incident X-ray region between 20 and 60 keV, while the second experiment examined incident X-ray energies below 20 keV. Each experiment established an upper limit for X-ray-induced emission of isomeric Hf-178 many orders of magnitude

below previously reported work, with the upper limit from the second experiment  $\sigma_{x\text{-ray}} < 10^{-26} \text{ cm}^2\text{-keV}$  for  $E_x \sim 6.5$  keV. The results of the two experiments are illustrated in Figure 1. Three important points regarding these results follow:

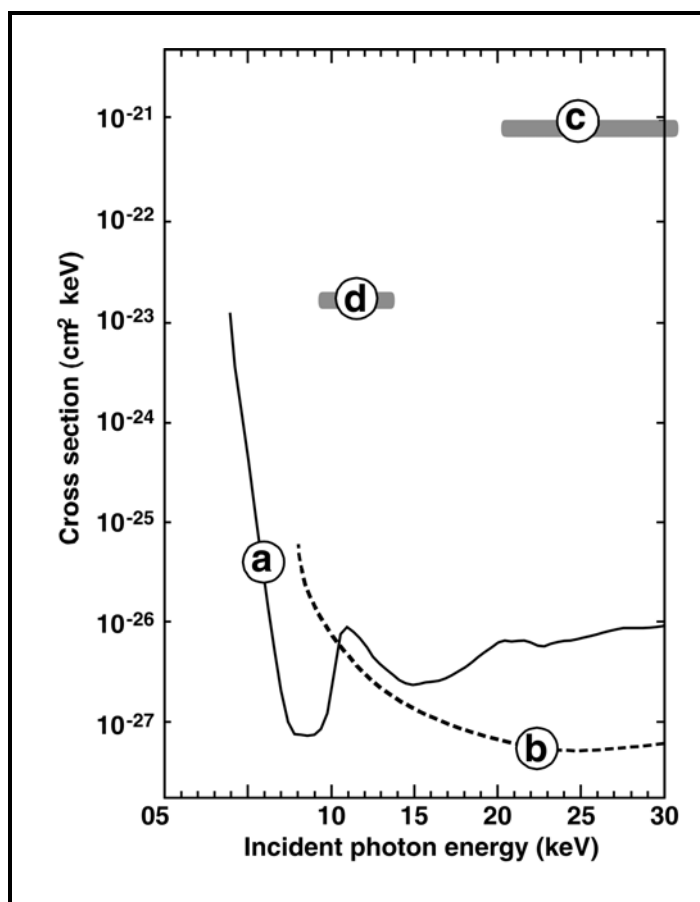


Figure 1. Upper limit of the integrated cross section for x-ray-induced decay of the 31-y Hf-178 isomer for incident energies  $6 < E_x(\text{keV}) < 30$  deduced from Ahmad, et al. Phys. Rev. C 67, 041395(2003) [a]. Earlier results are given for comparison: [b] Ahmad, et al. Phys. Rev. Lett. 87, 072503 (2001) [c] Collins, et al., Phys. Rev. Lett. 82, 695(1999), and [d] Collins, et al. Europys. Lett. 57, 677 (2002). See also preliminary results reported in H.E. Roberts, M. Helba, J. J. Carroll, J. Burnett, T. Drummond, J. Lepak, R. Propri, Z. Zhong and F.J. Agee, Hyp. Interact. 143, 111 (2002).

- The results of the two experiments conducted by a collaboration with Argonne National Laboratory (ANL), Lawrence Livermore National Laboratory (LLNL), and Los Alamos National Laboratory (LANL) are completely consistent.
- The upper limits quoted are valid for induced decay modes whether or not the supposed triggered decay mode proceeds through the 4-second isomer or bypasses it. This point does not seem to be well recognized.
- The upper limits presented in Figure 1 are consistent with known physics.

Researchers completed work on an analytic model of isomer energy release, which explores the conceptual engineering features of isomer energy supply systems (UCRL-ID-155561). Isomer power supply systems can be designed that will allow a large number of useful time varying power outputs, including constant power, power increasing linearly with time, power output increasing with the square of time, power output that is periodically switched on and off (square wave), and power output that varies with the square of time but is periodically switched off and on. Conceptual isomer energy systems based on super-radiance have very promising properties based on energy gain and power increase/decrease. These systems will require the identification of an appropriate isomer and excitation or de-excitation mode.

Work proceeded slowly on the study of an inverse internal conversion process in  $^{189}\text{Os}$ . The capture of an electron of appropriate energy into an atomic state of He-like  $^{189}\text{Os}$  would resonantly excite a nuclear level at 216.7 keV. This level decays to a 5.7-hour 31 keV metastable nuclear state. The experimental signature of this process is the decay of this metastable state. The effort has been slowed by operational issues with the LLNL Electron Beam Ion Trap (EBIT) in the high-voltage mode, which is required for this experiment.

Researchers have installed a microcalorimeter developed by National Aeronautics Space Administration (NASA) scientists on EBIT, which is operational. The device has superb energy resolution (75 eV at  $E_\gamma = 60$  keV) and it enables a precision measurement of the  $^{229}\text{Th}$  3.5 eV nuclear level to about 0.4 eV. The team has started the preliminary investigation into this measurement. A precision energy measurement is the first step to pumping this nuclear level with a laboratory laser.

**Task B: Coherent Emission.** Researchers on this task have accomplished the synthesis of potassium heptafluoroniobate crystals from an Nb-HF-KF aqueous solution. The needle-like crystals are shown in Figure 2. This procedure has the advantage of a greater chemical yield than epitaxial growth techniques. Crystalline needles of  $\text{K}_2\text{NbF}_7$  were grown from a solution containing 1 mg of Nb and spiked with a small amount of  $^{91\text{m}}\text{Nb}$ . One needle was removed and the activity was measured to estimate the amount of Nb in a typical crystal. The amount of activity found for this crystal was 9.6 percent of the starting activity, which means that the crystal contained approximately 0.096 mg of niobium.



Figure 2. Photomicrograph of potassium heptafluoroniobate.

## Planned Activities

The NERI project has been completed.



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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Random Grain Boundary Network Connectivity as a Predictive Tool for Intergranular Stress-Corrosion Cracking

PI: Mukul Kumar, Lawrence Livermore National Laboratory

Project Number: 01-084

Collaborators: University of Michigan, GE Global Research Center

Project Start Date: October 2001

Project End Date: September 2004

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### Research Objectives

Intergranular stress corrosion cracking (IGSCC) is one of the most pervasive degradation modes in current light water reactor systems (LWR) and is likely to be a limiting factor in advanced systems as well. In structural materials, IGSCC arising from the combined action of a tensile stress, a "susceptible" material, and an "aggressive" environment has been recognized for many years and the mechanisms widely investigated. Recent work has demonstrated that by sequential thermomechanical processing, properties such as corrosion, IGSCC, and creep of materials can be dramatically improved. The improvements have been correlated with the fraction of so-called "special" grain boundaries in the microstructure.

A multi-institutional team comprised of researchers from Lawrence Livermore National Laboratory (LLNL), University of Michigan (UM), and General Electric Corporate Research & Development (GECRD) propose an alternative explanation for these observations: *that the effect of grain boundary engineering is to break the connectivity of the random grain boundary network through the introduction of low energy, degradation resistant twins, and twin variants.* The team is carrying out a collaborative science and technology research project aimed at verifying the mechanism by which sequential thermomechanical processing ameliorates IGSCC of alloys relevant to nuclear reactor applications and prescribing processing parameters that can be used in the manufacture of IGSCC-resistant structures.

In this work, the team is developing methods to quantify the interconnectivity of the random grain boundary network and measuring the interconnectivity of a series of materials where the interconnectivity has been systematically altered. Researchers then perform property measurements on the materials, compare their performance ranking with the boundary network measurements, and characterize the

materials to correlate actual crack paths with the measurements of the random grain boundary network.

With this data, the team will evaluate and improve the methods that have been chosen to describe the random grain boundary network. Researchers will test the characterization method by evaluating the interconnectivity of the random grain boundary network in a series of as-received materials, rank their expected performance, and compare that result with property measurements.

The major accomplishments of this project are expected to be 1) the determination that the random boundary network connectivity (RBNC) is a major driver of IGSCC in low to medium stacking fault energy austenitic alloys, 2) the development of a predictive tool for ranking the IGSCC performance of these alloys, and 3) the establishment of thermomechanical processing parameters to be applied in the manufacture of IGSCC-resistant materials.

The outcome of the project will be identifying a mitigation strategy for IGSCC in current LWR conditions that can then enable the development of economically and operationally competitive water-cooled advanced reactor systems.

### Research Progress

#### Task 1. Preparation of Test Microstructures.

Researchers have reviewed candidate commercial heats of stainless steel and alloy 600 from among those archived at General Electric, and have identified type 304 stainless steel (SS304 [heat AJ9139]) and alloy 600 (heat 3110439) as optimal for this program. The first experimental test material, SS304, was subjected to cycles of sequential thermomechanical processing. Each processing cycle consisted of rolling at room temperature to a reduction of 20 percent and annealing at 1,000°C followed by water quenching. This was repeated up to four times with an

annealing time of 10 minutes in each cycle. The specimens were analyzed first in the as-received state and again after two and four processing cycles. Researchers observed that the processed condition had a lower special fraction than the reference condition, and that the grain size of the as-received condition (26 $\mu$ m) was larger than that on the CSLE sample (18 $\mu$ m). The team performed a further heat treatment after the fourth cycle for an hour at 1,100°C to get a grain size comparable to the as-received condition, with only a marginal effect on the other microstructural parameters. They observed that the alloy condition annealed for 1 hr at 1,100°C; SS304-CSLE+1hr/1,100°C maintained its low special fraction (0.49) with a grain size increase to 36  $\mu$ m. The researchers decided that this condition would be used for testing against the as-received condition. In addition, pieces of stock material in the AR and CSLE+1hr/1,100°C conditions were forged by 20 percent at 140°C at GE, and were tested at the University of Michigan and GE.

The microstructural observations for SS304 from these experiments are shown in the following figures. The random grain boundaries in all cases are in black and the colored boundaries in the background are crystallographically special boundaries. The as-received condition (Figure 1) is to be used as the baseline microstructure, as its properties are well understood. The sample after four

cycles of thermomechanical processing (Figure 2a) and additional heat treatment has a lower fraction of special boundaries as well as a more connected network of random grain boundaries. In addition, a representative from samples that were processed to boost the special fraction is shown in Figure 2b. Further data on the connectivity of grain boundary networks is also included for the two cases, and are shown in Figures 3 and 4.

Inconel 600 has been processed in a similar manner and the comparisons between the as-received and the processed microstructures are given in Figures 5-8. It is evident, both visually and from the data, that the connectivity of the random boundary networks is considerably broken in the processed condition. These samples are undergoing stress corrosion cracking (SCC) testing at both GE and University of Michigan.

### Task 2. Stress Corrosion Cracking Testing.

These research activities were carried out at the University of Michigan and General Electric and focused on determining whether modified grain boundary character distributions resulting from thermomechanical processing influenced the cracking behavior of SS304 under different water chemistry conditions. Researchers performed these experiments using fracture mechanics specimens (0.5T or 1T CT specimens) in sophisticated equipment, which involved precision control and monitoring of water chemistry and corrosion

potential, digital servo-control loading systems under computer control, high-pressure/high-temperature autoclave systems with digital temperature controllers, continuous high-resolution dc potential drop monitoring of crack length, and computer data acquisition and test control.

For this purpose, researchers at UM conducted constant extension rate testing (CERT) of SS304 alloy samples in both the as-received and processed conditions. The alloys used for CERT testing were SS304 in both the as-received, SS304-AR, and thermomechanically processed, SS304-PROC conditions. In addition to these conditions, an AR/PROC pair of samples was forged by 20 percent at 140°C in order to have similar conditions to those tested at GE. These alloy conditions were designated SS304-AR-DEF and SS304-PROC-DEF.

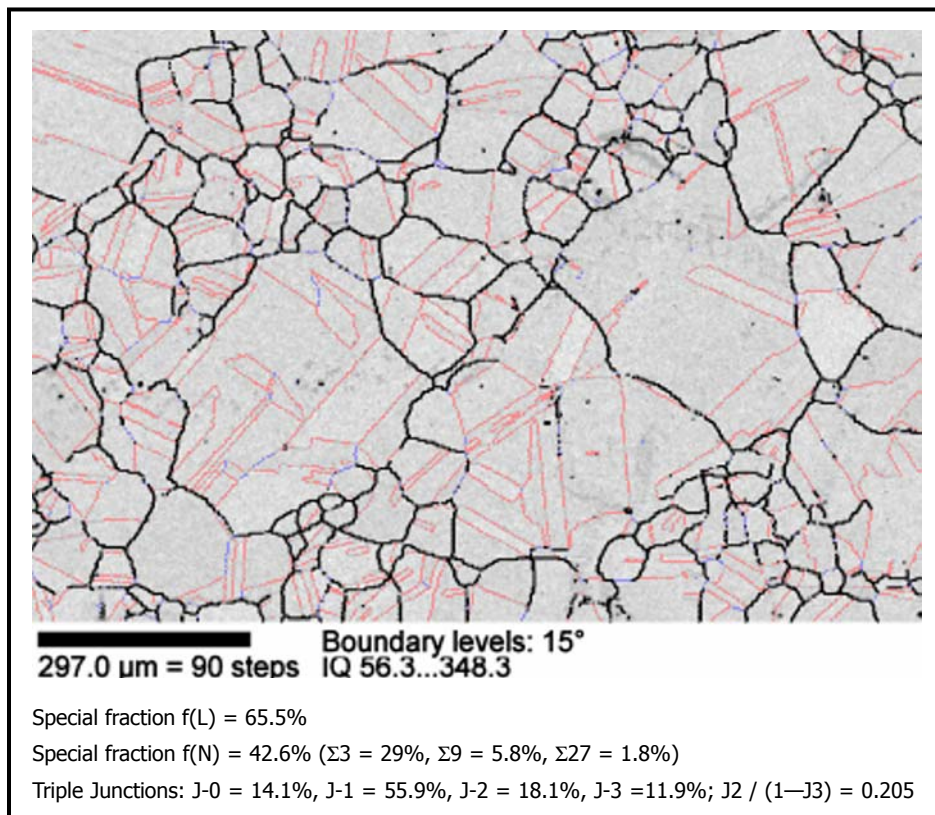


Figure 1. SS304 Series 1 & 2: As-received microstructure.



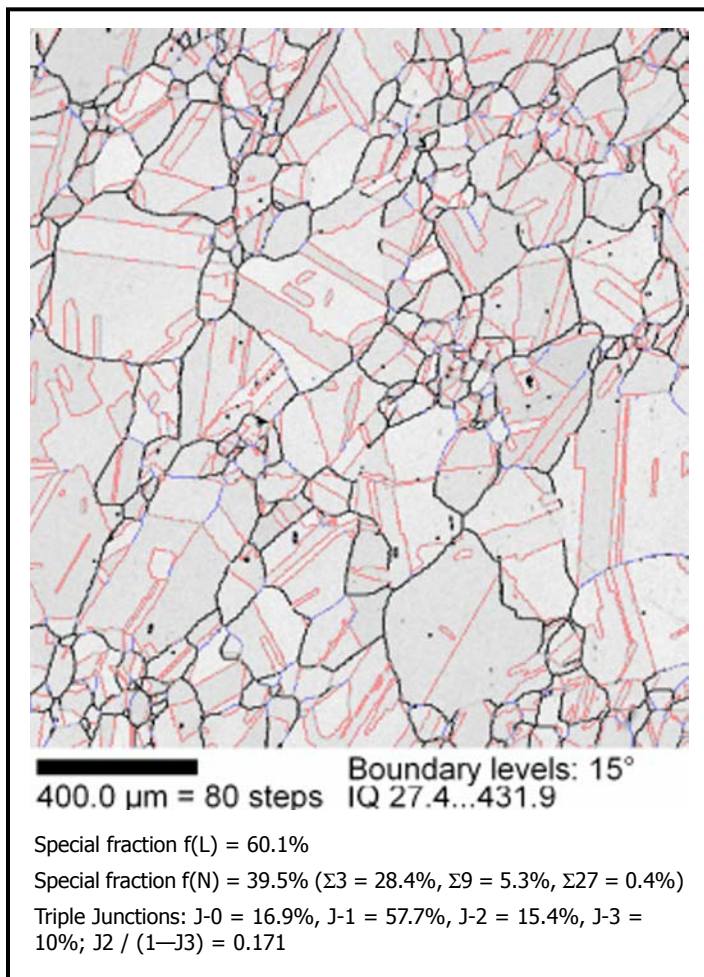


Figure 2a. SS304 Series 1: 4X processed + grain growth HT microstructure.

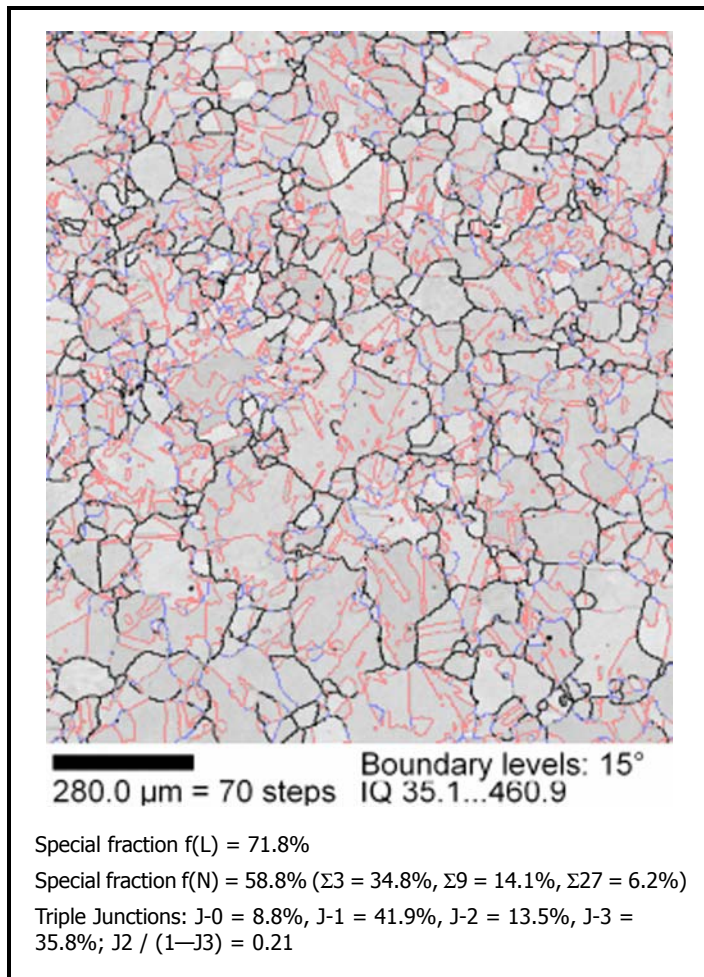


Figure 2b. SS304 Series 2: 4X processed.

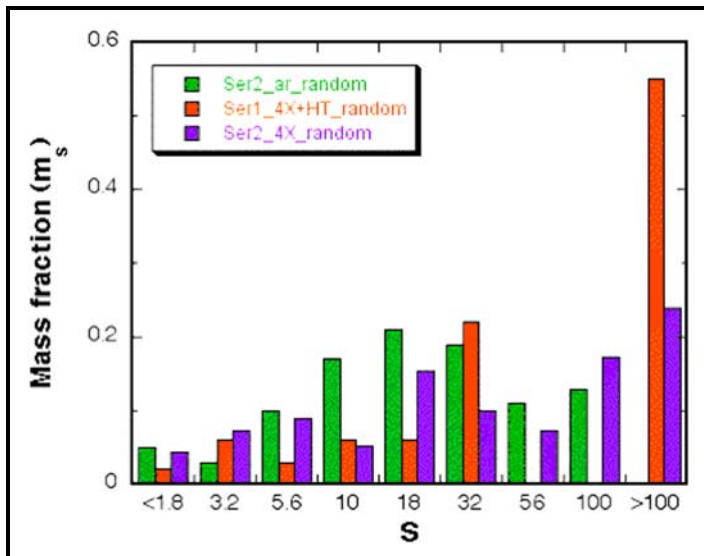


Figure 3. Random cluster mass distributions: As-received vs. processed microstructures (SS304).

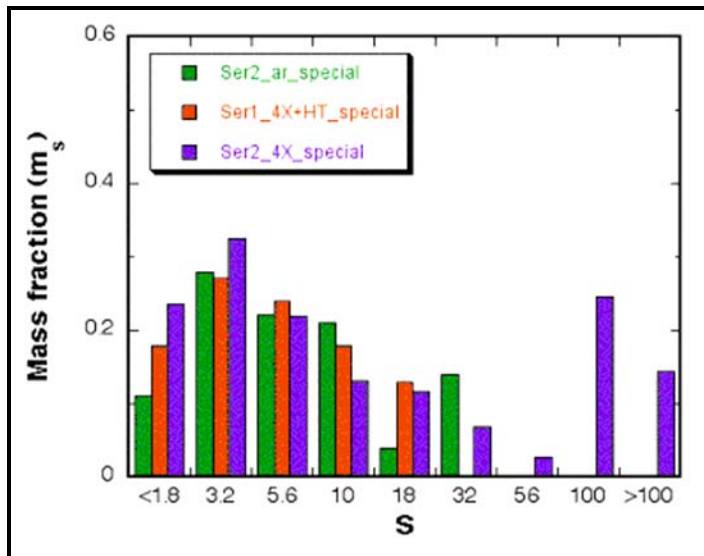


Figure 4. Special cluster mass distributions: As-received vs. processed microstructures (SS304).



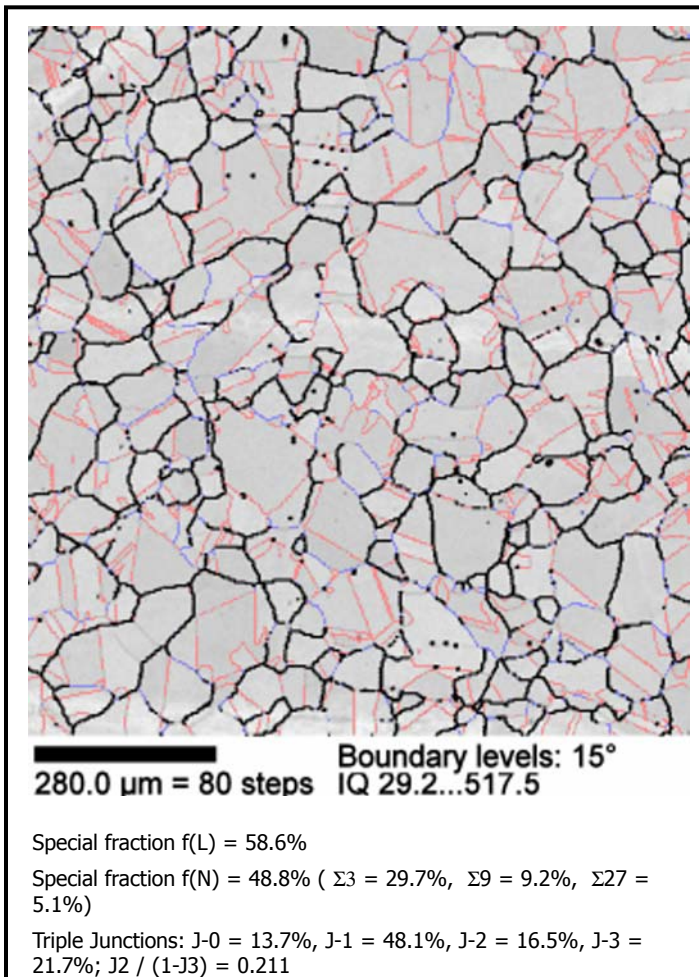


Figure 5. IN600: As-received microstructure.

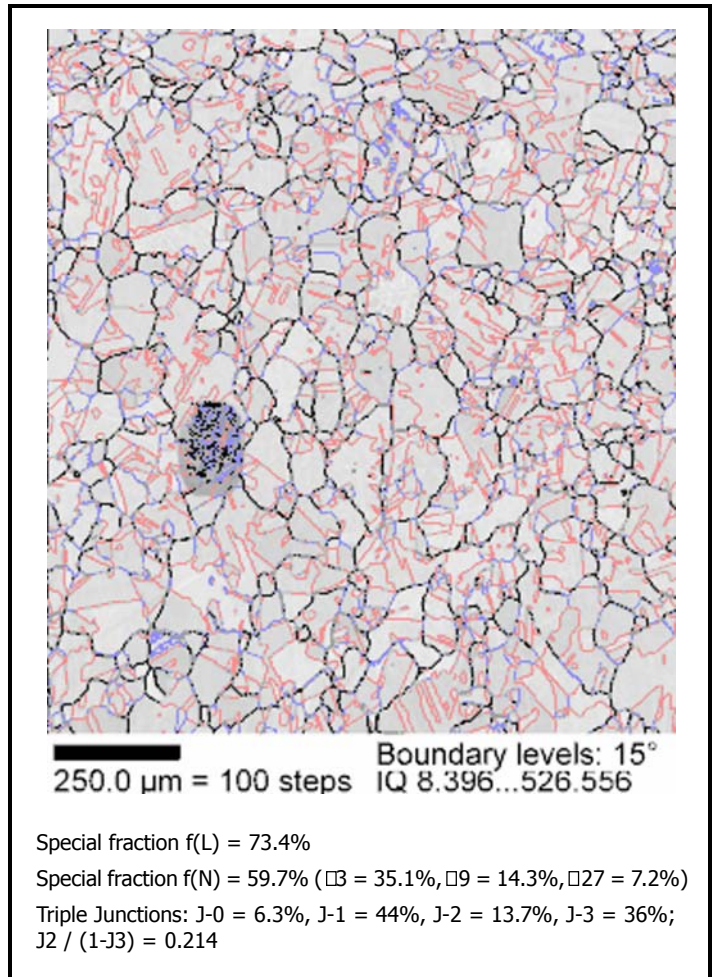


Figure 6. IN600: 4X processed.

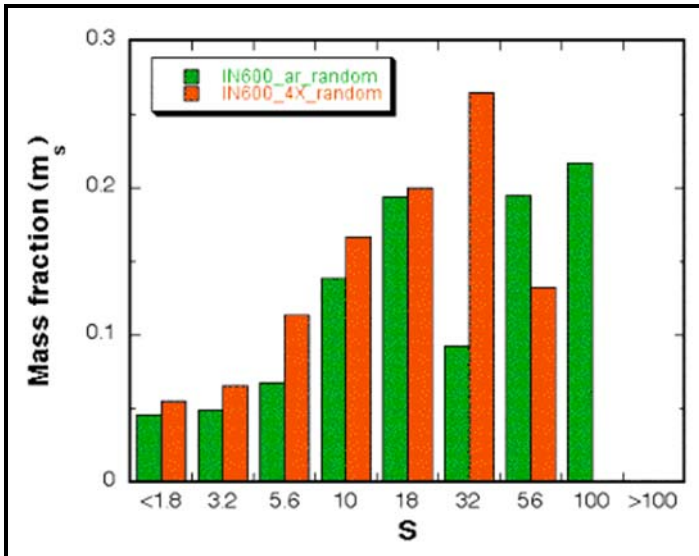


Figure 7. Random cluster mass distributions: As-received vs. processed microstructures (IN600).

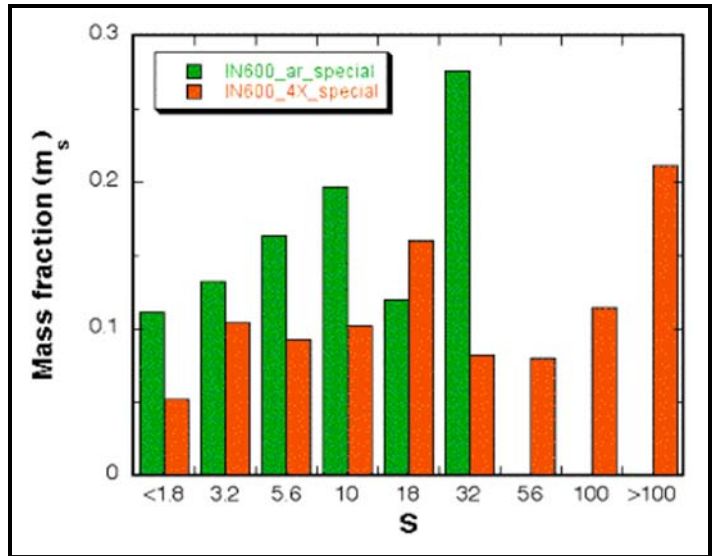


Figure 8. Special cluster mass distributions: As-received vs. processed microstructures (IN600).

The CERT experiment at UM was conducted in a 1.8 liter Korros Data autoclave system. Researchers strained all four tensile specimens simultaneously at an initial strain rate of  $3 \times 10^{-7} \text{ s}^{-1}$ . The testing environment proposed initially was already an oxidizing environment, consisting of high purity water at 288°C, containing 2,000 ppb  $\text{O}_2$ , and at a conductivity of  $0.2 \text{ } \mu\text{S/cm}$ . Nevertheless, SS304 has not been found to be susceptible to cracking in this environment in a non-irradiated condition. Therefore, a somewhat more aggressive environment was chosen for the test at hand: 288°C non-deaerated water ( $\sim 8,000$  ppb dissolved oxygen), and a conductivity of  $0.5 \text{ } \mu\text{S/cm}$ . In addition, straining was stopped twice, for a period of 24 hours at both 6 percent and 8 percent strain to maximize the exposure time under load in the environment, and thus promote cracking. The resulting stress-strain curves from this experiment are shown in Figure 9.

Only three samples reached 20 percent strain. One sample, SS304-PROC-DEF, failed at 8 percent strain. Inspection in the SEM of the EBSD scanned areas revealed that no significant cracking took place in the non-deformed samples in spite of the more aggressive environment. This observation is consistent with previous work on non-irradiated SS304 samples in similar experimental conditions.

On the contrary, the samples forged by 20 percent prior to CERT testing were found to develop cracks on the surface. Fewer than 20 such cracks were observed on the entire surface of either sample, and thus a quantitative measure of cracking propensity by sample condition or boundary type could not be determined for either sample. Nevertheless, the longest crack found on this sample at 20 percent strain allowed for an estimation of the crack growth rate (CGR). As such, the length of the crack measured  $342 \text{ } \mu\text{m}$  after 210 hours of exposure. Assuming that cracking initiated at the beginning of the CERT experiment, the estimated crack growth rate was:

$$\text{CGR}_{\text{SS304-AR-DEF}} \cong 4.52 \times 10^{-7} \text{ } \mu\text{m s}^{-1}$$

The low-CSL, low connectivity SS304-PROC-DEF sample failed after approximately 8 percent strain (Figure 9). Approximately seven cracks were counted on the surface of this sample, mostly in the vicinity of the fracture surface. Cracks in the vicinity of the fracture surface suggested that the failure of this sample might have initiated intergranularly. The fracture surface of SS304-PROC-DEF showed a transgranular fracture mode. However, high magnification images gave some indication of intergranular cracking, mostly near the sample surface.

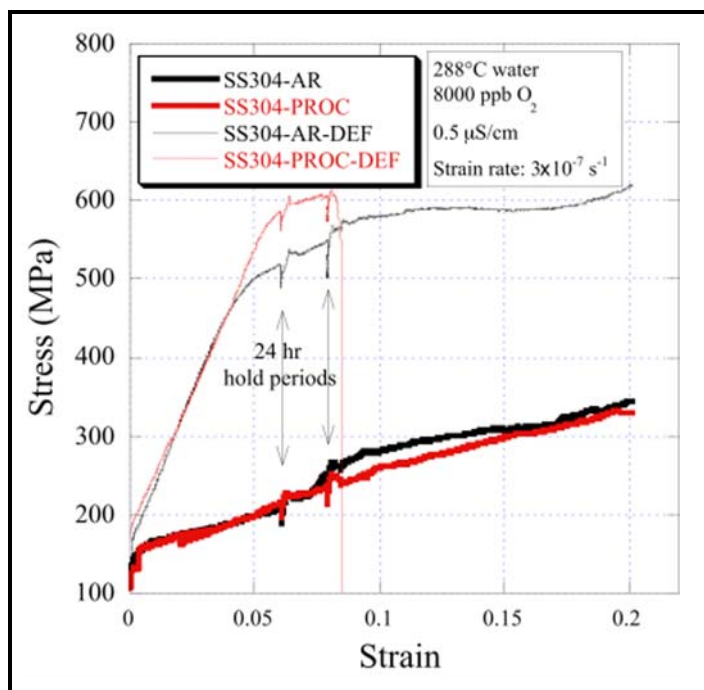


Figure 9. Stress-strain curves for the four samples tested.

Regardless of the failure mechanism, the low-CSL, low connectivity sample failed before its counterpart, SS304-AR-DEF. In the same manner, assuming that cracking initiated at the beginning of the CERT experiment, and considering that this sample lasted for 120 hours, a crack growth rate can be estimated at:

$$\text{CGR}_{\text{SS304-PROC-DEF}} \cong 5.09 \times 10^{-6} \text{ } \mu\text{m s}^{-1},$$

i.e., approximately an order of magnitude higher than that in the SS304-AR-DEF.

The objective of the testing at GE was to compare the SCC growth rate response of the different microstructures (with fatigue pre-cracking) under different water chemistry conditions. The experiments were performed using fracture mechanics specimens (0.5T specimens) in sophisticated equipment involving precision control and monitoring of water chemistry and corrosion potential, digital servo-control loading systems under computer control, high-pressure/high-temperature autoclave systems with digital temperature controllers, continuous high-resolution dc potential drop monitoring of crack length, and computer data acquisition and test control. The data were obtained at  $\approx 25 \text{ ksi/in}$  in 288°C high purity water containing 2,000 ppb  $\text{O}_2$  or 95 ppb  $\text{H}_2$  to represent typical boiling water reactor and pressurized water reactor conditions, respectively.

Figure 10 (a-d) shows a direct comparison between the specimens with a low and high fraction of special grain boundaries under essentially identical conditions of loading and water chemistry. Researchers can see their behavior



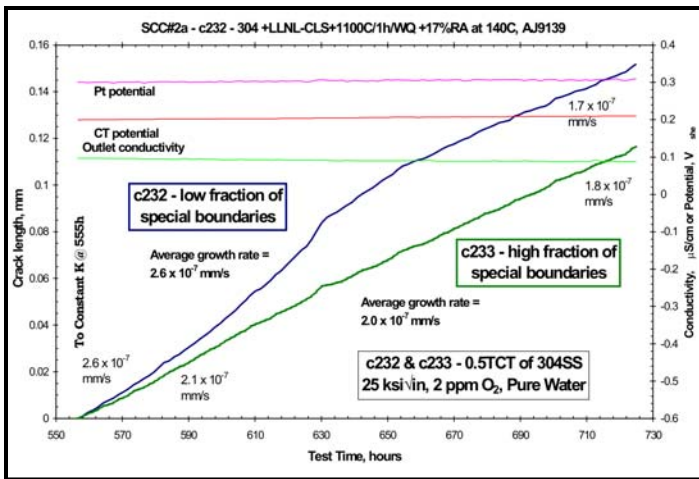


Figure 10a. Comparison of the crack growth rate during the same time period, same water chemistry, and same loading conditions between specimens possessing high and low fraction of special boundaries.

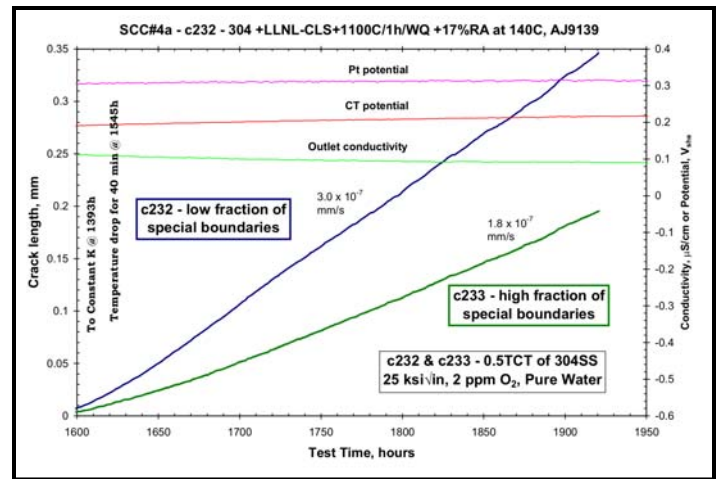


Figure 10b. Comparison of the crack growth rate during the same time period and same water chemistry and loading conditions between specimens possessing high and low fraction of special boundaries.

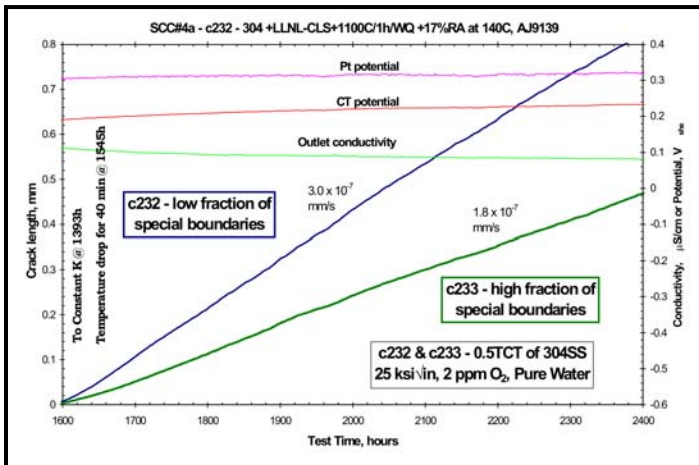


Figure 10c. Comparison of the crack growth rate during the same time period and same water chemistry and loading conditions between specimens possessing high and low fraction of special boundaries.

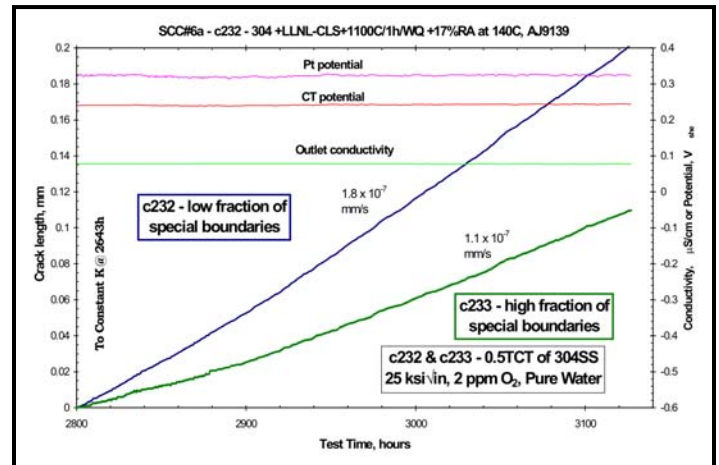


Figure 10d. Comparison of the crack growth rate during the same time period and same water chemistry and loading conditions between specimens possessing high and low fraction of special boundaries.

under constant K conditions in pure 288°C water containing 2,000 ppb O<sub>2</sub>. The crack growth rate for c232 (low fraction of special boundaries or SS304-PROC-DEF) was slightly higher initially, but during the last 100 hours the rates were essentially identical for both specimens. Later in the test, at about 1,400 hours, the crack growth rates for the two specimens were consistently different, although c232 only grew about 50 percent faster than c233 (or SS304-AR-DEF), which is not a large difference.

Later still in the test, the same differentiation between the two specimens was observed (c232 grew approximately 60 percent faster than c233). Near the end of the test, this still held true, with c232 growing about 60 percent faster

than c233. These results are promising in the sense that a higher fraction of special grain boundaries does retard SCC growth. Note also that the observed benefit is consistently increased at low stress intensity factor, which correlates with small crack sizes in plant components. Similarly, a more dramatic benefit is expected on smooth surfaces during the crack nucleation process.

### Planned Activities

Similar IGSCC tests will be performed on alloy 600 in FY04. The microstructural state of these samples has been described in this report.

# NUCLEAR ENERGY RESEARCH INITIATIVE

## Reactor Physics and Criticality Benchmark Evaluations for Advanced Nuclear Fuel

PI: William J. Anderson, Framatome ANP, Inc.

Project Number: 01-124

Collaborators: Sandia National Laboratories, Oak Ridge National Laboratory, University of Florida

Project Start Date: September 2001

Project End Date: August 2004

### Research Objectives

The objective of this project is to design, perform, and analyze critical benchmark experiments for validating reactor physics methods and models for fuel enrichments greater than 5-weight percent  $^{235}\text{U}$ . These experiments will also provide additional information for application to the criticality-safety bases for commercial fuel facilities handling greater than 5-weight percent  $^{235}\text{U}$  fuel. Because these experiments are to be designed not only as criticality benchmarks but also as reactor physics benchmarks, they will include measurements of critical boron concentration, burnable absorber worth, relative pin powers, and relative average powers.

### Research Progress

This project began in September 2001. Year 1, which ran from September 1, 2001, through August 31, 2002, focused primarily on designing the experiments using available fuel; preparing the necessary plans, procedures, and authorization basis for performing the experiments; and preparing for the transportation, receipt, and storage of the unirradiated Pathfinder fuel currently stored at the Pennsylvania State University (PSU).

In Year 1, Framatome ANP, Inc. (FANP), Oak Ridge National Laboratory (ORNL), and Sandia National Laboratories (SNL) designed the proposed experiments and prepared the safety authorization to perform these experiments at the SNL facility.

Work in Year 1 also included the development and submittal of a license application for a shipping package in support of the transportation of fuel from PSU to SNL. On February 10, 2003, the NRC issued the WE-1 Shipping Container Safety Evaluation Report and Certificate of Compliance. The WE-1, which is now approved for shipment of the Pathfinder fuel, is the only known shipping package capable of housing this fuel and licensed to

transport uranium dioxide fuel with enrichments up to 7.5-weight percent  $^{235}\text{U}$ . This major accomplishment required significant technical effort in the form of criticality benchmarking for fuels in the 7.5-weight percent enrichment range and structural design and analysis.

Year 2, which ran from September 1, 2002, through August 31, 2003, was the manufacturing and application phase of this project. Preparation for transportation, receipt, and storage of the Pathfinder fuel continued into Year 2. However, the primary focus of Year 2 was on actual experiments. These tasks included analyzing the proposed experiments using current industry computer codes, shipping the fuel from PSU to SNL, and fabricating fuel rods using the deconstructed Pathfinder fuel for use in the experiments. A code-to-code comparison report analyzing the proposed experiments was issued in February 2003.

Due to delays in the licensing of the shipping package and establishing the necessary paperwork for the shipments, the experiments will not begin until Year 3 of this project. However, the first shipment of fuel was completed on September 12, 2003 (see Figure 1). The remaining nine shipments were completed in November 2003. A total of ten shipments are necessary to move the entire inventory of Pathfinder fuel from PSU to SNL.



Figure 1. Loading pathfinder fuel in shipping container at Pennsylvania State University.

The detailed design of the hardware that is specific to this project is underway. Researchers will use as much of the existing hardware from the recent burnup credit critical experiment (BUCCX) as possible in these experiments. The same core tank and dump tank will be used as well as the Instrumentation and Control system. However, researchers will design and fabricate new grid plates and associated hardware to facilitate the proposed fuel lattice design. New control/safety rods will also be required.

The work on the Authorization Basis (AB) documentation continued through Year 2. The AB must be completed prior to the first critical experiment. Because the schedule for the arrival of the fuel has been stretched, this work is being allowed to proceed more slowly than originally scheduled. This allows late changes in the physical design of the experiment hardware to be incorporated into the first revision of the AB documents.

Researchers will fabricate new fuel elements using the  $\text{UO}_2$  pellets obtained from PSU. They will place the fuel in thin-walled aluminum tubes with a welded aluminum lower end plug. The upper closure will be made with an aluminum plug glued in place with a high-temperature epoxy. Prototypes of candidate upper closure designs have been fabricated and tested. The length of the fuel element cladding is set so that the upper closure is more than 15 cm away from the upper end of the fuel pellet stack to protect the closure during a design basis accident.

Researchers have installed a glovebox in the Hot Cell Facility at SNL to accommodate the disassembly of the Pathfinder fuel elements and the fabrication of fuel elements for the critical experiments. At the end of the project year, the disassembly of a Pathfinder fuel element was underway. Initial efforts to download the fuel have been successful. The cost of removing the fuel pellets from the Pathfinder fuel assemblies will be a significant part of the cost of the project at SNL. Researchers on this project are exploring techniques for efficiently removing the fuel from the assemblies.



Figure 2. Downloaded fuel pellets from a pathfinder fuel assembly.

This project also involves evaluating typical fuel-processing operations to determine the limits and restrictions required for fabricating higher-enriched fuel. The University of Florida is considering the following: 1) storage and handling of uranium hexafluoride ( $\text{UF}_6$ ), 2)  $\text{UF}_6$  processing to powder, 3)  $\text{UO}_2$  powder handling and storage, 4)  $\text{UO}_2$  pellet production, 5) fuel-pellet handling and storage, 6) fuel-rod processing and storage, 7) fuel-assembly processing and storage, 8) fuel-assembly transportation, and 9) on-site fuel assembly storage.

To date, the fuel cycle analysis has focused on the fuel cycle beginning at the shipment of  $\text{UF}_6$  to a fuel fabricator where the  $\text{UF}_6$  is converted into  $\text{UO}_2$ . The University of Florida analyzed wet processing of  $\text{UF}_6$  (ADU) and considered the dry conversion process (IDR) including the kiln, calciner, and sintering furnace. The calciner proved to be the limiting process. Calculations show that the current calciner containing 5-weight percent  $^{235}\text{U}$  reached the 0.95  $k_{\text{eff}}$  limit under accident conditions. The calculations demonstrated that the kiln would be limited to approximately 8-weight percent  $^{235}\text{U}$  without modifications, and the current sintering furnace results show that the furnace would be limited to approximately 12-weight percent  $^{235}\text{U}$ .

## Planned Activities

The remaining activities planned through the end of this project include:

- Transporting the remaining Pathfinder fuel elements to SNL.
- Downloading the Pathfinder fuel.
- Re-fabricating the fuel into shorter, aluminum-clad fuel rods.
- Procuring the remaining hardware.
- Performing the experiments.
- Analyzing the experiments using industry methodology.
- Documenting the experiments.
- Evaluating and documenting the experiments for inclusion in the International Handbook of Evaluated Criticality Safety Benchmark Experiments.
- Completing the analysis of the generic fuel-cycle.
- Documenting the results of the fuel-cycle scoping analysis.



# NUCLEAR ENERGY RESEARCH INITIATIVE

## Fundamental Understanding of Crack Growth in Structural Components of Generation IV Supercritical Light Water Reactors

PI: Iouri I. Balachov, SRI International

Project Number: 01-130

Collaborators: VTT Industrial Systems, Finland

Project Start Date: August 2001

Project End Date: August 2004

### Research Objectives

The objective of this project is to develop a fundamental understanding of corrosion and stress corrosion cracking (SCC) behavior of alloys in supercritical water. Theoretical and experimental results of this project will aid in international efforts to select structural materials for supercritical light water reactors (SCWRs). This NERI project uses a unique combination of two advanced materials characterization techniques 1) controlled distance electrochemistry (CDE) and 2) fracture surface topography analysis (FRASTA) to meet the objective as follows:

- **Alloy screening.** In-situ characterization of the oxide films formed on candidate structural materials allows researchers to rank materials according to their susceptibility to general and localized forms of environmentally assisted degradation.
- **Understanding basic phenomena.** Kinetic parameters of the charge and mass transport processes in the metal/oxide film/supercritical water system are derived from in-situ oxide film studies to understand and quantify the rate controlling processes and, eventually, the fundamentals of metal oxidation phenomenon at supercritical temperatures.
- **Providing a basis for development of new alloys.** Integration of the in-situ experimental information on oxide film resistance to charge and mass transport for alloys of various

composition with fracture surface analysis and current theoretical understanding of the relationship between properties of the oxide films and stability of materials is expected to aid in material selection and in the development process by providing recommendations on chemical compositions of the alloys depending on their expected locations in the reactor (or more specifically, depending on the local temperature and oxidizing conditions).

### Research Progress

Following is a summary of the major accomplishments during the first two years:

- Researchers designed and built a test system for parallel electrochemical and fracture mechanics studies in supercritical water (Figure 1).



Figure 1. General view of the experimental system: supercritical test reactors and high-temperature loop, low pressure loop, and data acquisition system.

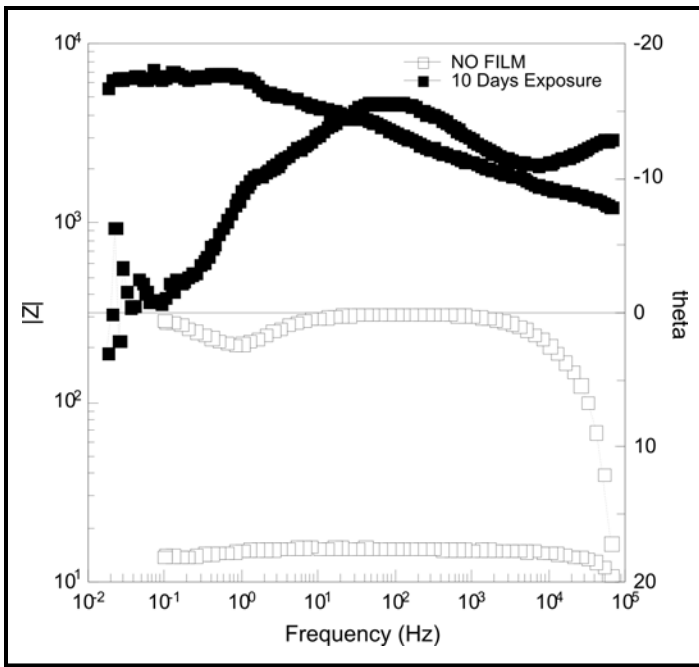


Figure 2. Evolution of the measured impedance spectra with formation and growth of the oxide film.

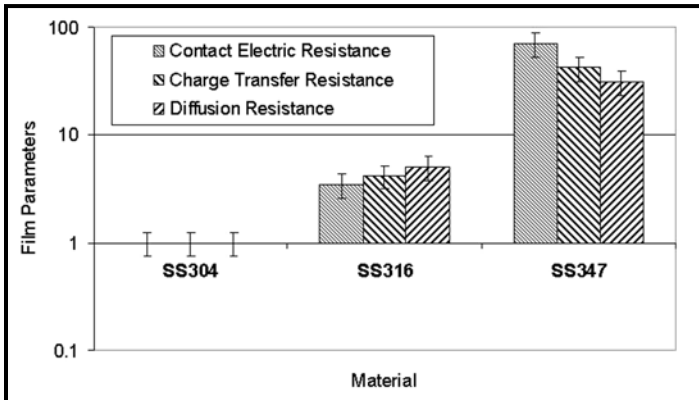


Figure 3. Transport properties of the oxide films on austenitic steels relative to SS304.

- Researchers have been using a test system for more than a year for obtaining continuous in-situ information on the film formation and growth (Figure 2) and on the rates of charge and mass transport processes in the oxide films formed on candidate structural materials in supercritical water.
- Researchers have obtained systematic experimental data on the charge and mass transfer properties of the oxide films on austenitic steels.
- From CDE measurements, researchers determined kinetic parameters of the charge and mass transfer processes in the oxide, which are in good agreement with independent results obtained at VTT.

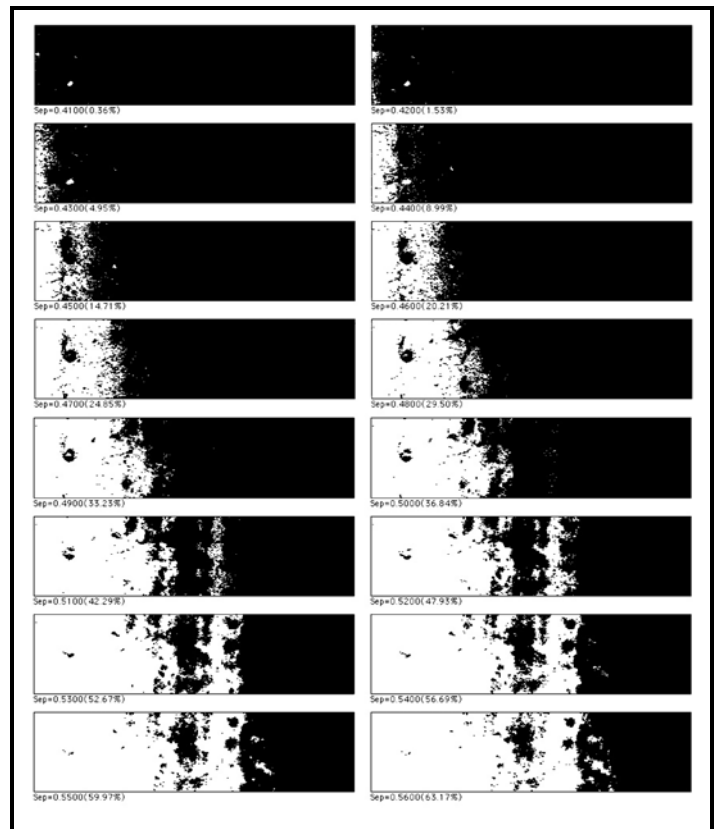


Figure 4. Crack front movement.

- Researchers ranked the first group of candidate structural materials (austenitic stainless steels SS304, SS316, and SS347) against their susceptibility to environmentally assisted degradation based on the in-situ data on film stability. They observed that the resistance to both electronic and ionic charge was the lowest for SS304, the highest for SS347, and in between for SS316 (Figure 3).
- Researchers observed a correlation between measurable oxide film properties and susceptibility of austenitic steels to environmentally assisted degradation. Experimental proof of the existence of this correlation is one of the major goals of present work.
- One of the major practical results of the present work is the experimentally proven ability of the CDE technique to supply in-situ data for ranking candidate structural materials for Generation IV SCWR.
- Researchers evaluated a potential use of the CDE arrangement developed at SRI for building in-situ sensors for monitoring oxide films and water chemistry in the heat transport circuit of Generation IV SCWR. This was proven to be feasible.

- Researchers performed post-examination of the fracture surfaces using the FRASTA technique to obtain information on a sequence of the fracture events: the development of crack initiation sites, the movement of the crack front, and, eventually, crack initiation times and crack growth rates.
- FRASTA analysis of the crack front movement revealed that the crack in austenitic stainless steels advanced by forming discontinuities ahead of the crack front followed by their coalescence (Figure 4).
- Experimental data obtained during the reporting period allowed researchers to estimate the crack growth rates for the first group of candidate structural materials— austenitic stainless steels. This group included SS304 as a "baseline" material and SS316 and SS347 as candidate materials.

## Planned Activities

The following work will be performed during Year 3 for the remaining two groups of candidate structural materials—ferritic-martensitic steels and nickel-based alloys:

- Characterize the oxidation and reduction kinetics and mechanisms of metals as well as the properties of metal oxide films by using CDE measurements.
- Rank the influence of ionic species on the oxide films forming on metal surfaces.
- Quantify and interpret the rate-limiting processes in the corrosion phenomena and the role of electrochemical reactions and properties of oxide films in the crack growth mechanism under supercritical conditions.
- Identify candidate remedial actions (changes in water chemistry, material chemical composition, and metallurgical parameters) that can decrease the susceptibility to stress corrosion cracking.
- Examine fracture surfaces using the FRASTA technique to determine crack front formation and movement, and estimate crack extension and growth rates.
- Correlate electrochemical information on material-environment interactions with crack nucleation and growth.



# NUCLEAR ENERGY RESEARCH INITIATIVE

## New Design Equations for Swelling and Irradiation Creep in Generation IV Reactors

PI: Wilhelm G. Wolfer, Lawrence Livermore National Laboratory

Project Number: 01-137

Collaborators: Pacific Northwest National Laboratory, University of California-Berkeley

Project Start Date: October 2001

Project End Date: September 2004

### Research Objectives

The objectives of this research project are to develop physical models for radiation-induced microstructural changes in structural materials to be used in Generation IV nuclear reactors. Researchers will derive from these models the constitutive laws for void swelling, irradiation creep, and stress-induced swelling, as well as changes in mechanical properties. The approach is based on modeling the cause-effect relationships—from the fundamental atomistic processes to the macroscopic constitutive laws. The many levels of the cause-effect hierarchy and cross connections are illustrated in Figure 1.

Researchers are testing and validating both the microscopic models and the macroscopic constitutive laws by analyzing electron microscopy data, density data, irradiation creep data, diameter changes of fuel elements, and

post-irradiation tensile data. Validation of both microstructure models and macroscopic constitutive laws will provide a more stringent test of the consistency of the underlying science for radiation effects in structural materials for nuclear reactors.

### Research Progress

Figure 1 shows that researchers must develop and integrate a multitude of models to arrive at some of the constitutive descriptions of radiation-induced property changes. Below is a brief explanation on the progress achieved for various models.

- Researchers have developed a model to predict the changes in mechanical properties of irradiated materials. The microscopic radiation damage is in the form of small helium bubbles or voids, prismatic dislocation

loops, and line dislocation defects. The coarse-grained model groups all these different defect microstructures into two irradiation-induced defect densities with average defect sizes for both. Researchers use these four microstructural parameters to predict the stress strain response of irradiated alloys with different levels of accumulated damage. The predictions of the model developed suggest that as the level of radiation damage increases the strength of the material should increase, while the strain hardening of the material will decrease. The plastic deformation of the material will be more prone to flow localization as the level of radiation damage increases; but, if it

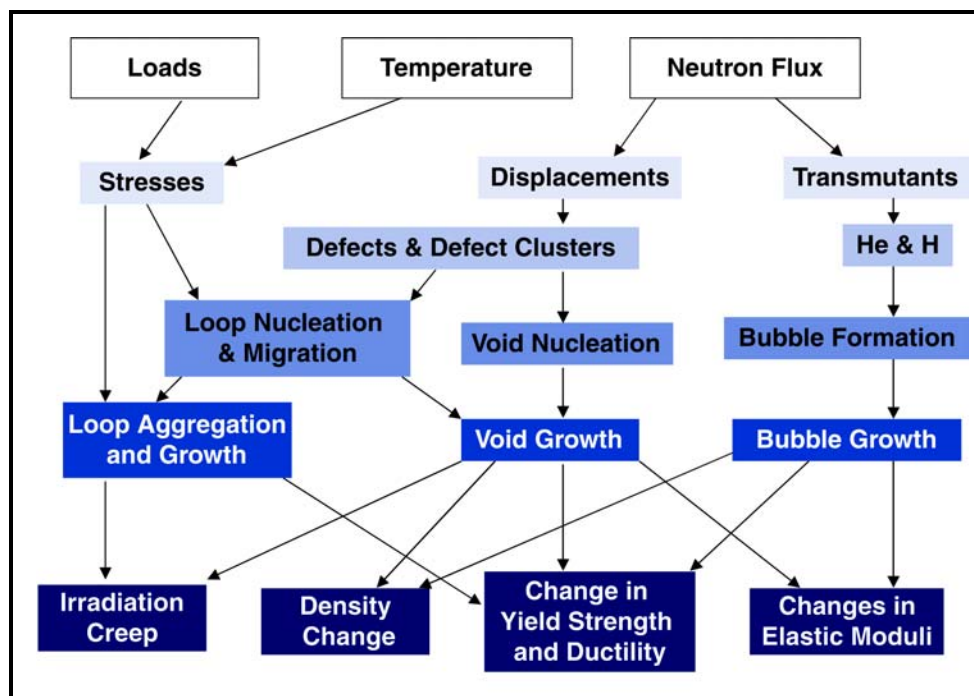


Figure 1. The many levels of the cause-effect hierarchy and cross connections.

possesses high strain rate sensitivity to begin with, it may not show any strain softening behavior.

- b) Dislocation loops play an important role in radiation-enhanced creep and in stress-induced void swelling. These loops form by the aggregation of small mobile loops. In preparation of developing the constitutive laws for irradiation creep, researchers have carried out new theoretical studies on the effects of internal and external stresses on loop migration and their orientations in stress fields.

Researchers on this project have derived the complete and consistent expressions for glide force and torque exerted by an arbitrary stress field on a glissile dislocation loop, and for the self-torque of the loop. They have obtained a solution for the loop orientation as a function of its location, and this solution is employed to derive the actual interaction energy or glide force for the combined motion and rotation of a loop in a general stress field. Researchers have demonstrated that stress-induced rotation can significantly enhance the glide force. The rotation caused by the stress is seen to significantly enhance the glide force at large distances. Although the force is weak in absolute terms at these large distances, it is there where this force begins to impose a drift on the otherwise random motion of the loop, leading to its eventual capture in close vicinity of a dislocation, other loops, or voids.

The collective interaction among prismatic dislocation loops is an important aspect of the interrelationship between stress-affected swelling and irradiation creep. This interaction is a consequence of image stresses that had not been derived correctly by previous researchers. In this project, researchers have developed, for the first time, correct theories for image stresses produced by dislocation loops and have shown that they depend on the loop radius relative to an atomic scale parameter, namely the Burgers vector. With increasing loop radius, keeping the loop volume constant, the image stresses are found to gradually disappear. Such a situation can actually be realized in metals irradiated at low temperatures and subsequently annealed. The initial high density of small prismatic loops coarsens into a low density of larger loops, and the lattice parameter recovers to its original value before the irradiation. Results found in this project are in marked contrast to results obtained earlier and reported in the literature. These earlier results led to the paradoxical conclusion that the image stresses, and the changes in lattice parameter they produce, are

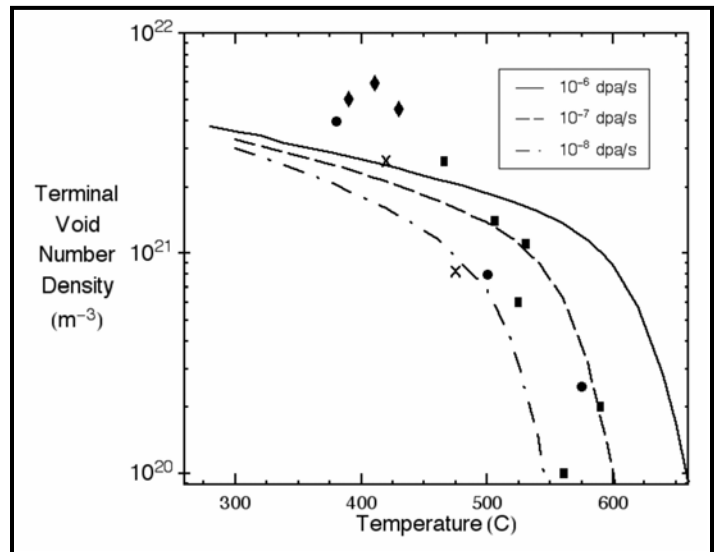


Figure 2. Terminal visible void density is shown versus temperature for a fixed dislocation density of  $2 \times 10^{13} \text{ m}^{-2}$ . The terminal density is achieved within a few dpa, at most. Experimental measurements are shown for comparison.

independent of the loop diameter. The new, correct results have been published in the *Philosophical Magazine Letters*.

- c) Researchers applied the recently developed Master equation and Fokker-Planck method for cluster-nucleation and growth simulations to impurity-free type-316 stainless steel under irradiation. The evolution of the void size distribution is treated in full generality, although the dislocation density is held constant versus time and temperature. The simulations reproduce several observed characteristics of irradiation swelling, involving a brief incubation delay followed by quasi-steady swelling. The predicted incubation period shows a clear dose-rate response—lower irradiation flux requires less total fluence to complete the incubation process. This trend is consistent with some recent experimental reports. Predicted and observed void number densities are in fair agreement.

## Planned Activities

During the coming year, researchers from Lawrence Livermore National Laboratory (LLNL) and University of California-Berkeley will develop models for irradiation creep and for stress effects on the incubation period for void swelling. The coupling between irradiation creep and swelling is believed to originate from the formation and growth of prismatic dislocation loops and from their coalescence into a dislocation network. When the climb motion of this network is affected by the growing voids, irradiation creep rate is reduced. This impediment of climb motion by

voids is the subject of a doctoral thesis. The results of the research as part of this thesis will be incorporated into the development of constitutive equations for irradiation creep and swelling.

In addition, researchers will analyze radiation effects data for ferritic steels and model the data with the void nucleation code. Researchers will attempt to develop a design equation for void swelling in this class of materials. However, several important fundamental materials parameters are not known from experiments, and researchers will have to use theoretical estimates.

Researchers from Pacific Northwest National Laboratory will compile irradiation creep data for both austenitic and ferritic steels, which they will use to validate both micro-

structural models and constitutive laws developed jointly with LLNL. Researchers have retained irradiated stainless steel reflector hex blocks of SS304 from reflector subassembly U-9807 of the EBR-II reactor, and will carry out dimensional and density measurements. These blocks are expected to have significant gradients of swelling both across as well as along the block. The differential swelling will have generated stresses that must have been relaxed by irradiation creep and stress-induced swelling. Researchers have made dimensional examinations, and will make subsequent destructive examinations to measure the spatial variation of swelling and determine the impact of the internal stresses.





# NUCLEAR ENERGY RESEARCH INITIATIVE

## Development and Validation of Temperature-Dependent Thermal Neutron Scattering Laws for Applications and Safety Implications in Generation IV Nuclear Reactor Designs

PI: Ayman I. Hawari, North Carolina State University

Project Number: 01-140

Collaborators: Oak Ridge National Laboratory

Project Start Date: September 2001

Project End Date: August 2004

### Research Objectives

The overall objectives of this work are: 1) to critically review the currently used thermal neutron scattering laws for various moderators and fuel cells as a function of temperature; 2) to use the review as a guide in examining and updating the various computational approaches in establishing the scattering law; 3) to understand the implications of the results obtained on the ability to accurately define the operating and safety characteristics (e.g., the moderator temperature coefficient) of a given reactor design—that is, to know not only the reactivity coefficients but also their errors, sensitivity coefficients, and covariance matrices; and 4) to test and benchmark the developed models within the framework of an experiment to slow neutrons.

In particular, the studies will concentrate on investigating the latest ENDF/B thermal neutron cross sections for

reactor-grade graphite, beryllium, beryllium oxide, zirconium hydride, high purity light water, heavy water, and polyethylene at temperatures greater than or equal to room temperature. These materials are neutron moderators that will be used in developing Generation IV nuclear power reactors and in many other applications in the nuclear science and engineering field. Graphite is an important material as it is the moderator in the modular pebble bed reactor (MPBR) that is being examined internationally as a possible Generation IV power reactor, as the subcritical reactor in accelerator-driven concepts, and as the incinerator of radioactive waste and weapon-grade plutonium. Researchers are studying the use of a newly developed, highly conductive form of graphite, known as graphite foam, as a reactor material.

### Research Progress

During the second year, researchers on this project evaluated the thermal neutron scattering laws for certain key materials and tools that were established in the first year. Specifically, two materials have been studied extensively: beryllium and graphite. Beryllium represented an ideal material for testing the utility of the ab-initio technique for generating the phonon frequency distributions and subsequently the scattering law. To do this, researchers used the Vienna ab-initio Simulation Package (VASP) to calculate the phonon frequency spectra. In principle, VASP solves the Kohn-Sham equations using a given pseudopotential to generate the Hellmann-Feynman (HF) forces between the atoms in a perfect supercell. Once such forces are computed, the results are imported into the PHONON code to perform a lattice dynamics calculation and to produce the characteristic dispersion relations and the vibrational frequency spectrum,  $\rho(\beta)$ . Researchers examined the results to ensure that the model is producing physically acceptable results (e.g., only positive frequency

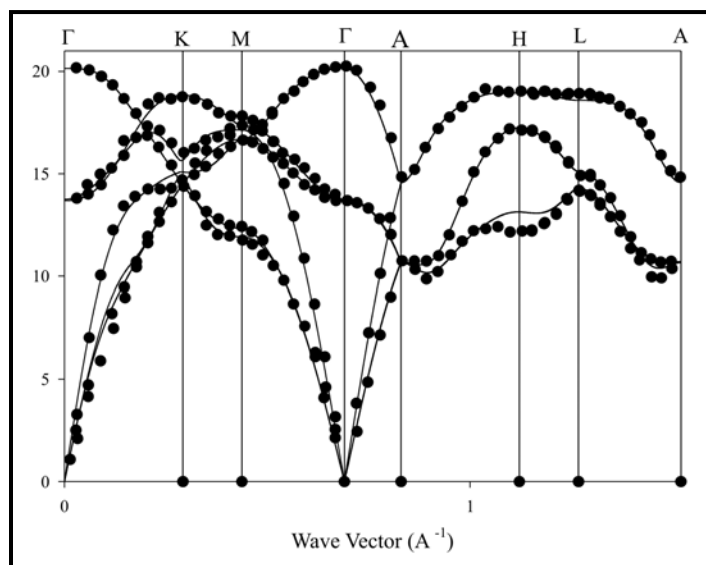


Figure 1. A comparison of calculated (lines) and measured dispersion relations for Be. The calculation was performed for a 96-atom supercell. The measured data is from R. Stedman et al., *J. Phys. F*, 6, 157 (1976).

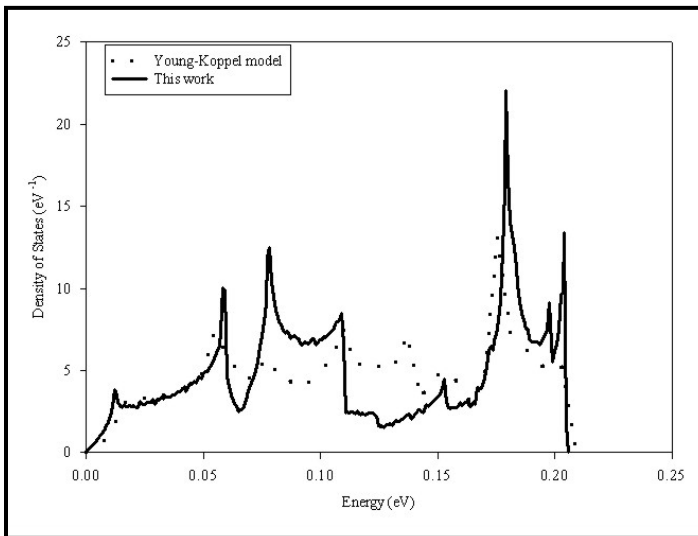


Figure 2. The phonon frequency spectrum of graphite based on a 144-atom supercell VASP model. The spectrum is compared to that of Young-Koppel, which is used in standard data libraries (see J. A. Young, J. U. Koppel, *J. Chem. Phys.*, 42, 357 [1965]).

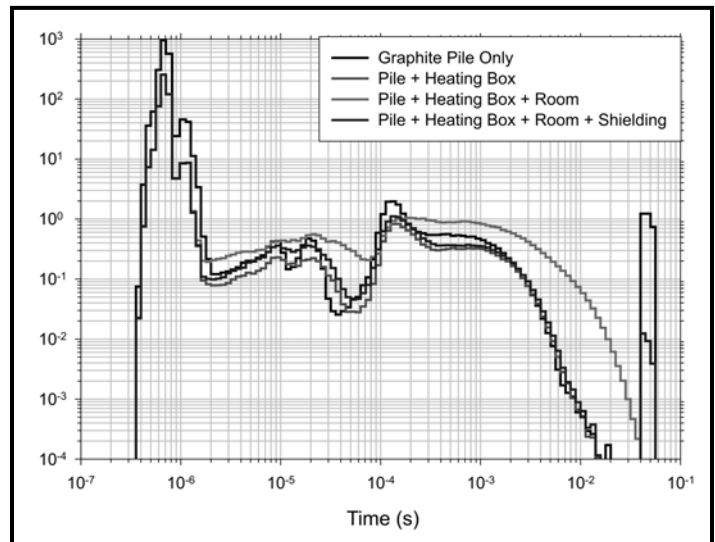


Figure 4. The calculated response of a Pu-239 detector at 25-cm from the surface of the experimental setup. The calculation simulates an ORELA pulse slowing down in a graphite pile at room temperature.

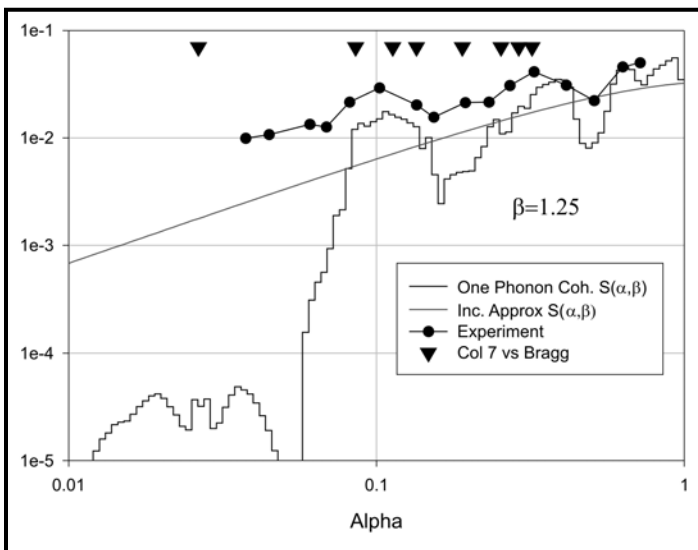


Figure 3. A comparison of the scattering law for beryllium as calculated using the 1-phonon formulation and the incoherent approximation. Raw experimental points are shown that demonstrate consistency with the data that was generated using the 1-phonon approach.

values are generated). Figure 1 shows the calculated dispersion relations for Be (using the ab-initio approach) compared to measured data that are based on neutron-scattering experiments. Six vibrational modes appear in the figure—as expected for the Be unit cell, which has 2 atoms. Researchers calculated the dispersion relations along the high symmetry directions ( $\Gamma$ , K, M, H, and L) in the hexagonal Brillouin zone. The lowest three branches, starting from  $\Gamma$ , are known as the acoustic modes, while the highest three branches are the optical modes. As the figure shows, the agreement between the measurement

and the calculation is excellent, which verifies the models and methods applied in this calculation.

Figure 2 shows the ab-initio based phonon frequency spectrum for graphite, which is based on force constants derived from a 144-atom supercell model. In general, the spectrum is comparable to that of Young-Koppel, which is used in generating the common thermal neutron scattering libraries (e.g., the data libraries distributed with the MCNP code). However, differences between the two spectra can be seen in the low energy extreme of this figure. Researchers are currently studying these differences, which are important for low-energy neutron scattering.

Based on the above, researchers on this project have generated thermal neutron scattering libraries for Be and graphite. Currently they are testing these libraries using simulated experiments. In addition, they have implemented an approach to produce the scattering law that relaxes the "incoherent approximation," which is applied in the familiar codes GASKET and NJOY/LEAPR. This approach is based on an exact calculation of the one-phonon coherent inelastic expression using the dispersion relations derived from the ab-initio calculations. After evaluating the influence of this new treatment, they will, if necessary, extend the calculation to the higher order terms in the phonon expansion. The researchers have generated and are currently examining the preliminary results.

Figure 3 shows the results obtained for the Be  $S(\alpha, \beta)$  in comparison to experimental data. The experimental data were not corrected for background contamination. The results of the incoherent approximation are also shown, as

well as the alpha values that correspond to the lowest Bragg peaks.

During Year 2, researchers concluded the design work for the heating system to be used for the graphite benchmark experiment planned to take place at the Oak Ridge Linear Electron Accelerator (ORELA). The system has been ordered and is expected to be built by early 2004. In addition, the research team has submitted the experiments report to the ORELA staff for review. After the design and optimization of the heating system, researchers performed further studies to evaluate the effects of room return and to design the most suitable shielding to minimize this effect. Figure 4 presents the simulated response of the Pu-239 detector for different experimental conditions. The figure shows the effect of room return on the ideal detector response. This effect is minimized using 1-inch polyethylene shields containing 5 percent boron that surround the experimental setup.

## Planned Activities

During Year 3, researchers will perform the temperature-dependent graphite benchmark experiment at ORELA. The results of this experiment will be combined with the computational results to produce recommended thermal neutron scattering cross section libraries for graphite to use in the design calculations of Generation IV reactors. In addition, researchers will perform reactor and non-reactor based benchmark simulations (using published experimental data) for all materials of interest to this work. These simulations will validate the computational models and methods that are used in the generating of the thermal neutron scattering cross sections. Finally, researchers on this project plan to continue their development of improved methods for calculating the scattering law, which includes the implementation and testing of the one-phonon formulation.



# NUCLEAR ENERGY RESEARCH INITIATIVE

## The Oxidation of Zircaloy Fuel Cladding in Water-Cooled Nuclear Reactors

PI: Digby D. Macdonald, Pennsylvania State University

Collaborators: None

Project Number: 02-042

Project Start Date: September 2002

Project End Date: September 2005

### Research Objectives

This work seeks to develop a comprehensive model that can be used to predict performance, and assess the risk of failure, of Zircaloy fuel cladding in commercial boiling water reactors (BWR) and pressurized water reactors (PWR) under high burn-up conditions.

### Research Progress

**Task 1: Modified Boiling Crevice Model.** Under this task, researchers have modified the Boiling Crevice Model to describe the evolution of the environment in crud pores and, hence, in contact with the cladding Zircaloy surface under low super heat (nucleate boiling in PWRs) and high super heat (sustained boiling in BWRs) heat transfer conditions. The Modified Boiling Crevice Model calculates the evolution of the solution contained within the pores of the crud layer on the fuel cladding. As boiling occurs within the crevice, the concentration of the electrolyte increases and eliminates the super heat. The concentration process begins at the bottom of the pore where the temperature is highest. Thus, a concentrated solution is produced in the pore from the pore base and gradually expands to fill the pore.

Boiling is believed to be the mechanism for concentrating  $\text{Li}^+$  and  $\text{B}(\text{OH})_4$  in crud pores on the fuel and, ultimately, for the precipitation of  $\text{LiB}(\text{OH})_4$  resulting in the Axial Offset Anomaly (AOA). Therefore, researchers have derived the volume-averaged concentration for  $\text{LiB}(\text{OH})_4$  in the pore as follows:

$$C^* = \theta S_0 C_0 \exp(-t/\tau) + \theta S_0 C_{\text{lim}} (1 - \exp(-t/\tau)) \quad (1)$$

$S$  is the saturation;  $\theta$  is the porosity; subscription 0 means the mouth of the pore;  $C_{\text{lim}}$  is the limiting concentration in the pores  $\tau = \frac{\theta S_0 C_{\text{lim}}}{C_0 B}$ . Figure 1 shows a

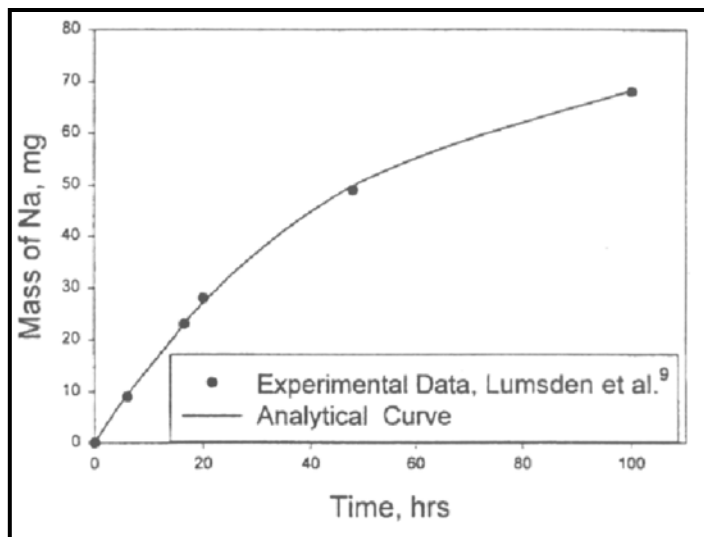


Figure 1. Comparison between theory and experiment for the average volume concentration of  $\text{Na}^+$  in a boiling crevice in contact with a bulk solution containing 40 ppm  $\text{NaOH}$ . The theory was fit to the first two experimental points.

comparison between theory and experiment for the concentration of  $\text{NaOH}$  in a crevice under boiling conditions, demonstrating the accuracy of the model.

### Task 2: Development of Point Defect Model.

In this task, researchers have developed two models for the passive corrosion of Zircaloy in reactor coolants. Each model depends on the type of barrier layer formed on the alloy. The first model applies to highly hydrogenated coolants (conventional PWRs), where the barrier layer is a hydride ( $\text{ZrH}_x$ ,  $1 < x < 2$ ) and the outer layer is a precipitated oxide ( $\text{ZrO}_2$ ). The second model applies to normal, oxidizing BWR conditions, where the passive film comprises a tetragonal  $\text{ZrO}_2$  barrier layer and a monoclinic  $\text{ZrO}_2$  outer layer.

The derived equation for the thickness of the hydride barrier layer under PWR coolant conditions is as follows:

$$L_{bl} = \frac{(1-\alpha)}{\varepsilon} V_{bl} - \frac{\beta}{\varepsilon} pH_{BOI} - \frac{1}{\alpha_3 \gamma \varepsilon} \ln \left( \frac{c_{H^+}^n a_w^{BOI} k_{11}^0 \theta}{k_3^0} \right) \quad (2)$$

The activity of water ( $a_w^{BOI}$ ) is taken to be 1; the parameter  $\alpha$  is the polarizability of the barrier layer/outer layer interface (BOI, dimensionless constant);  $\beta$  is a constant with units of voltage;  $pH_{BOI}$  is the local pH at the BOI;  $\gamma = F/RT$ ;  $\alpha_j$  is the dimensionless transfer coefficient for Reaction  $j$ ;  $k_j^0$  is the standard rate constant for  $j^{\text{th}}$  reaction;  $\varepsilon$  is the electric field of barrier layer (the  $\varepsilon$  in the hydride has a negative value), and  $\theta$  is the porosity of the outer layer. Reaction 3 corresponds to the growth of the barrier layer into the metal, whereas Reaction (1) corresponds to dissolution of the barrier layer at the BOI. The corresponding equation for the formation of an oxide barrier layer is as follows:

$$L_{bl} = \frac{1 - \alpha(1 - \alpha_6 / \alpha_3)}{\varepsilon} V_{bl} - \frac{\beta}{\varepsilon} (1 - \alpha_6 / \alpha_3) pH_{BOI} - \frac{1}{\alpha_3 \gamma \varepsilon} \ln \left( \frac{a_{V_{O_2}}^{BOI} a_w^{BOI} \hat{k}_6 \theta}{k_3^0} \right) \quad (3)$$

Researchers have completed work on deriving the theoretical expressions for the transfer function in order to interpret electrochemical impedance data and to derive model parameters. The necessary algorithms and software are nearing completion. Researchers have successfully tested the analysis of impedance data on a variety of other systems, including Alloy C-22, Type 316 SS, and nickel, while they await their first impedance data for zirconium.

**Task 3: Experimental Measurement of Model Parameters.** This task involves the experimental measurement of critically important model parameters, such as the electrochemical kinetic parameters for the redox reactions (oxidation of  $H_2$  and the reduction of  $O_2$ ) that occur on the metal surface. Under this task, researchers

are measuring these parameters using the controlled hydrodynamic system shown in Figure 2(a). By using very high mass transfer rates, the region of potential over which charge transfer effects can be studied is greatly expanded, thereby providing for more accurate parameter determination. Researchers will also measure other parameters, including passivity breakdown potentials, corresponding to the onset of "nodular attack," using potentiodynamic techniques as a function of voltage sweep rate and as a function of heat treatment (i.e., distribution of second phase particles [SPPs]).

Finally, researchers are also performing electrochemical transient (ET) and electrochemical impedance spectroscopic (EIS) studies on the oxide films grown on Zircalloys under simulated BWR and PWR primary coolant conditions. The purpose of these studies is to measure the thickness of the passive film as a function of voltage and exposure time and to ascertain the appropriate oxidation mechanism through the use of the diagnostic criteria discussed in the original proposal. These measurements will also be used to extract information on important model parameters (e.g., diffusivity of oxygen vacancies in the barrier layer).

Researchers on this project have successfully carried out potentiodynamic experiments to study the oxidation of hydrogen on platinized nickel at 300°C to test the apparatus using a well-defined reaction. Figure 2(b) shows typical potentiodynamic polarization curves for the oxidation of hydrogen in 0.1 M NaOH solution at 300°C, at a hydrogen concentration of 1.4 ppm, and for a voltage step rate of 50

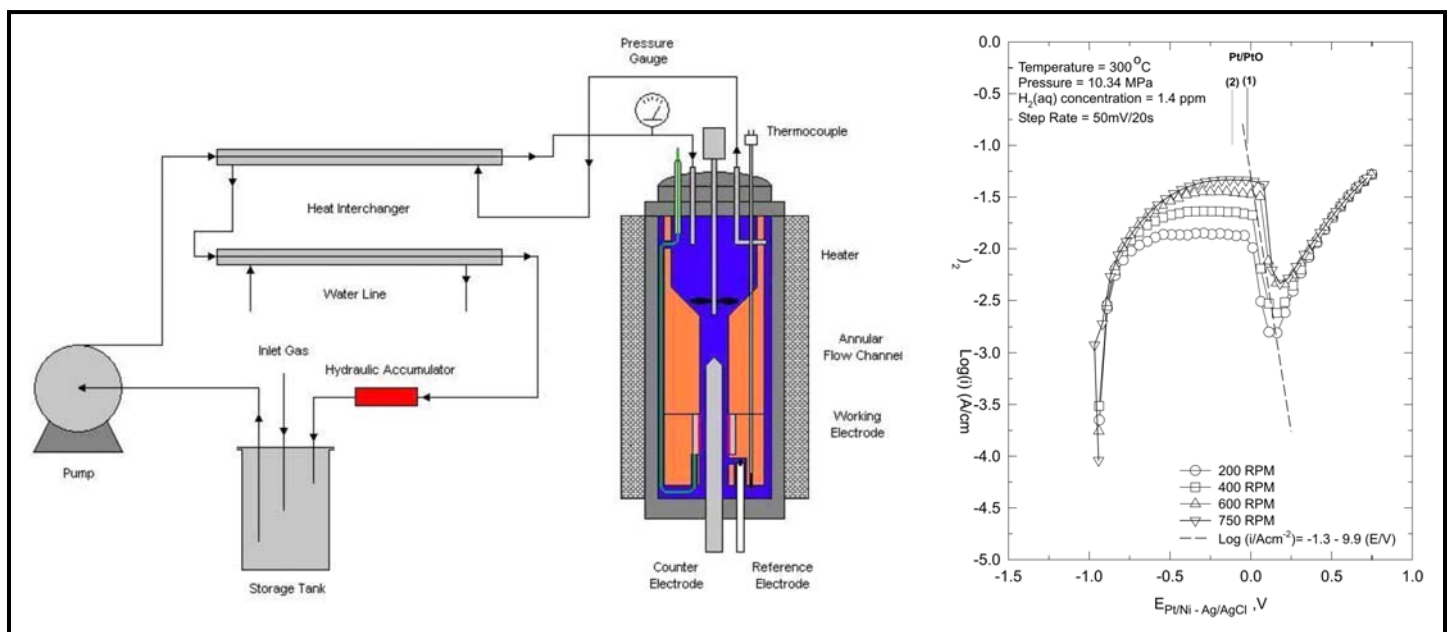


Figure 2. (a) Once-through recirculating flow loop and the high-temperature/high-pressure controlled hydrodynamic test cell. (b) Typical polarization curves for the oxidation of hydrogen (1.4 ppm) on platinized nickel in 0.1 M NaOH at 300°C as a function of the rotational velocity of the flow activating impeller.



mV/20s, as a function of the rotational velocity of the flow activating impeller. The broken line corresponds to the prediction of the perfect defect model (PDM), assuming that charge transfer is due to direct quantum mechanical tunneling across a PtO barrier layer.

Researchers are currently carrying out similar potentiodynamic experiments on zirconium at 300°C. To simulate the PWR working conditions, researchers are using aqueous solutions containing 1,000 ppm boric acid and 5 ppm LiOH. PWRs operate with boric acid as a nuclear shim to control the nuclear reactivity. LiOH is added to control the release of corrosion products into the coolant and subsequent deposition onto fuel surfaces. The pH of this solution is 7.42 at 300°C.

## Planned Activities

Work will continue over the next reporting period on model development, with particular emphasis on the PDM. Researchers expect to begin optimizing the PDM on experimental EIS data, in order to extract values for important model parameters. As the models are completed, they will be integrated with the other models being developed in this study to eventually produce a comprehensive theory for the oxidation of Zircaloy fuel sheathing under BWR and PWR operating conditions.



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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Incorporation of Integral Fuel Burnable Absorbers Boron and Gadolinium into Zirconium-Alloy Fuel Clad Material

PI: Kumar Sridharan, University of Wisconsin

Project Number: 02-044

Collaborators: Sandia National Laboratories,  
Westinghouse Science and Technology  
Department

Project Start Date: September 2002

Project End Date: September 2004

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### Research Objectives

Long-lived fuels require the use of higher enrichments of  $^{235}\text{U}$  or other fissile materials. Such high levels of fissile material lead to excessive fuel activity at the beginning of life. To counteract this excessive activity, integral fuel burnable absorbers (IFBA) are added to some rods in the fuel assembly. The two commonly used IFBA elements are gadolinium, which is added as gadolinium-oxide to the  $\text{UO}_2$  powder, and boron, which is applied as a zirconium-diboride coating on the  $\text{UO}_2$  pellets using plasma spraying or chemical vapor deposition techniques. The incorporation of IFBA into the fuel has to be performed in a nuclear-regulated facility that is physically separated from the main plant. These operations tend to be very costly because of their small volume and can add 20 to 30 percent to the manufacturing cost of the fuel. Other manufacturing issues that impact cost and performance are: maintaining the correct levels of dosing, reducing the fuel melting point due to gadolinium-oxide additions, and absorbing parasitic neutron at the fuel's end-of-life.

The goal of this research is to develop an alternative approach that involves incorporating boron or gadolinium into the other surface of the fuel cladding material rather than as an additive to the fuel pellets. This paradigm shift will allow for the introduction of the IFBA in a non-nuclear regulated environment and will obviate the necessity of additional handling and processing of the fuel pellets. This could represent significant cost savings and potentially lead to greater reproducibility and control of the burnable fuel in the early stages of the reactor operation.

### Research Progress

This project is being performed collaboratively between three participating institutions. The University of Wisconsin-Madison is the lead organization and is responsible for

materials preparation and characterization before surface treatment of materials, after surface treatment, and in the post-autoclave testing materials analysis. They are also responsible for project coordination and the educational aspects of the project. Sandia National Laboratories, Albuquerque, is responsible for the ion-based surface treatment of the alloys and computer simulations of the surface alloying process. Westinghouse Science and Technology, Pittsburgh, is responsible for autoclave testing of the surface-treated samples and evaluating the manufacturability of the process.

The research program initially focused on identifying and resolving a number of technical issues brought forth by the three collaborating groups. These included detailed discussions on issues such as sample size and thickness, surface roughness, IFBA sputter layer thickness, the type of energetic ion to be used for the ion-based surface treatment, and scheduling.

Westinghouse supplied sheet stock of two widely used zirconium alloys, Zirlo and Zircaloy-4, to the University of Wisconsin. The sheet stock was pickled (process of removing surface oxides present from previous hot forming operations) and metallographically polished at the University of Wisconsin and cut into samples 0.75 inch by 0.75 inch and sent to Sandia National Laboratories for ion-based surface treatment. Surface treatment at Sandia was initiated on gadolinium incorporation into the zirconium alloys, which was performed by sputter depositing a thin layer of gadolinium on the samples and surface alloyed by near surface melting and rapid solidification using the ion beam surface treatment (IBEST) process. Initial optimization of this process required a number of iterations of processing and analysis, and was supported by computer simulations using an ion-materials interaction code and surface melting codes. The goal of these initial experi-

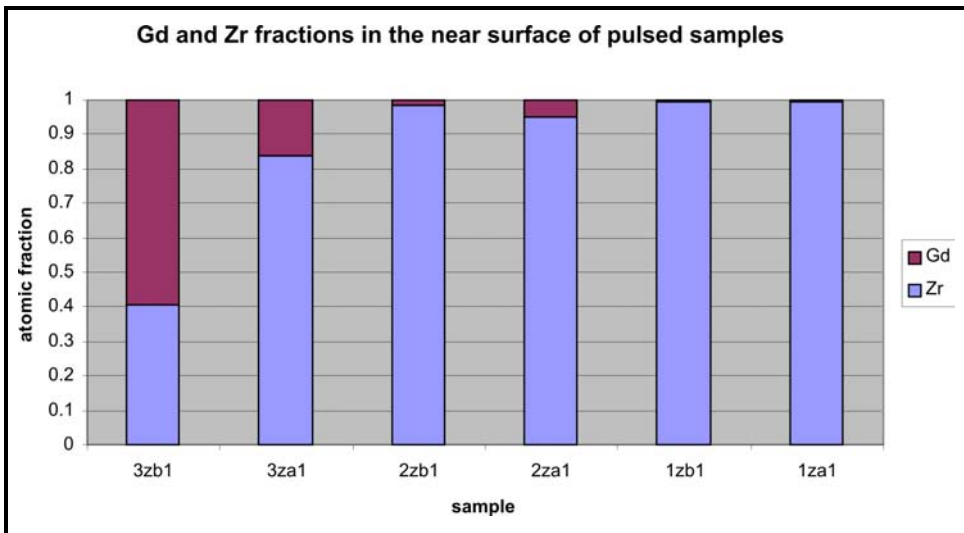


Figure 1. Rutherford Backscattering Spectroscopy (RBS) results showing the co-existence of gadolinium and zirconium in the near-surface regions of the material. Results are shown of samples that experienced different process conditions. Sample 3zb1 shows the best alloying between Gd and Zr.

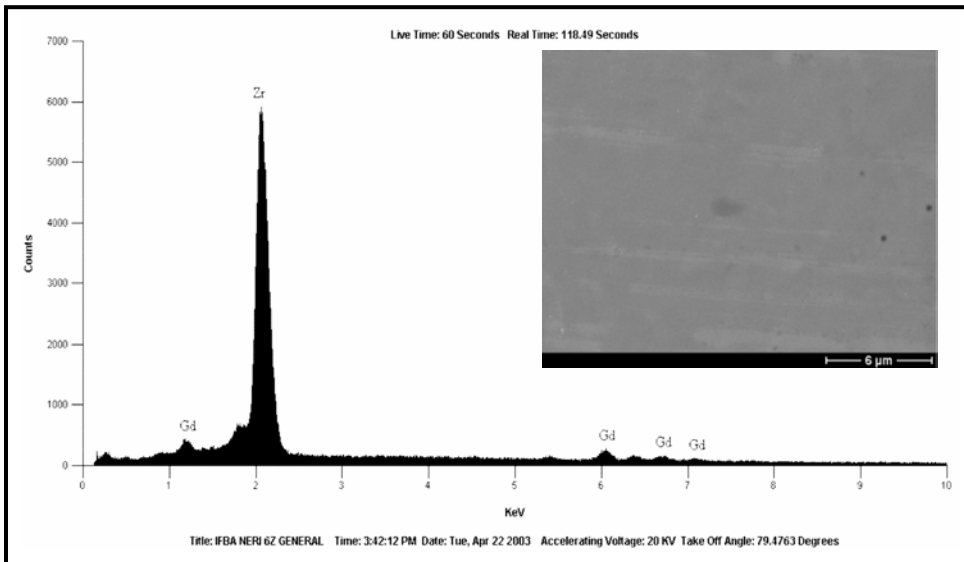


Figure 2. Scanning Electron Microscopy Energy Dispersive Spectroscopy (SEM-EDS) analysis showing the presence of Gd in the near-surface regions of the Zr-alloy. Gd signals are attenuated because the electron penetration depth exceeds the alloyed layer depth. High magnification imaging shows a homogeneous structure devoid of phase separation.

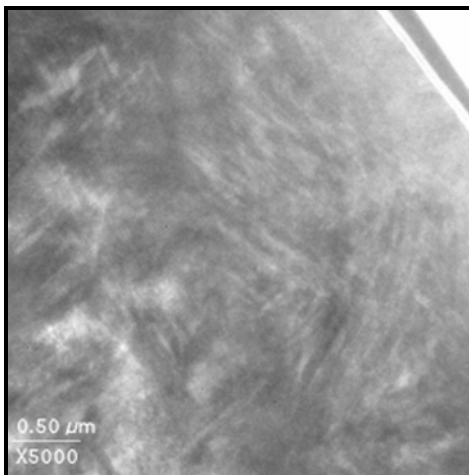


Figure 3. Transmission Electron Microscopy image of Gd-incorporated Zr-alloy. The taper in the top right side is the sample surface. The structure is homogeneous and there is no evidence of phase separation. Samples were prepared by Focus Ion Beam (FIB) technique.

ments and simulations was to determine the required gadolinium film thickness and appropriate ion-bombardment energies. The necessity for such optimization is driven by two competing physical effects occurring at the materials surface, namely, ablation due to evaporation and sputtering and surface alloying due to liquid phase mixing. The goal of the initial experiments, analysis, and simulations was to ensure that surface alloying outpaces ablation.

Figure 1 shows the results of near-surface chemical analysis of the zirconium alloys after gadolinium surface alloying, as determined by Rutherford Backscattering Spectroscopy (RBS). The results show that a substantial amount of gadolinium co-exists in the near-surface regions of the sample along with the substrate material Zr. Figure 2 shows the Scanning Electron Microscopy-Energy Dispersive Spectroscopy (EDS) result of the gadolinium-incorporated samples. The presence of gadolinium is confirmed by the EDS analysis (Gd signal is attenuated because the material's volume affected by electron beam can extend up to  $3\mu\text{m}$ ) and the surface structure is very homogeneous and devoid of any phase segregation.

To further confirm the observation relating to the structure, researchers performed Transmission Electron Microscopy (TEM) using the Focused Ion Beam (FIB) approach for sample preparation. Figure 3 shows the high-magnification, high-resolution TEM image of the near-surface region of the sample. Even at these nanometer levels of detail, no segregation or phase separation of Gd and Zr or their enriched phases is observed. These observations and results are significant because they demonstrate that, despite the negligible mutual solubility between Gd and Zr, they can be homogeneously alloyed using non-equilibrium ion bombardment and rapid solidification approaches.

An example of computer simulations that researchers are using to gain a predictive capability of the process is shown in Figure 4, which shows a 1-D simulation performed on Gd and on Zr using a neon beam energy of 2.4 J/cm<sup>2</sup> and beam pulse ranging from 0 to 450ns. The code indicates that a Gd layer fully melts after which the Zr melts to depths of 1.5 $\mu$ m. Zr melt duration is about 1.3 $\mu$ s and Gd melt duration is 3 $\mu$ s.

Initial autoclave tests at Westinghouse have shown that oxide scaling began to occur on the sample surface when tested in 800°F steam for one day. Figure 5 shows a high-

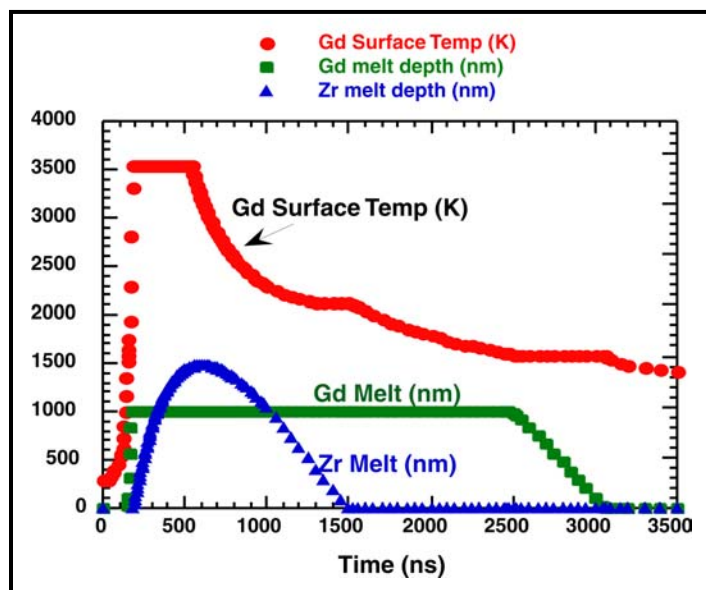


Figure 4. An example of 1-D simulation code that is being used to determine the required Gd layer thickness and process parameters.

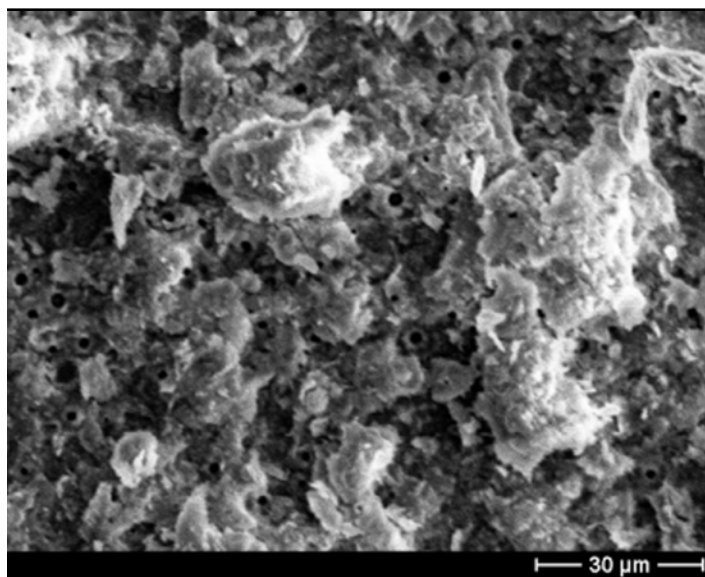


Figure 5. Scanning Electron Micrograph showing surface oxidation after autoclave testing at 800°F. EDS analysis showed the oxide to be that of gadolinium. Researchers are presently examining ways of mitigating the scaling of gadolinium-oxide by changing IBEST process parameters and Gd film thickness.

magnification Scanning Electron Micrograph (SEM) image of the oxide formation and scaling. SEM-EDS analysis indicated that some samples showed predominantly gadolinium-oxide. Researchers on this project are presently investigating this and will be performing another Gd-IBEST run shortly by adjusting process parameters with the goal of enhancing resistance to scaling.

Westinghouse has performed a detailed evaluation of scale up and manufacturability costs of this research concept, and has published a report. The task identified the manufacturing issues encountered when the IFBA, either boron or gadolinium, is sputtered on the outside of the fuel cladding tube and melted into the surface using the ion beam apparatus. The task estimated the capital and operating costs for introducing an IFBA material on the outside of the fuel tube. The study took into account issues such as power requirements, ventilation requirements, hazardous materials handling, waste generation, and zirconium tube inventory. The basis for the analysis was a production rate of 6 million feet per year of zirconium tubing of which 5 million feet are coated with IFBA, which translates into a uranium production rate of about 1,000 metric tons of U as UO<sub>2</sub> per year. The baseline constraints and assumptions used were those that reflect the current permitting and operational constraints at Westinghouse Nuclear Fuel plants in Columbia, South Carolina. The product cost was estimated to be at \$34/tube or \$17/kg of U.

## Planned Activities

Activities in the coming quarters are as follows:

1. Gain a fundamental understanding of the oxidation of behavior of Gd-alloyed samples in autoclave testing and improve the resistance to oxide scaling.
2. Continue autoclave testing of samples at Westinghouse.
3. Continue post autoclave testing analysis using x-ray diffraction and Scanning Electron Microscopy at University of Wisconsin to establish oxidation modes.
4. Perform ion-materials interaction and surface melting simulations for boron IFBA into zirconium.
5. Perform IBEST surface alloying process to alloy IFBA element boron into the zirconium alloys.
6. Perform autoclave testing of boron-alloyed samples.



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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Neutron and Beta/Gamma Radiolysis of Supercritical Water

PI: David M. Bartels, Argonne National Laboratory

Project Number: 02-060

Collaborators: University of Wisconsin

Project Start Date: August 2002

Project End Date: September 2005

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### Research Objectives

Current pressurized water reactors (PWR) run at roughly 300°C and 100 atmospheres pressure. Advanced water-cooled designs under consideration in the Generation IV initiative would operate at 500°C and 250 atmospheres, i.e., well beyond the critical point of water. This would improve the thermodynamic efficiency by about 30 percent, and provide considerable capital cost savings due to plant simplifications. However, a major unanswered question is: What changes occur in the radiation-induced chemistry in water as the temperature and pressure are raised beyond the critical point, and what does this imply for the limiting corrosion processes in the materials of the primary cooling loop?

The cooling water of any water-cooled reactor undergoes radiolytic decomposition, induced by gamma, fast-electron, and neutron radiation in the reactor cores. Unless mitigating steps are taken, oxidizing species produced by the coolant radiolysis can promote intergranular stress-corrosion cracking and irradiation-assisted stress-corrosion cracking of iron- and nickel-based alloys. These will alter corrosion rates of iron- and nickel-based alloys and zirconium alloys in reactors. One commonly used remedy to limit corrosion by oxidizing species is to add hydrogen in sufficient quantity to chemically reduce transient radiolytic primary oxidizing species (OH, H<sub>2</sub>O<sub>2</sub>, HO<sub>2</sub>/O<sub>2</sub><sup>-</sup>). This stops the formation of oxidizing products (H<sub>2</sub>O<sub>2</sub> and O<sub>2</sub>); but, it is still unclear whether this will be effective at the higher temperatures proposed for future reactors. While an earlier FY 1999 NERI project (99-276) investigated some of the most important radiation chemistry in supercritical water (SCW), there is no information at all on the effect of neutron radiolysis, which is the main source of the troublesome oxidizing species.

The objective of this project is to discover most of the fundamental information necessary for a predictive model of radiation-induced chemistry in a supercritical water

reactor core. Electron pulse radiolysis coupled with transient absorption spectroscopy is the method of choice for measuring kinetics of radiation-induced species and product yields for fast electron and gamma radiation. Researchers are measuring second-order free radical reaction rates in high-temperature water using the Argonne Chemistry Division electron linear accelerator. The University of Wisconsin (UW) Nuclear Reactor Facility is a very convenient source of neutron radiation that can be exploited for radiolysis experiments from room temperature to 500°C. The combined capabilities will make it possible to create a quantitative model for water radiolysis in both current PWR systems and supercritical, water-cooled plants in the future.

### Research Progress

The first major task was to design, construct, and test an apparatus that could be inserted into UW's nuclear reactor to obtain information on the chemistry induced by neutron interaction with SCW. This was a challenging endeavor because several operational factors had to be considered, which added constraints on the materials, size, and operation of the loop components. Also of concern was shielding for and safety of operators of the SCW loop facility. In this experiment, researchers pump aqueous solutions containing certain well-characterized reagents into an irradiation zone next to the reactor core, give an exposure on the order of ten seconds, and collect the cooled, irradiated solution within one to two minutes at the exit of the beam port for analysis. The reagents are chosen to produce simple, highly stable gas molecules that can be stripped out and analyzed with very sensitive mass spectroscopy. To remove most of the uncertainties inherent in previous reactor experiments, researchers need to carry out the analyses immediately, and control the temperature within 0.1°C in the irradiation zone.

Figure 1 shows an overall schematic of the loop, which is comprised of several different sections. Also shown is a schematic representation of the instrumentation necessary



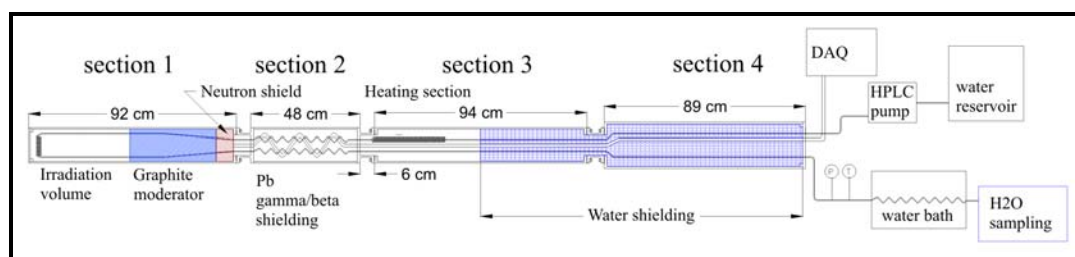


Figure 1. Overall schematic of the SCW in pile loop facility.

for operation and for measurement of the neutron-induced chemistry in high-temperature water.

Researchers have completed the design and construction of the flow loop and are now in the testing phase to ensure proper operation of the thermal hydraulics and chemistry measurement procedure before it is inserted into the reactor beam port for radiolysis experiments.

Measurement of the gas products with this apparatus will be fruitless unless careful measurements are also made of the energy deposited by fast neutrons into the water solutions. To this end, researchers have carried out extensive modeling of the UW reactor core and the experimental irradiation volume during the first year of the program using the MCNP neutron transport code. One critical result of these simulations is shown in Figure 2: the vast majority of energy deposited in the flow tube will occur within the irradiation volume near the core, where the temperature is to be carefully controlled. As a quantitative test, researchers carried out initial irradiation foil experiments on the inside face of the innermost concrete plug of the beam port and compared this to the calculated fluxes at the same location. Results of these initial measurements were somewhat scattered, though of the correct order of magnitude. Researchers will perform further direct calibration of the absorbed dose as part of the experimental program.

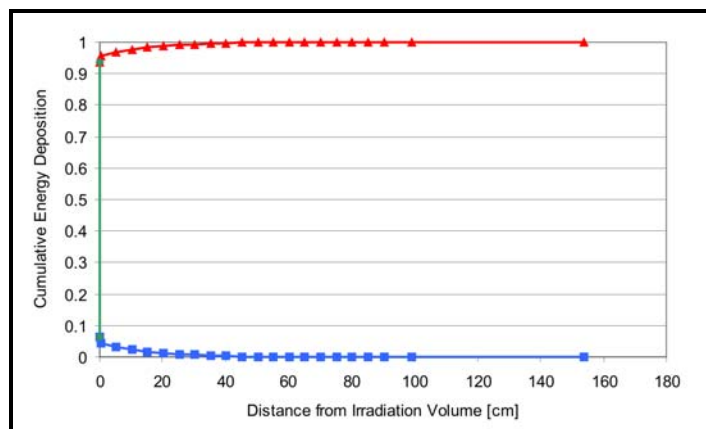


Figure 2. Cumulative energy deposition in the incoming feed line (blue), 2-meter-long irradiation volume (green), and outgoing return line (red).

Experiments carried out at Argonne during this first year continued work toward a comprehensive kinetic model in high-temperature water. This work directly supported the analytical chemistry for UW efforts.

Researchers have taken measurements with several visible-light-absorbing competition reagents and also direct UV detection of OH to determine the rate constant for  $\text{OH} + \text{OH} \rightarrow \text{H}_2\text{O}_2$ . Testing of a coating for tubing to allow direct analysis of hydrogen peroxide radiolysis product proved unsuccessful. The hydrogen peroxide decomposes to molecular oxygen and water on the tubing walls at elevated temperatures. Therefore, researchers are measuring the sum of oxygen and hydrogen peroxide produced in the neutron radiolysis by measuring the total  $\text{O}_2$  produced. They performed extensive work to demonstrate the sensitivity of the gas stripping and mass spectrometry detection technique. To conveniently analyze dissolved gas at the micromolar level, researchers needed to use an electron multiplier detector. Therefore, the team purchased an improved mass spectrometer for the Wisconsin experiments. Researchers hoped that formate ion could be used at elevated temperatures to produce stable  $\text{CO}_2$  gas from reacting with OH radicals. Experiments at Argonne have demonstrated, in agreement with previous work, that the formate thermally decomposes above  $200^\circ\text{C}$ , so that it cannot be used for this purpose in the Wisconsin experiments; researchers are searching for an alternative chemistry.

## Planned Activities

The testing phase for the Wisconsin neutron radiolysis apparatus has now begun, and it will be inserted into the reactor beam port once this phase is complete. The first experiments will simply measure  $\text{H}_2$  and  $\text{O}_2$  produced by neutrons in water at high temperature, to find out how large the radiolysis problem might be. The next experiment will test the efficacy of added  $\text{H}_2$  to suppress the production of  $\text{O}_2$  in supercritical water. It remains unclear whether this will be more difficult or less difficult relative to PWR conditions around  $300^\circ\text{C}$ . More detailed experiments to determine yields of H atoms, OH radicals, and hydrated electrons will follow. In addition, studies at Argonne will continue to focus on the very difficult measurement of second-order free radical recombination rates. Researchers will carry out the measurement of the very critical reaction rate of  $\text{H}_2$  with OH radicals in supercritical water.

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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Innovative Approach to Establish Root Causes for Cracking in Aggressive Reactor Environments

PI: Stephen M. Bruemmer, Pacific Northwest National Laboratory

Project Number: 02-075

Collaborators: General Electric Global Research Center

Project Start Date: September 2002

Project End Date: September 2005

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### Research Objectives

This research project focuses on the characterization of critical Fe- and Ni-base stainless alloys tested under well-controlled conditions where in-service complexities can be minimized. Researchers use quantitative assessments of crack-growth rates to isolate effects of key variables and high-resolution analytical transmission electron microscopy, which provides mechanistic insights by interrogating crack-tip corrosion/oxidation reactions and crack-tip structures at near atomic dimensions. Reactions at buried interfaces, not accessible by conventional approaches, are being systematically interrogated for the first time. Researchers on this project will use novel, mechanistic "fingerprinting" of crack-tip structures tied to thermodynamic and kinetic modeling of crack-tip processes to isolate causes of environmental cracking. They will compare the results on failed components removed from light water reactor (LWR) service (funded separately by industry collaborators).

This research strategy capitalizes on unique national laboratory, industry, and university capabilities to generate basic materials and corrosion science results with immediate impact to next generation nuclear power systems. Project activities will be integrated with other research projects, such as fundamental research funded by the DOE Office of Basic Energy Sciences and U.S. and international projects dealing with current LWR degradation issues. This leveraged approach will facilitate revolutionary advances by combining basic and applied science to understand and develop next generation materials that meet advanced reactor performance goals.

### Research Progress

**Single-Variable Stress Corrosion Cracking (SCC) Experimentation.** An essential first step to elucidate environmental cracking mechanisms is experimentation under well-controlled material, environmental, and stress

conditions. The selection of these conditions is critical to produce degradation where crack initiation and advance processes are best understood. Researchers on this project are controlling material, environmental, and electrochemical conditions to promote degradation by slip dissolution, hydrogen-induced cracking, or internal oxidation. This produces unique samples with known cracking mechanisms that can be used for crack-tip characterizations in the following task. A key limitation in extracting useful information from examinations on failed service components (e.g., from LWRs) is that material and environmental conditions are uncontrolled. As a result, off-normal conditions often contribute to the cracking process and complicate interpretation of basic environmental degradation mechanisms.

Researchers completed critical SCC experimentation in several areas, including crack-growth rate measurements on warm-worked stainless steels in high-temperature water environments and static tests on sensitized stainless steels comparing effects on key solution impurities (chloride, thiosulfate, fluoride, and lead). These tests provided unique samples for crack-tip characterizations that complemented contributions from other collaborators who supplied cracked service components from operating commercial nuclear power plants.

**Crack-Tip Characterization.** The goal of this task is to generate a library of high-resolution, crack-tip "fingerprints" of different known mechanisms of environmental cracking. This can then be used to verify model predictions and to compare with in-service cracking. The analytical transmission electron microscopy (ATEM) examination of crack tips has proved particularly effective in discriminating different mechanisms of degradation in Ni-base alloy, steam-generator tubes and in stainless steel components removed from high-temperature water service.

Researchers documented crack and crack-tip corrosion structures at near atomic dimensions for environment-induced cracks in several key nickel-base alloys. They made first-of-a-kind comparisons between Pb-assisted SCC of alloy 600 in high-temperature water for controlled laboratory tests and pressurized water reactor (PWR) secondary-side steam generator tube failures. Contrary to current accepted theories, caustic crack solutions were not required to promote rapid intergranular (IG) SCC in alloy 600. Researchers found nearly identical crack and crack-tip structures in both the laboratory and service samples with high Pb concentrations in nanocrystalline oxides at the leading edges of attack, as illustrated in Figure 1. Although present in parts per million levels in solution, Pb enriches to greater than 10 weight-percent in the corrosion product oxides. Researchers also investigated crack tips in alloy

182 weld metal for the first time. The researchers removed this material from dissimilar metal weldments in a PWR outlet nozzle. They identified stress-corrosion cracks following high-angle grain boundaries—not interdendritic boundaries as reported in the literature. Researchers performed detailed examinations to investigate solidification-induced segregation and evidence of hot cracking that could be a precursor to subsequent environment-induced crack growth. Significant segregation was limited to interdendritic boundaries where no cracking was discovered. The team did not identify hot cracking in these weldments.

**Modeling Crack-Tip Corrosion Reactions.** The final key area of research during the first year was in modeling crack-tip corrosion reactions. Researchers made predictions of solution thermodynamics and corrosion-product

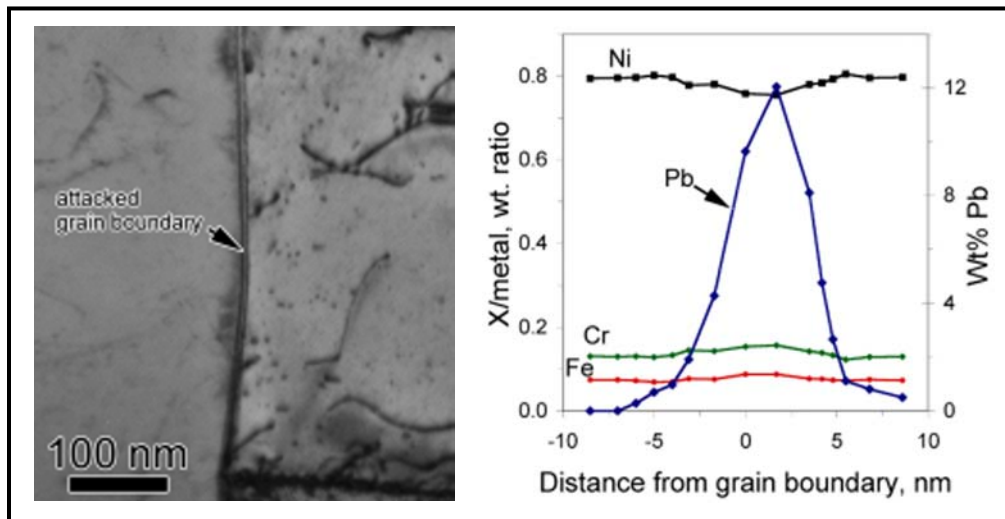


Figure 1. Intergranular attack in Alloy 600: (a) TEM image of oxidized grain boundary and (b) fine-probe composition profile across corroded boundary showing Pb enriched to ~12 wt percent.

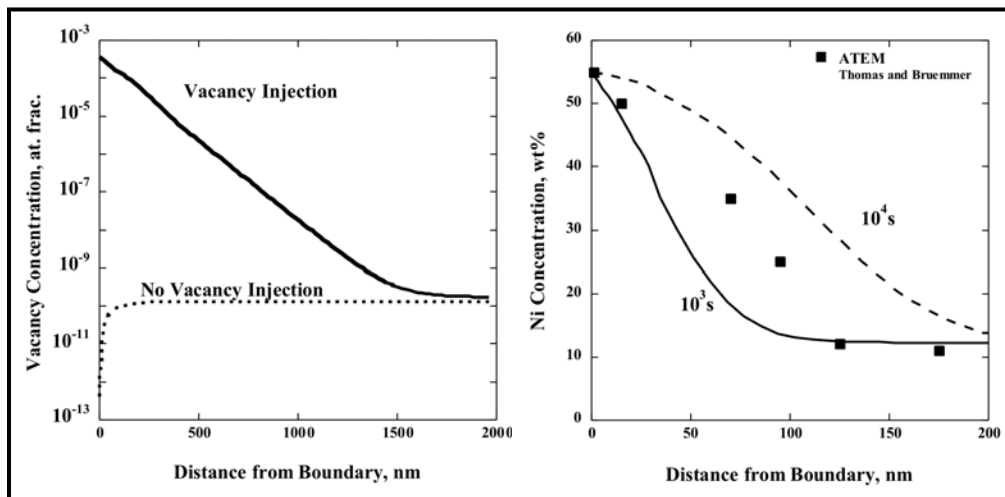


Figure 2. Model predictions for crack-tip corrosion-induced vacancy injection: (a) vacancy profiles ahead of tip with and without injection and (b) predicted Ni concentration ahead of crack tip for two delays between crack advance steps compared to ATEM measured concentration.

phase stabilities focusing on high-temperature water system with Pb as an impurity. They are now exploring important aspects of Pb migration down cracks and enrichment at crack tips. Researchers also modeled solid-state processes occurring ahead of a growing IGSCC crack to interpret mechanisms of crack advance. They made key comparisons to recent high-resolution microchemistry measurements on crack tips in a 304SS top guide after more than 30 years of reactor service. They evaluated possible explanations for unexpected observations of significant Cr/Fe depletion and Ni enrichment extending up to 100 nm ahead of the tips relative to crack advance rates and known diffusion processes. Selective dissolution and corrosion-induced vacancy injection were required to develop the measured crack-tip compositional changes (Figure 2).

## Planned Activities

**Single-Variable SCC Experimentation.** Researchers are continuing crack-growth and static SCC tests under well-controlled material, environmental, and stress conditions. Materials issues being isolated are bulk composition, grain boundary structure and composition, and matrix strength on cracking response along with environmental issues such as solution composition and electrochemical potential. This research will produce clear examples of cracking where the mechanism of crack growth is well established, i.e., slip-oxidation, hydrogen-induced cracking, and internal oxidation. Much of this work will be on current stainless steels and nickel-base alloys with new tests starting on advanced replacement materials.

**Crack-Tip Characterization.** High-resolution ATEM characterizations will continue to generate the library of crack-tip "fingerprints" of different known mechanisms of environmental cracking for model verification and comparisons with service failures. Researchers will use well-controlled, crack-growth samples to establish SCC crack-tip and crack-wall signatures in high-temperature water

environments. They will investigate structure, composition, and kinetics of crack-wall film growth. They will also examine solution impurity effects on crack advance and corrosion-product characteristics using static test samples focused on isolating the influence of chloride, thiosulfate, fluoride, and lead. Research on hot cracking and SCC in nickel-base alloy weldments will expand with the intent to document processes that control cracking mechanisms in current and advanced weld metals.

### **Modeling Crack-Tip Corrosion Reactions.**

Researchers will continue mechanistic modeling to relate measured SCC response and crack-tip corrosion products to predictions using activity, solubility, and kinetics of corroding species and to rationalize stable and metastable phases observed at crack tips. Three modeling subtasks will be pursued: 1) thermodynamically favored phases, 2) kinetically allowed phases, and 3) SCC crack growth.



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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Design of Radiation-Tolerant Structural Alloys for Gen IV Nuclear Energy Systems

PI: Todd Allen, University of Wisconsin-Madison

Project Number: 02-110

Collaborators: Argonne National Laboratory, University of Michigan, Pacific Northwest National Laboratory, Japan Nuclear Cycle Development Institute

Project Start Date: September 2002

Project End Date: September 2005

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### Research Objectives

The aim of the project is to focus on methods to improve the radiation tolerance of both austenitic and ferritic-martensitic (F-M) alloys projected for use in Generation IV (Gen IV) systems. The expected materials limitations of Gen IV components include higher temperature creep strength, dimensional stability, and corrosion/stress corrosion compatibility. The research focuses on three main concepts for achieving increased radiation tolerance in these alloys: 1) grain boundary engineering, 2) the addition of oversized solutes to the matrix, and 3) microstructural/nanostructural control by matrix precipitate addition. Each approach is aimed at mitigating specific irradiation effects. Grain boundary engineering will increase the fraction of special boundaries, reducing radiation-induced segregation (RIS) to those boundaries and strengthening grain boundaries against creep from sliding and deformation. Oversized solute additions will promote recombination, reducing RIS and altering the dislocation microstructure. Matrix precipitate additions provide a high density of interfaces to promote recombination and trap He, and also strengthen the matrix against high-temperature creep.

### Research Progress

**Grain Boundary Engineering.** Grain boundary engineering involves a series of thermo-mechanical treatments designed to convert a fraction of the high-energy boundaries to low-energy boundaries identified as Coincident Site Lattice (CSL) boundaries, thus reducing cracking susceptibility and improving creep strength. This project developed the first treatment to enhance the fraction of CSL boundaries in an advanced, F-M steel-T91. F-M alloys present a unique challenge due to their complicated microstructure. T91 is a low-carbon, 9Cr-1MoVNb steel that is used in the two-phase, F-M structure. The standard

heat treatment consists of 1) a solution anneal at 1,066°C to completely austenitize the microstructure and dissolve the carbides and 2) a tempering treatment at 790°C to relieve the stresses and enhance toughness. The resulting microstructure consists of tempered martensitic laths forming subgrains in a ferrite matrix, with (V, Nb) carbonitrides precipitated mainly on dislocations within the subgrains and  $M_{23}C_6$  precipitated on the prior austenite grain boundaries and on sub-grain boundaries. The sub-grain structure produced by martensitic transformation and the precipitation of carbides and carbonitrides are the primary microstructural features responsible for its excellent high-temperature creep strength.

The challenge was to enhance the grain boundaries without disturbing the original microstructure. Since the microstructure is critical to achieving high-temperature properties, the heat treatment process requires strict control. Researchers developed a treatment in which the CSL boundaries fraction of T91 was enhanced over the as-received case while maintaining the other critical features of the microstructure: grain size, carbide size and location (see Figure 1), density, and hardness. Improved creep strength should result from the preservation of all the microstructural features decisive for creep strength in T-91, and from an increase in fraction of low-angle boundaries.

**Oversized Solute Additions.** The second task was to study the effect of oversized solute additions on reducing radiation damage. The addition of oversized solutes is expected to restrict the development of deleterious microstructural features through interaction of the oversized solutes and radiation-induced point defects. Researchers attempted to fabricate a series of alloys by adding an oversized solute. Scandium, yttrium, hafnium, and zirconium were added to 316 stainless steel. Alloys with hafnium and zirconium were the easiest to fabricate and

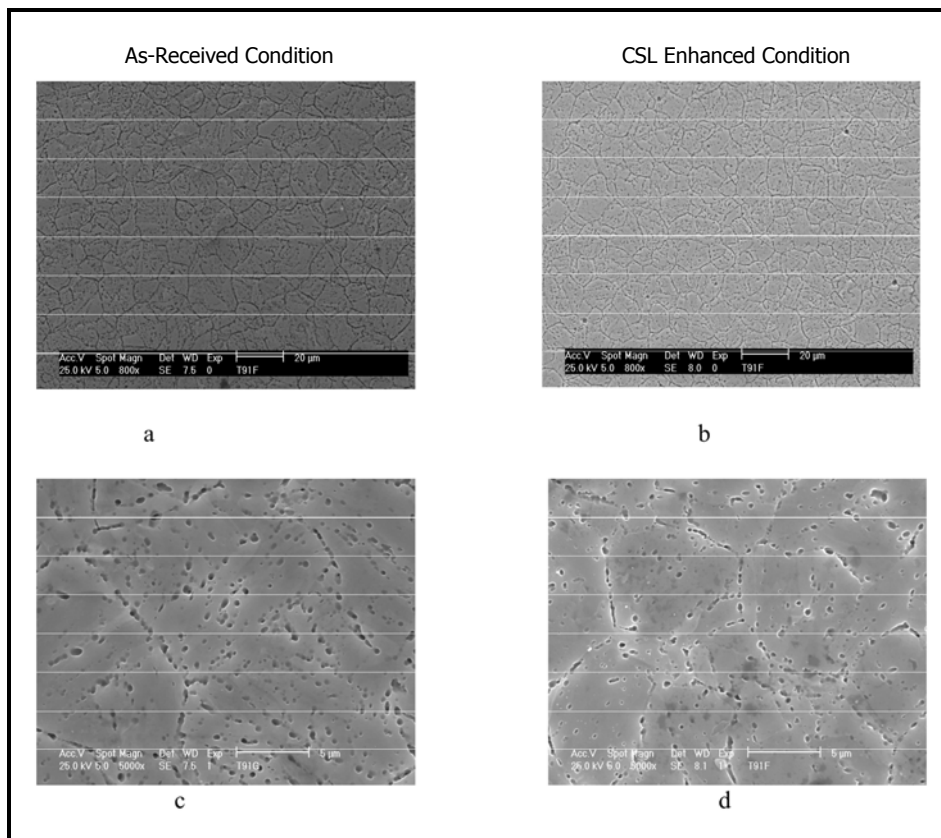


Figure 1. T91 and CSL-enhanced T91 showing: a, b) grain size; c, d) carbide size and location.

were ultimately chosen for radiation testing. Researchers developed treatments to maximize the amount of hafnium or zirconium in solution.

Researchers irradiated hafnium- and zirconium-containing alloys with either high-energy nickel ions or with reactor neutrons. The reactor-irradiated samples received their exposure in the Fast Flux Test Facility (FFTF). For hafnium- and zirconium-containing alloys irradiated with high-energy nickel ions, the addition of hafnium or zirconium reduced or delayed the formation of voids significantly compared to alloys without the additions. This is consistent with results from previous NERI studies (Project No. 99-155) using ion irradiations and work in Japan using neutron irradiation. The reduction or delay of swelling could be an improvement in austenitic alloys. This would allow their use to much higher doses than that achieved in the U.S. fast reactor development program. Changing the pre-irradiation heat treatment to take the hafnium out of solution and into precipitates reduced the effectiveness of hafnium in preventing void swelling.

Zirconium additions to a high-purity stainless-steel alloy did not reduce void swelling after high-dose irradiation in FFTF. In Year 2, researchers will perform a detailed study

of the microstructure of the nickel-ion irradiated and neutron-irradiated samples to better understand the differences in response and evaluate effects of the oversized element on the incubation time for swelling.

**Stability of Nano-particulate Additions.** The final task in Year 1 of this project was to evaluate the stability of the oxide particles in a 9Cr ferritic-martensitic oxide dispersion strengthened (ODS) stainless steel. ODS steels are being developed to increase the high-temperature strength of alloys while maintaining excellent swelling resistance. The dispersed oxide particles are critical to improving the high-temperature strength. The oxide stability in a radiation field is critical to continuous, adequate performance to high-radiation dose. The 9Cr ODS steel was irradiated to 5, 50, and 150 dpa using high-energy nickel ions; researchers

examined the resulting microstructure at each dose. As the dose increased, the average oxide particle size decreased slightly from 11.8 nm to 9.1 nm. But, even at this high dose, the resulting oxide distribution is expected to support the high-temperature creep strength required of an ODS alloy. No voids were seen in the ODS alloy, even up to 150 dpa.

## Planned Activities

In Year 2 of this project, the grain boundary engineering task will focus on creep testing of the CSL-enhanced T91 alloys to verify that the CSL enhancements did improve the creep resistance. Researchers will perform additional irradiation and examine the resulting microstructure on alloys with oversized solute additions. Finally, the team will perform tests on other candidate Gen IV ferric-martensitic steels and examine the changes in hardness and microstructural features.



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# NUCLEAR ENERGY RESEARCH INITIATIVE

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## Enhanced Control of PWR Primary Coolant Water Chemistry Using Selective Separation Systems for Recovery and Recycle of Enriched Boric Acid

PI: Ken Czerwinski, University of Nevada-Las Vegas

Project Number: 02-146

Collaborators: University of California-Berkeley, Los Alamos National Laboratory, Pacific Southern Electric & Gas Company, Florida Power & Light, (n, p) Energy, Inc.

Project Start Date: October 2002

Project End Date: September 2005

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### Research Objectives

The fundamental science of operating existing and advanced pressurized water reactors (PWRs) clearly shows that increasing nuclear fuel enrichment will produce more energy. However, to operate within the nuclear reactor safety requirements, the concentration of natural boric acid used as a flux chemical shim would have to be increased. The key objective of this research project is to develop systems for efficiently and selectively recovering special purpose isotopes that are added to primary coolant water in light water reactors (LWRs) for neutron flux control and water chemistry. Typically,  $^{10}\text{B}$ -enriched boric acid,  $\text{B}(\text{OH})_3$ , is favored over natural boron for neutron flux control. This is because it allows the use of a lower  $\text{LiOH}$  concentration to maintain operational pH, which helps to decrease the extent of corrosion cracking resulting from the  $\text{LiOH}$ . However, the cost of producing and using enriched isotopes such as  $^{10}\text{B}$  and  $^7\text{Li}$  requires a means to cost-effectively recover and reuse them.

The goal of this project is to develop and field test polymeric sequestering systems designed to efficiently and selectively recover enriched boric acid/lithium hydroxide from the primary coolant water of LWRs. These advanced separation materials will reduce the cost of operating existing and advanced LWR systems by improving the chemical control of the primary reactor coolant. Researchers on this project will characterize contaminants present in the coolant system according to their potential for interfering with the selective recovery of  $^{10}\text{B}$  and  $^7\text{Li}$ , with an effort to assess the impact of actinides and activation products on target isotope separation. Then they will develop counter measures to mitigate the interference of non-target radionuclides. Cost benefits will result from greater energy production per reactor unit, reduced operational radiation

exposure, and protection from accelerated corrosion of critical core components.

### Research Progress

Project researchers currently at University of California-Berkeley, and University of Nevada-Las Vegas, expanded the existing boron/polymer chemical speciation model to include polyborate ion paired species. In order to model behavior of the polymer filtration chemical system, researchers made assumptions as to the actual chemical species involved. As shown in Figure 1, previous models had only little success at predicting binding fractions at low total boron concentrations, and diverged even more widely at higher concentration values, both in the pH of the maximum binding and the total bound value. The model does not predict the shift on the pH of maximum binding that scientists observed experimentally—from near 9.5 at dilute boron concentrations to near 6.2 at the highest boron concentrations. By adding four ion pair species to the CHESS database, researchers produced a much closer agreement to the experimental data. Each of the four species added represented an ion pair species where one of the four borate anions known to exist in aqueous solution binds to the positively charged protonated polymer backbone sites. Researchers analyzed  $^{11}\text{B}$  NMR (Nuclear Magnetic Resonance) data to determine appropriate CHESS formation constants. The modeling utilized experimental binding results provided by researchers at Los Alamos. By adding polyborate ion pair species, researchers on this project made two significant improvements in the model prediction. As illustrated in Figure 2, the model now begins to predict the experimentally observed shift on the pH of maximum binding to a lower pH. It also improves the agreement in the prediction of binding fraction at high boron concentration to within a factor of two.

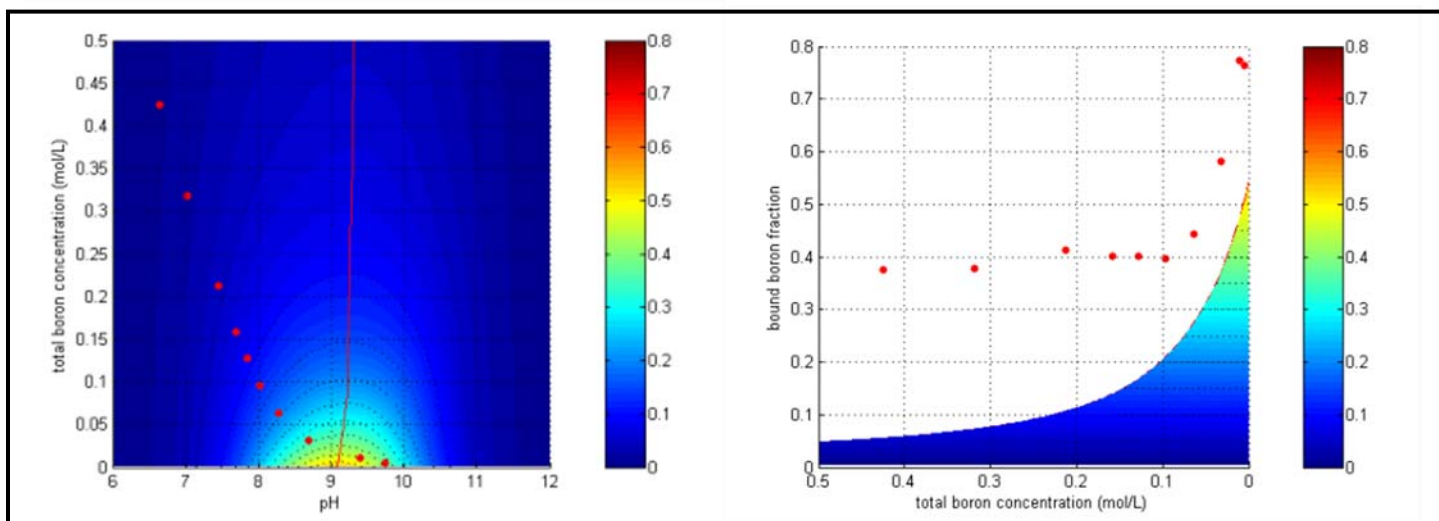


Figure 1 – Previous Model: The colored surface represents the fraction of boron bound to the polymer as calculated by the model. Experimental data points are represented by red dots. Without any polyborate species or ion pair species, this model fails to predict the system behavior under any conditions.

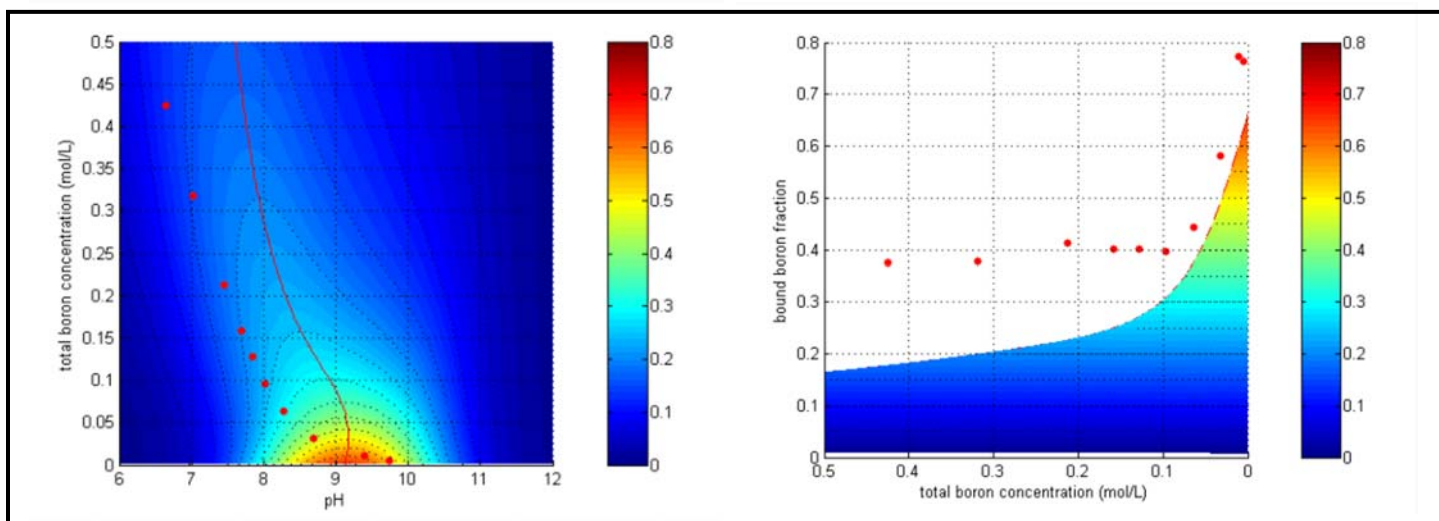


Figure 2 – Current Model: The colored surface represents the fraction of boron bound to the polymer as calculated by the model. Experimental data points are represented by red dots. With the addition of polyborate ion pair species, the model begins to predict a shift on the pH of maximum binding to a lower pH. It also improves the agreement in the prediction of binding fraction at high boron concentration.

Researchers at UC Berkeley prepared terephthalamide functionalized polyethylenimine (PEI) for use in the on-site industrial investigations. In previous work, terephthalamide ligands proved useful in separating actinide metal ions in polymer filtration when incorporated into water soluble chelating polymers, such as PEI. In current work, researchers are examining the boron and boric acid binding of a variety of catecholamide (CAM), terephthalamide (TAM), and hydroxypyridinone (HOPO) ligands.

Researchers at the Los Alamos Laboratory completed model compound studies using simple primary (1°), secondary (2°), and tertiary (3°) nitrogen-containing compounds. The reactions were followed by NMR and

selected peaks were integrated to determine the loss of starting material and the gain of product. Researchers performed the synthesis of the last polymer of the series, the triol. The material was characterized by H and C-NMR and verified to be the target polymer. Subsequently, researchers performed an extraction series, and found the extraction order for boron to be triol, diol, and monol, from greatest to least, respectively. In addition, they performed ion-pairing suppression studies in an attempt to get an estimate of the ratio of ion pairing to diol ester formation. At 0.1 M ionic strength, the monol was essentially suppressed while the diol retained 28 percent of its original 79-percent binding.

## Planned Activities

The following work is being planned for Year 2 of the project:

- Researchers plan to further develop the reactor contamination model, use experimental data to evaluate species interference with B and Li, and develop methods to remove interferences.
- Researchers will develop other polymers and look at the specifics of interfering elements such as actinides, fission products, and activation products.
- Researchers will continue to look at the extraction of boric acid and Li with ultrafiltration membranes, focusing on temperature effects.
- Researchers will complete procedures and training for the in-plant demonstration phase and coordinate with plant operators to develop extraction flow sheets.



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