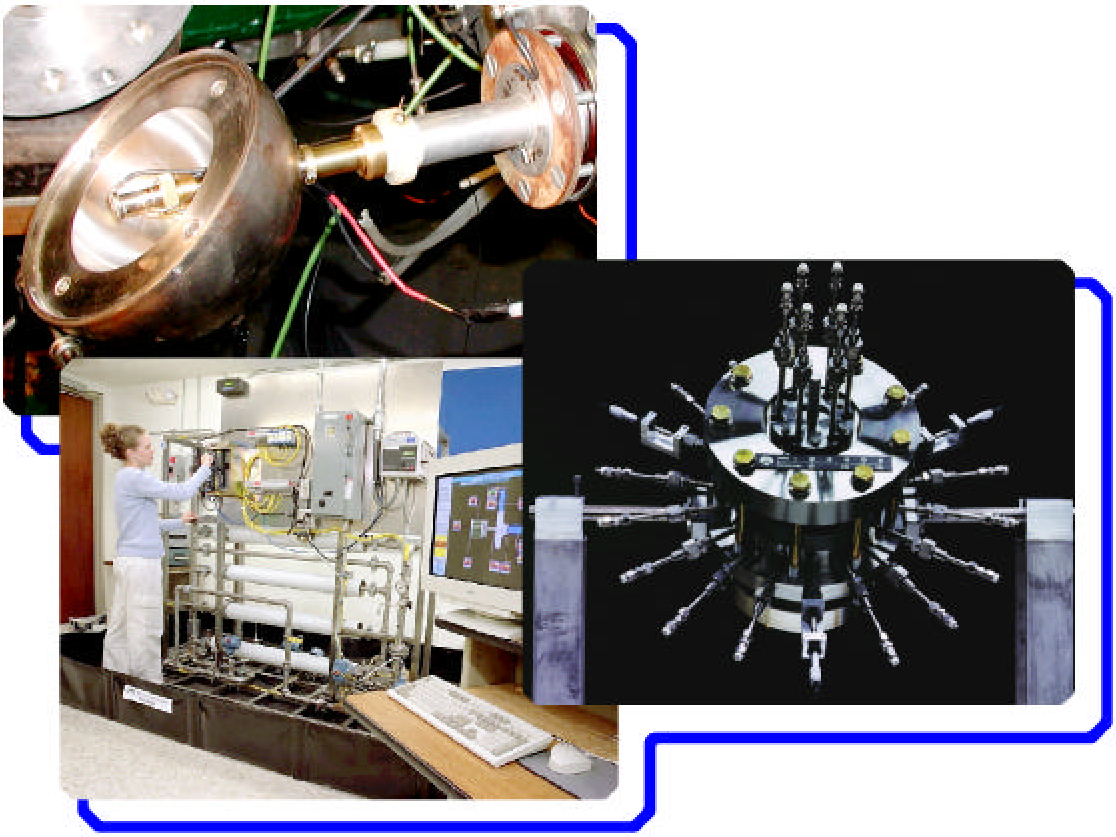
DOE/NE-0121

# Nuclear Energy Research Initiative



## Annual Report 2001

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## FOREWORD

The Nuclear Energy Research Initiative (NERI) began in fiscal year 1999 as the core of a new, restructured Federal effort to develop advanced nuclear energy. NERI grew out of the recommendations made in the November 1997 report by the President's Committee of Advisors on Science and Technology on Federal energy research and development. Its purpose is to apply the successful methodologies to select quality research projects that have been used for years by scientific agencies such as the National Science Foundation. Using independent, expert peer-review to competitively select project proposals from a wide range of researchers in academia, national laboratories, and industry.

Adapting this methodology to the more applied nature of nuclear energy technology development has been a challenging and rewarding experience for the Department. Excellent research covering many areas of science and technology that might never have been conducted using more traditional approaches to funding research is now underway, adding significantly to the body of knowledge. NERI has supported innovative solutions to the key issues facing the generation of electric energy using nuclear fission—namely, proliferation, safety, waste generation and disposal, and economics. NERI has pointed the way for efforts such as the Generation IV Nuclear Energy Systems initiative and spawned a significant increase in international cooperation. Furthermore, NERI has helped maintain the Nation's nuclear science and engineering infrastructure.

This Annual Report summarizes research progress based on information submitted by the principal investigators for each of the NERI projects initiated in FY1999. Also included in this document are the abstracts for the FY2000 NERI research awards. This report is a first step in disseminating the results of NERI research to the wide R&D community to spur yet more innovation to assure a bright future for nuclear energy in the United States and the world.

William Magwood IV, Director
Office of Nuclear Energy, Science and Technology

# NUCLEAR ENERGY RESEARCH INITIATIVE

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# NUCLEAR ENERGY RESEARCH INITIATIVE

## 1. INTRODUCTION

The Department of Energy (DOE) created the Nuclear Energy Research Initiative (NERI) to sponsor nuclear energy science and technology research and development in order to address and help overcome the principal barriers to the future use of nuclear energy in the United States. NERI will also help preserve the nuclear science and engineering infrastructure within our nation's universities, laboratories, and industry and will advance the development of nuclear energy technology, enabling the United States to maintain a competitive position worldwide. DOE believes that in funding creative research ideas at the nation's science and technology institutions and corporations, solutions to important nuclear issues will be realized and a new potential for nuclear energy will emerge in the United States.

The Nuclear Energy Research Initiative Annual Report serves to inform interested parties of progress made in NERI on a programmatic level, as well as research progress made in individual NERI projects during the initial year of the program.

Section 2 of this report provides background on the events that led to the creation and implementation of NERI, a discussion of the goals and objectives of NERI, the NERI research focus areas, as well as information on the management of the program.

Section 3 provides a summary of NERI's fiscal year (FY) 1999 awards and accomplishments, FY2000 awards and accomplishments, and FY2001 planned activities.

Sections 4 through 7 provide an index and research summary of the individual FY1999 NERI projects. These reports discuss NERI projects that have advanced sufficiently to enable the Department to report their progress. Research objective, research progress to date, and planned activities for the next research phase is described for each of the funded projects.

Finally, an index and abstracts for each of the FY2000 research awards can be found in Section 8.

## 2. BACKGROUND

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

In its November 1997 report, the PCAST Panel on Energy Research and Development determined that establishing nuclear energy as a viable and expandable option was important and that a properly focused R&D effort to address the potential long-term barriers to 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 research and development activities in an R&D effort to address these potential barriers with a new nuclear energy research initiative. This new initiative would fund research based on competitive selection of proposals from the national laboratories, universities and industry.

The Department endorsed the PCAST recommendations and received Congressional appropriations in FY1999 for NERI to sponsor innovative scientific and engineering R&D to address the key issues affecting the future use of nuclear energy and to preserve our nations nuclear science and technology leadership.

To achieve these long-range goals, NERI has the following objectives:

- Develop advanced reactor and fuel cycle concepts and scientific breakthroughs in nuclear technology to overcome the principal scientific and technical obstacles to expand future use of nuclear energy in the United States, including issues involving nuclear material proliferation, unfavorable economics, and nuclear waste disposition.

- Advance the state of U.S. nuclear technology to maintain a viable nuclear power options for the near and long-term.

- Promote and maintain a nuclear science and engineering infrastructure to meet future technical challenges.

In order to determine the initial focus of the NERI research areas, DOE convened a workshop in April 1998 of nuclear community stakeholders, including national laboratory, university, and industry representatives. As a result of this NERI workshop, DOE focused its initial scientific and engineering R&D on the following:

- 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.

The Department also changed the method by which it selected R&D projects to support. The Department solicited researcher-initiated R&D proposals from universities, national laboratories, and industry in very broad R&D areas.

The researchers selected research topics of interest and defined the scope and extent of the R&D in their proposals. The Department employed an independent, expert peer review process to judge the scientific and technical merit of the R&D proposals. For those proposals judged to have the highest scientific and technical merit, the Department conducted a programmatic review to ensure conformance of selected projects with DOE policy and programmatic requirements. The two reviews resulted in award selection recommendations to the Department's Selection Official.

To help guide this R&D effort and shape the future direction of nuclear energy R&D, the Secretary of the Department of Energy established an independent advisory committee, the Nuclear Energy Research Advisory Committee (NERAC). A NERAC chartered subcommittee developed a *Long-Term Nuclear Energy Science and Technology Research Plan* to guide nuclear energy research out to the year 2020. In addition, NERAC issued a report on *Technology Opportunities for Increasing the Proliferation Resistance of Global Nuclear Power Systems (TOPS)*. The Department intends to use this long-term R&D Plan and TOPS report to guide future NERI research activities.

## 3. NERI ACCOMPLISHMENTS

In FY1999, the Department received 308 investigator-initiated R&D proposals from U.S. universities, national laboratories, and industry. The initial FY1999 NERI procurement was completed with the award and issuance of grants, cooperative agreements, and laboratory work authorizations for 46 R&D projects involving research participants from 45 U.S. universities, laboratories and industrial organizations. Thirty-two of the projects involved collaborations of multiple organizations. In addition, 11 foreign R&D organizations participated in NERI collaborative projects.

The FY1999 NERI appropriation was $19 million. The duration of these annually funded awards is one to three years, with most being for a three-year period. The total cost of these 46 research projects for the three-year period is over $52 million.

Figure 1 depicts the number of FY1999 research projects in each of the four noted R&D areas. Proliferation resistant technologies, though not specifically mentioned, are incorporated in most of the advanced nuclear fuels and new reactor designs and technologies research projects. Additionally, the fundamental nuclear science area includes research projects in materials science, fundamental chemistry, computational and engineering science, and nuclear physics.

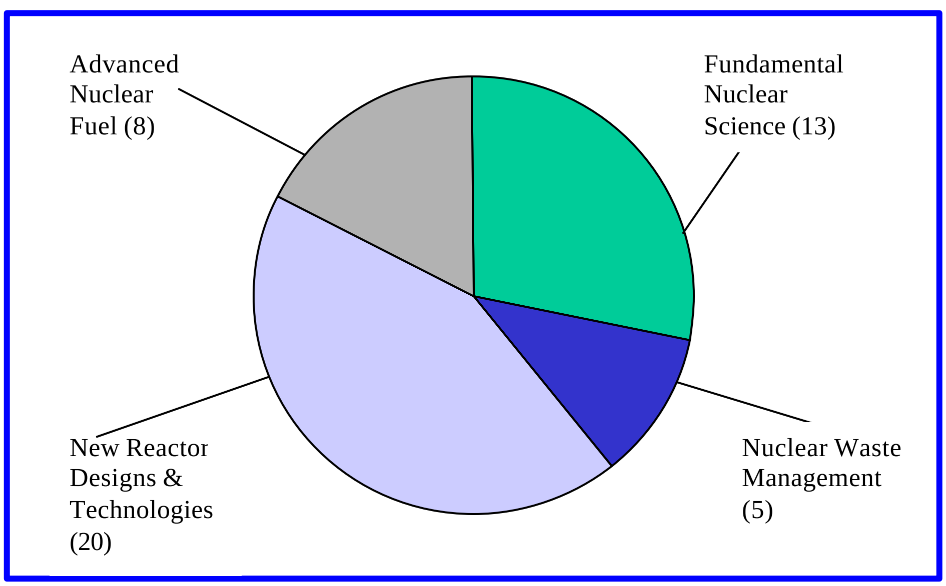



**FIGURE 1**

NERI R&D Areas (FY1999)

In FY2000, scientific knowledge and technology development was advanced through the continuation of research efforts begun in FY1999 and through the award of ten new NERI R&D projects involving 18 U.S. and six foreign R&D organizations. Figure 2 provides a funding summary of the participating organizations based on the FY1999 and FY2000 project funding. FY2000 appropriations totaled $22.5 million.

The Department as part of the NERI Program has not funded foreign participation in existing projects. It has been supported by foreign nuclear organizations interested in the research being conducted. Although the principle investigators have been responsible for soliciting such support, the Department does approve all project participants.

In FY2001, DOE anticipates awarding approximately 15 new NERI projects and continuing ongoing research projects begun in FY1999 and FY2000. Approximately $28 million has been appropriated for this effort.

In addition, the 1999 PCAST report on International Cooperation on Energy Innovation recommended that an international component to NERI be created to promote "bilateral and multilateral research focused on advanced technologies for improving the cost,

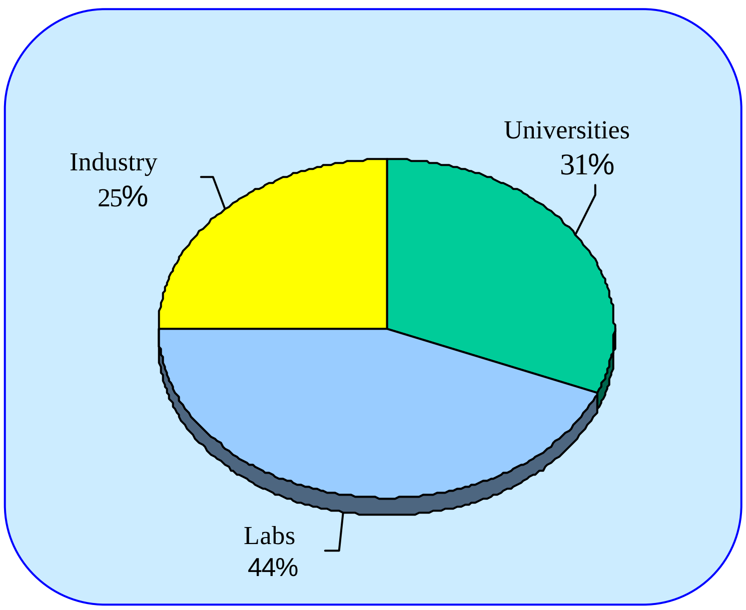



**FIGURE 2**

NERI Overall Funding Profile (FY1999 + FY2000)

safety, waste management, and proliferation resistance of nuclear fission energy systems." In FY2001, the Department will launch a new initiative, the International Nuclear Energy Research Initiative (I-NERI) for bilateral and multilateral nuclear energy research. Approximately $7 million has been appropriated for bilateral, cost-shared research work under the I-NERI program with countries such as Japan, South Korea, France, South Africa, and the European Union.

I-NERI would allow DOE to leverage federal investment with international resources through specific cost-share arrangements with each participating country on a wide range of nuclear technology topics. I-NERI would further enhance the United States and the Department's influence in international policy discussions on the future direction of nuclear energy.

I-NERI will also feature competitive researcher-initiated R&D selected through an independent peer-review process by international experts from the U.S. and each participating country.

## 4. NEW REACTOR DESIGNS AND TECHNOLOGIES

This program element focuses on two of the NE long-term R&D goals. The first of these goals addresses the need to develop advanced nuclear reactor technologies that will allow the deployment of highly safe and economical new nuclear power plants that would be a competitive electricity production alternative in the U.S. and foreign markets, while being responsive to environmental, waste management, and proliferation concerns. The second addresses the need to develop instrumentation, controls, information management and decision making tools for use in nuclear power plants that employ or adapt the latest technological advances in digital instrumentation and controls, communications and man-machine interface technology including micro-analytical devices and/or smart sensors, on-line signal validation and condition monitoring.

As noted in the long-term R&D goals, competitive nuclear plant costs are necessary to restore nuclear power as a viable option to help meet our future electrical power demands. Therefore, this program element also includes projects intended to identify and evaluate alternative methods, analyses, and technologies to reduce the costs of constructing future nuclear power plants.

Additionally, this element includes research projects to improve the intrinsic proliferation resistance 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 and utilization of plutonium and other actinide isotopes generated in the fuel.

Project selected under this element involve the investigation and preliminary development of advanced reactor and power conversion system concepts that offer the prospect of improved performance and operation, design simplification, enhanced safety, and reduced overall cost. They also include innovative reactor, system, or component designs; alternative energy/power conversion cycles, advanced instrumentation and control systems; or other important design features and characteristics.

Specifically, projects involving advanced reactors under this program element address, among other items, the characteristics, principal attributes, feasibility, safety features, proliferation resistance, economic competitiveness, and additional research that may be required. These reactor concepts include advancements in light water reactor technology to achieve higher performance or development of other higher temperature advanced reactor designs for higher efficiencies. These concepts also include compact or modular reactor designs suitable for transport to remote locations, alternative energy production or co-generation reactor applications. Desirable features include long-lived reactor cores that minimize or avoid altogether the need for refueling and concepts that maximize fuel burn-up or employ advanced energy conversion technology.

# NUCLEAR ENERGY RESEARCH INITIATIVE

## NUCLEAR ENERGY RESEARCH INITIATIVE

**Application of Innovative Experimental and Numerical Techniques for the Assessment of Reactor Pressure Vessel Structural Integrity**

| | |
|---|---|
| PI: | T.Y. Chu, Sandia National Laboratories (SNL) |
| Collaborators: | U.S. Nuclear Regulatory Commission (NRC), Organization for Economic Cooperation and Development (OECD)/Nuclear Energy Agency |
| Project Start Date: | August 1, 1999 Projected End Date: September 30, 2002 |
| Project Number: | 99-0018 |

## Research Objective

The lower head of the reactor pressure vessel (RPV) can be subjected to significant thermal and pressure loads in the event of a core meltdown accident. The mechanical behavior of the reactor vessel lower head is of importance both in severe accident assessment and the assessment of accident mitigation strategies. For severe accident assessment the failure of the lower head defines the initial conditions for all ex-vessel events, and in accident mitigation the knowledge of mechanical behavior of the reactor vessel defines the possible operational envelope for accident mitigation. The need for validated models of the lower head in accident scenarios is accomplished by well-controlled, well-characterized large-scale experiments simulating realistic thermal/mechanical loads to the reactor pressure vessel.

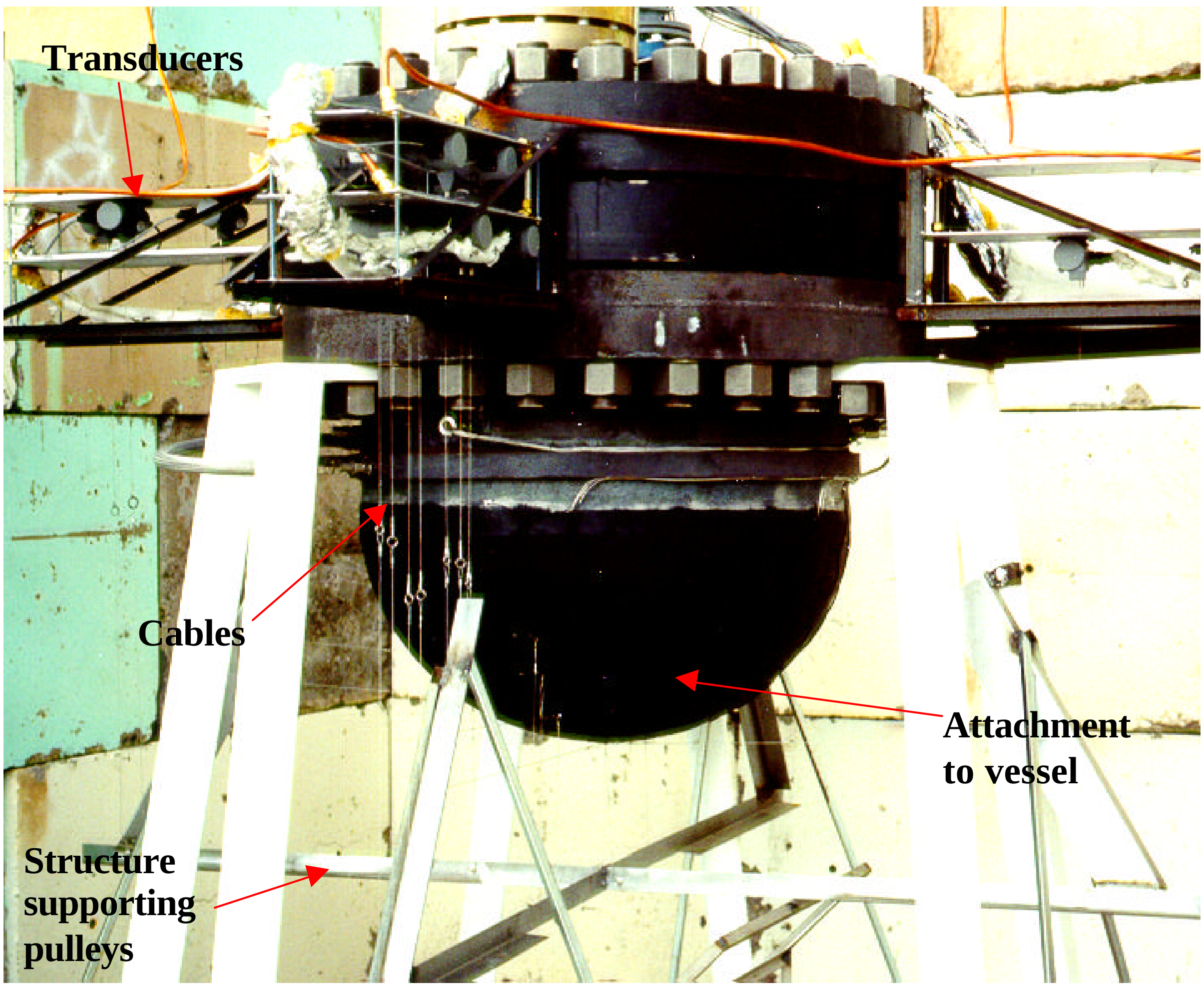
This project consists of both experimental and analytical efforts in investigating the structural integrity of reactor pressure vessels. Experiments simulating the thermal/mechanical loads to a reactor pressure vessel generate data that can be implemented into a finite element code, such as the commercially available code ABAQUS, to assess the ability of the code to capture the response of the pressure vessel to severe accident conditions. In addition, the pressure vessel material (SA533B1 steel) used in these experiments is prototypic of reactor pressurized water reactor vessel material and is well characterized by material property testing as part of this program.

The Nuclear Energy Research Initiative (NERI)/NRC/OECD sponsored program consists of eight international partners: Belgium, Czech Republic, Finland, France, Germany, Spain, Sweden, and the United States. U.S. support is provided by the NRC and the Department of Energy NERI program. This experimental/analytical program builds on the accomplishments of a previous NRC-sponsored Lower Head Failure (LHF) program (NUREG/CR-5582). The current program is referred to as the OECD Lower Head Failure (OLHF) program to distinguish it from the previous program and to recognize the international participation of the OECD.

**Research Progress**

The purpose of the OLHF project is to investigate lower head failure for conditions of low reactor coolant system (RCS) pressure (2-5 MPa) and prototypic temperature difference across the vessel wall ($\Delta T_W$) (200K-400K) where the previous NRC sponsored research investigated the condition of high RCS pressures and small $\Delta T_W$. Low RCS pressure is chosen because of the desire to use the data to develop models for assessing accident management strategies involving RPV depressurization. Pressure transient data is useful in assessing the effect of water injection as part of an accident management strategy. Prototypic $\Delta T_W$ is important because the need to provide data where stress redistribution in the vessel wall (as a result of decreasing material strength with temperature) is important.

The OLHF experiments are being performed using 1 to 4.85 linear scale models of a typical PWR lower head. Below is a picture of the OLHF test assembly. The test vessel is geometrically scaled to a typical PWR reactor to preserve the membrane stress.




**OHLF Test Assembly**

The test vessel consists of a 91.4-cm ID, nominally 70-mm-thick SA533B1 steel hemisphere welded to a 45-cm upright cylinder assembly closed off on top by a blank flange. The vessel is heated from within with a unique induction-heated graphite-radiating cavity. Large $\Delta T_W$ is achieved by increasing (with respect to geometrical scaling) the wall thickness and leaving the wall un-insulated. The membrane stress is preserved by increasing the test pressure by a factor corresponding to the wall thickness distortion ($R_W$), i.e., $P_{test} = R_W \cdot P_{RCS}$. The prototypical material for U.S. PWRs, SA533B1, was used to preserve material behavior. There are a total of five tests planned, two of which have already been performed. Both of these were conducted at constant RCS pressure tests. The bottom of the test vessel was uniformly heated for both the OLHF-1 and OLHF-2 tests. The equivalent RCS pressures for OLHF-1 and OLHF-2 were nominally 5 MPa and 2 MPa.

An extra vessel was fabricated from the SA533B1 steel from which samples were prepared for material property testing. This material underwent essentially the same heat treatment and work history as actual test vessels to minimize variability in material properties. Five tensile tests were performed at high temperature (925 K to 1275 K) and 21 creep tests were performed at about 75 percent and 95 percent of yield stress at high temperature (925 K to 1275 K). Two replicate creep tests were performed to provide a means of assessing the reproducibility of test results. Supplemental tests will also be performed by several of the OECD partners to extend and/or verify the database. The results of these tests are used to construct a constitutive model for implementation into structural analysis models.

**Planned Activities**

The test matrices for the remaining three tests are still evolving. Future tests will consider the effects of pressure transients as well as the effects of vessel penetrations. Also of interest is the effect of a pressure transient in the phase transition temperature range.

Analyses of the first tests are underway. Finite element simulations for each test will be performed at SNL using the commercially available ABAQUS code. The thermal data collected for each test is analyzed and implemented into the finite element method calculations. Additional analyses will be performed by several of the participating partners and a benchmark calculation has been proposed for at least one of the tests.

Simple “engineering” methodologies are required in Severe Accident Codes (e.g., MELCOR, SCDAP/RELAP5, and MAAP4) that model the full sequence of events that occur in a core melt accident. It has been demonstrated (NUREG/CR-5582) that the creep-based methods utilizing the semi-empirical lifetime rule nominally correlate both the time for onset of creep and failure times observed in the NRC-sponsored LHF tests. It is important to extend the methodology to the OLHF tests, namely applications with large through-wall temperature gradients resulting in significant redistribution of internal stress from the hot inside surface to the cooler outside surface of the lower head.

## The Secure Transportable Autonomous Light Water Reactor— STAR-LW (IRIS Project)

PI: Mario D. Carelli, Westinghouse Electric Company LLC

Collaborators: University of California – Berkeley; Massachusetts Institute of Technology; Polytechnic Institute of Milan, Italy
Additional IRIS Team Members: British Nuclear Fuels Limited (BNFL), United Kingdom; Commissariat a l'Energie Atomique (CEA), France; Japan Atomic Power Company (JAPC), Japan; Mitsubishi Heavy Industries (MHI), Japan; Tokyo Institute of Technology, Japan; Bechtel Corporation; University of Pisa, Italy

Project Start Date: August 1999 Projected End Date: September 2002

Project Number: 99-0027

### Research Objective

This program, currently known as the International Reactor Innovative and Secure (IRIS) project, has the objective of investigating a novel type of water-cooled reactor which can satisfy the four objectives of the Generation IV reactors: proliferation resistance; enhanced safety; improved economics; and reduced waste. The research objectives over the three-year program are as follows.

- First year: Assess various design alternatives and establish main characteristics of a point design.
- Second year: Perform feasibility and engineering assessment of the selected design solutions.
- Third year: Complete reactor design and performance evaluation, including cost assessment.

IRIS is an integral, modular, water-cooled reactor. In order to be economically competitive, the small size IRIS has to be deployed worldwide, and therefore, an international consortium has been formed to design and promote IRIS. The original proponents, Westinghouse, University of California–Berkeley, Massachusetts Institute of Technology, and Polytechnic of Milan were joined at various times during the first year activities by: CEA, BNFL, MHI, JAPC, the Tokyo Institute of Technology, Bechtel, and the University of Pisa. All of the additional participants and the Polytechnic of Milan are working under their own funding.

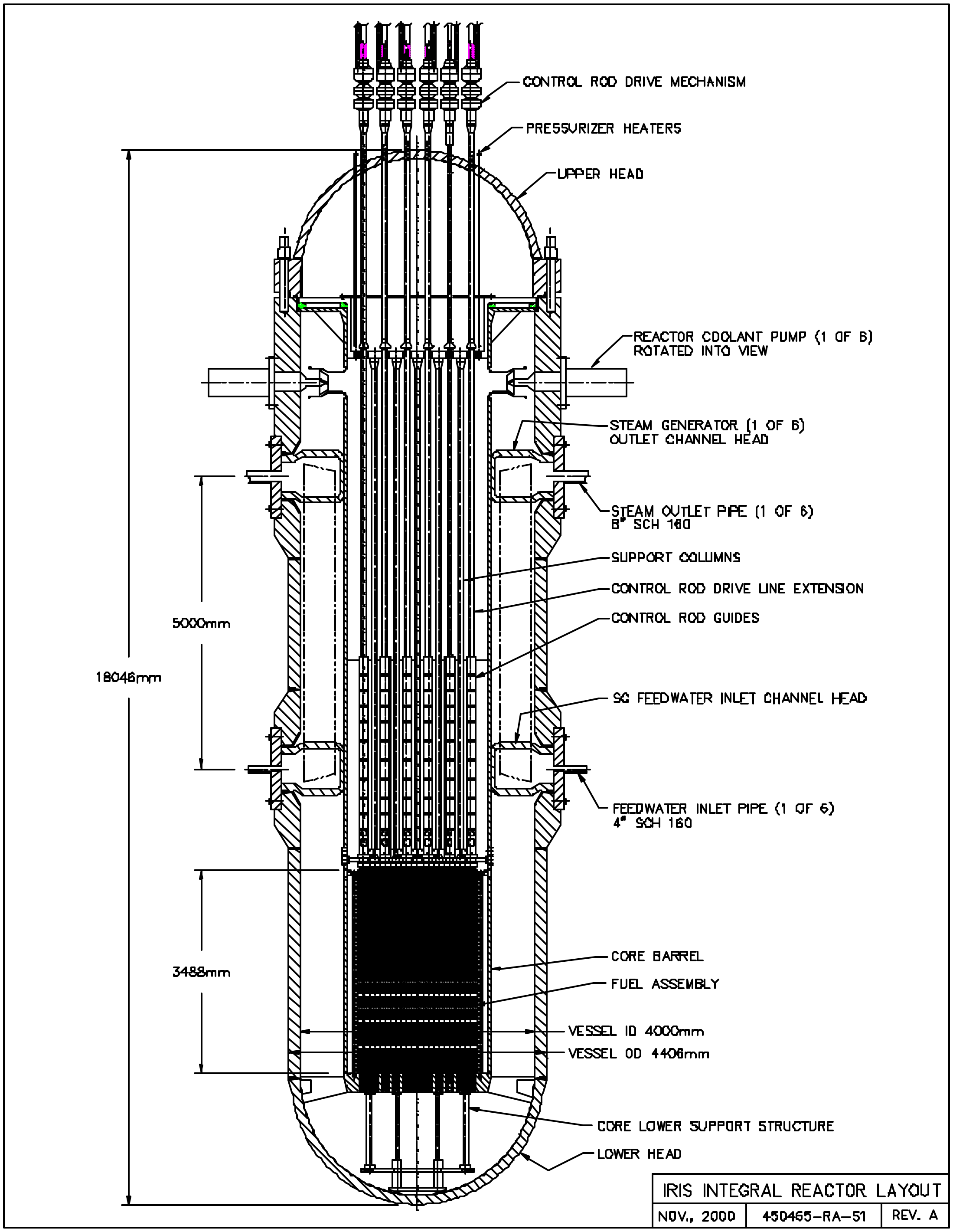
**Research Progress**

Various design alternatives have been examined and, at the end of the first year, an IRIS configuration has been established which would be developed into a conceptual design during the second year. Parametric studies indicated that a core lifetime of the order of eight years without shuffling or refueling was about the highest attainable within the specified enrichment limitation and still having reasonable power ratings to yield an economic design. Various types of fuels were considered in terms of form (oxide, carbide, nitride, metal) and of element composition (uranium [U], plutonium [Pu], thorium [Th]). The selection was narrowed to enriched uranium oxide and mixed oxide (MOX) fuels. The choice between the two is mostly programmatic, since they have similar performance and economic characteristics. IRIS will be able to operate with either one and, since the entire core is changed at end of life, it is possible to switch from a $UO_2$ to a MOX core and vice versa. Presently a $UO_2$ core is considered for domestic deployment, while the option to use MOX fuel is of interest to the international members of the IRIS team. Various types of cladding materials were considered and the choice was an advanced zirconium (Zr) alloy for burnup lower than 100,000 MWd/ton (current IRIS design) and stainless steel for higher burnup (attainable in future IRIS modules with a fast spectrum).

Core neutronics analyses were performed and indicated that a long (eight years) core life was indeed attainable with the tightly packed (triangular pitch, pitch to diameter ratio [p/d] = 1.1) core lattice envisioned in the proposal. However, the core void reactivity coefficient was positive at the end of life for both $UO_2$ and MOX fuels and throughout life for MOX. On the other hand, parametric studies indicated that high burnup was also obtainable for well-moderated cores with lattices having a p/d (triangular) of the order of 2.0. In the absence of chemical shim, well-moderated lattices yielded negative void and overall power reactivity coefficients throughout life. At the end of the first program year, effort was therefore moving in two directions: for the reference IRIS core, determination of the characteristics of a well moderated core; and, for a future, more advanced IRIS design, determination of the type of configuration yielding negative power coefficients in tight lattices (alternate layers of Th and U seem quite promising, and the use of Th further improves proliferation resistance).

Tradeoff studies were performed to assess the impact of full natural circulation, degree of boiling allowed in the core and lowering of the reactor inlet temperature. It was determined that full natural circulation would have a negative impact on the plant cost and performance (excessively tall vessel in single phase and excessive degree of boiling in two-phase) while the advantages of lowering the inlet temperature were overshadowed by the negative effect on plant efficiency and steam generator performance. The chosen solution was to have "aided natural circulation"; i.e., forced single-phase convection plus a sufficient degree of natural circulation (preliminarily estimate is 20 percent) for not exceeding design limits in case of a loss of flow accident.

A preliminary layout of the integral vessel has been completed, as shown in figure below, and sizing of steam generators is in progress.




**Layout of IRIS Integral Vessel for a 100 MWe Module**

In a tight lattice configuration, heat transfer to the coolant is critical. Thus, an investigation has been conducted to identify novel rod geometries, which offer a larger heat transfer area than conventional cylindrical rods. A variety of geometries were considered starting from cylindrical rods as a reference and moving to annular rods, cylindrical rod inside an annulus, cylinder in an octagon and various polygonal shapes obtained by using the mathematical tiling theory. Spacers considered were grid, wire wrap and bearing pads. Performance was established in terms of pressure drop, critical heat flux, cladding temperature distribution and fuel centerline temperature. The chosen reference configuration is a conventional wire wrapped cylindrical rod in a hexagonal array. The backup is a more exotic arrangement of hexagonal fuel pins in a triangular array. The backup design has lower pressure drops, larger critical heat flux (CHF) margin (by a factor of two), lower fuel temperature and more uniform circumferential temperature than the reference design. A computational fluid dynamics (CFD) approach to calculate temperature and flow distribution in exotically shaped channels was initiated.

A preliminary cost evaluation has been conducted which shows that IRIS is competitive with other nuclear and non-nuclear power sources over a large range of internal rate of return (IRR) values.

**Planned Activities**

Activities planned for the second year are those necessary to arrive at a conceptual design. They will include:

- Sizing of the main components (vessel, steam generators, pumps).
- Preliminary assessment of the balance of plant requirements and characteristics.
- Completion of the core neutronics and thermal-hydraulic evaluation.
- Assessment of maintenance optimization options to lengthen the time between scheduled shutdowns (since refueling outages occur only every eight years, the IRIS goal is to limit maintenance outages to once every four years or longer).
- Assessment of the reactor system delivery and disposal.
- Preliminary cost evaluation from a bottoms-up approach.

One very important IRIS feature is its approach to safety where accidents are prevented by design, rather than coping with and minimizing their consequences by active or passive means. The practical implementation of this approach will be addressed in the second year of effort.

## Monitoring and Control Technologies for the Secure Transportable Autonomous Reactor (STAR)

PI: Hussein S. Khalil, Argonne National Laboratory

Collaborators: Lawrence Livermore National Laboratory, Texas A&M University

Project Start Date: August 1999 Projected End Date: September 2002

Project Number: 99-0043

### Research Objective

A new reactor and fuel system concept designated as the Secure Transportable Autonomous Reactor (STAR) has been proposed for meeting the needs of developing countries for small, economical nuclear power stations while at the same time addressing proliferation concerns. This NERI project supports this goal through development of operations monitoring, control and remote surveillance strategies that exploit the passive safety and autonomous operation attributes of the STAR plant, and development and demonstration of advanced technologies for implementing these strategies such that operational reliability and nuclear materials security are assured. Specific objectives of the research are to simplify active control and safety protection systems, minimize reliance on on-site operating staff, and assure high levels of operational safety, reliability and facility security. Research tasks include: evaluating the ability of candidate STAR plants to operate autonomously with minimal reliance on active control for load adjustment and burnup reactivity compensation; identifying design and operating features that enhance operational autonomy and passive safety; developing simplified control strategies on the basis of the passive plant response; and developing and demonstrating computer-based technologies for remote monitoring of operational and safeguards information at centralized surveillance facilities.

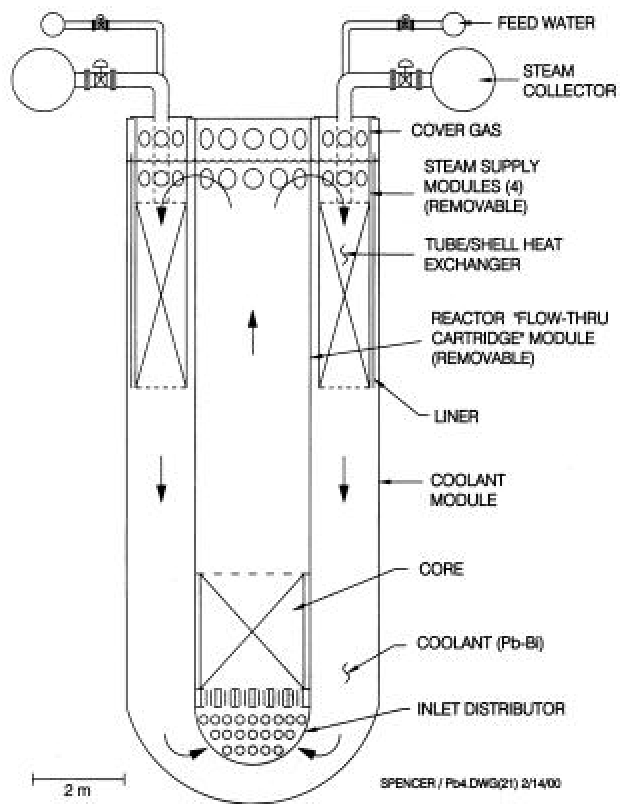
Although proposed in the framework of the STAR system development effort, the research addresses issues of fundamental importance to the operation of passively safe and autonomous plants. Resolution of these issues will increase the immunity of passively safe plants to operator and control system errors and will provide a technical basis for reducing the cost of plant control and safety protection systems.

### Research Progress

First year accomplishments include:

- Autonomous Operability of Star Designs: The startup, load and unprotected upset behavior of the liquid metal (lead-bismuth eutectic [LBE])-cooled STAR design concept were analyzed using a computer code specifically adapted for these evaluations. The STAR-LBE concept (see figure below) is substantially simpler than conventional sodium-cooled liquid metal reactors in that it employs no intermediate heat transport loop (steam generator modules are placed in the LBE pool within the reactor vessel) or primary coolant pumps (natural convection is used for primary system heat transport). Initial results verified that plant startup objectives could be met without active adjustment of primary flow, by using control rod reactivity, feedwater flow, and steam pressure to control the plant. In addition, a simplified control strategy for responding to load changes while yielding acceptable primary- and secondary-system temperatures was formulated; this strategy controls reactor power solely through the use of feedwater flow rate and steam pressure in the secondary system. Preliminary analysis of unprotected upset conditions showed that the most limiting transient is the reactor chilling event; it appears that this event can be accommodated, provided sufficient bypass flow around the steam generator has been designed for should the primary coolant in the steam generator freeze.

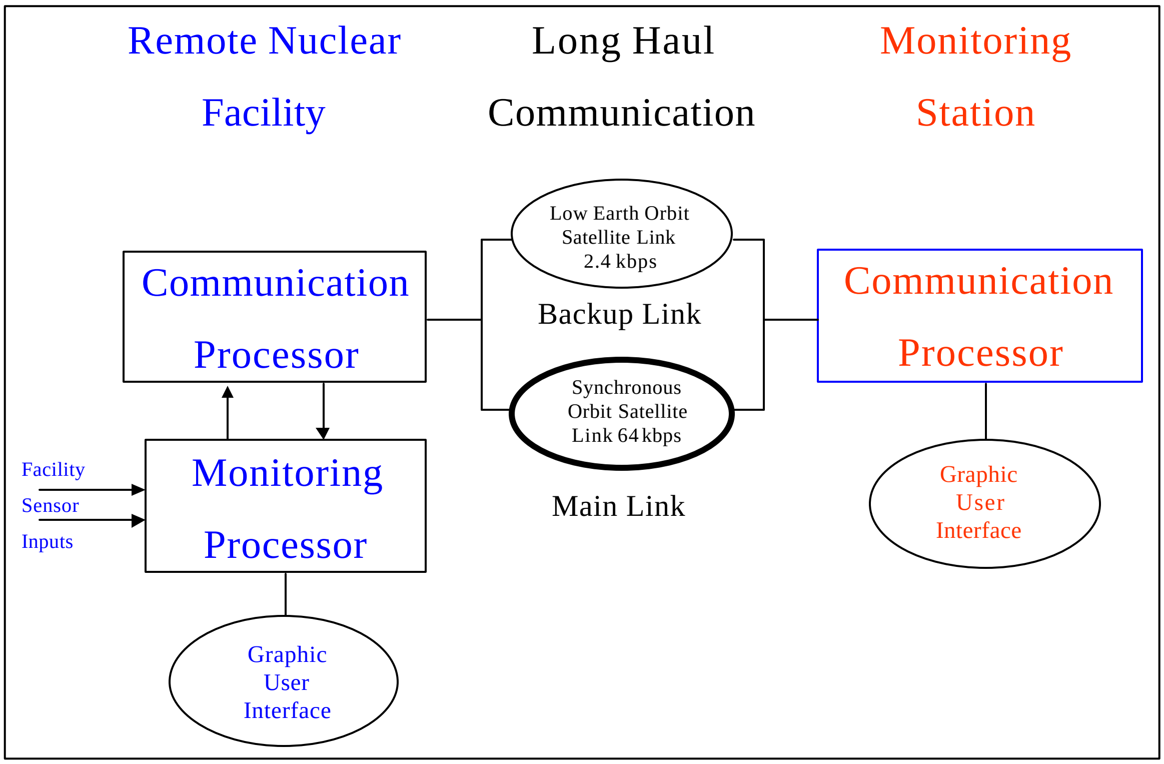
- Analyses of water-cooled STAR system concepts were also initiated to evaluate the feasibility of maneuvering core power without use of control rods. Preliminary results derived with a simple plant model indicated that with a pressurized water (non-boiling) reactor concept, the power coefficient is probably too large to allow full-range power maneuvering without exceeding primary-side thermal-hydraulic limits. A boiling water concept was also evaluated and shown to provide significantly greater potential for maneuvering within the power range without using control rods.




**STAR-LM Simplified, Modular, Small Reactor Featuring Flow-thru Fuel Cartridge**

- Remote Monitoring System Design: A remote monitoring system design was developed to meet anticipated security and operational monitoring requirements for a STAR plant. A schematic illustration of this system is shown in below. In this system, key plant security signals are acquired, digitized, encrypted and sent via the communication system to the remote monitoring site. Security requirements were defined assuming all persons with normal access to the plant may be a threat. Accordingly the security requirements start at the sensors and extend through the communications system. Many of the sensors have dual use for security and operation (e.g., reactor temperatures and flux levels), while others are dedicated to security (e.g., motion or volume sensors, video cameras, etc.). This data is transmitted to the remote site with a sampling rate appropriate to the data, but no more frequently than once each second. This data would be monitored at the remote site essentially in real time and would be stored for trending displays and additional analyses. Features to thwart potential attempts to subvert the monitoring system include limiting access to system components and use of a robust combination of tamper detecting devices and information analysis capabilities based on "machine intelligence" techniques.

**Monitoring System Overview**




- <u>Initial Demonstration of Remote Reactor Monitoring</u>: A basic capability for remote monitoring of the Texas A&M University Nuclear Science Center Reactor (NSCR) was developed and implemented. This capability uses standard hardware components and a software package (LabVIEW) available from National Instruments Co. for data and image acquisition, information analysis and storage, and remote monitoring of this information on the World Wide Web. The new hardware and software were installed to provide a capability for internet-based viewing of the NSCR main control room console, the fuel and water system temperatures, and the reactor log and linear power readings. In addition, a video-based surveillance system for Internet viewing of the NSCR core has been designed and partially implemented. The required video equipment was procured and interfaced with the LabVIEW software for display at the monitoring site using a standard web browser. Since the transfer of video images requires substantial computer memory and data transmission bandwidth, approaches for enhancing the efficiency of the monitoring system design (e.g., a system employing LabVIEW applications at the monitoring site) are currently being investigated.

**Planned Activities**

STAR system design features that enhance operational autonomy will be investigated during the remainder of the project. For the liquid metal (LBE)-cooled STAR plant, additional analysis is needed to characterize and confirm adequacy of startup behavior at very low power (<1 percent rated power), verify the adequacy of safety margins for unprotected upset conditions, and optimize the design parameters and operating conditions of the core and the steam generator modules to provide the desired load follow behavior while satisfying passive safety criteria and cost minimization goals.

Future efforts related to the light water cooled STAR system will be focused on the boiling water reactor option, because this option is judged at present to offer greater potential for power maneuvering over the full power range without use of control rods. Efforts planned for the second year include: evaluation of desired reactivity coefficient magnitudes and core design implications; implementation of appropriate two-phase models for evaluating autonomous control strategies in boiling water systems; and adaptation of control algorithms and operating modes previously developed [e.g., for the Simplified Boiling Water Reactor (SBWR)] or implemented (e.g., for the Dutch 183-MWt Dodewaard natural convection BWR) to the unique requirements and features of a water-cooled STAR system.

Future efforts on remote monitoring of STAR plants will be directed to further development of the monitoring system design. Data communication alternatives will be evaluated to determine the performance/cost tradeoffs and to choose the most favorable option for STAR remote monitoring applications. In addition, requirements for ensuring reliability and authenticity of the monitored information will be formulated, and the technologies meeting these requirements will be identified and incorporated in the monitoring system design. An integrated demonstration of the monitoring system, using the Texas A&M Nuclear Science Center reactor is planned for the third year of the project.

## Risk Informed Assessment of Regulatory and Design Requirements for Future Nuclear Power Plants


| | | |
|---|---|---|
| PI: | Stanley E. Ritterbusch, Westinghouse Electric Company | |
| Collaborators: | Sandia National Laboratories, Idaho National Engineering & Environmental Laboratory, Massachusetts Institute of Technology, North Carolina State University, Duke Engineering Services Inc., Egan Associates | |
| Project Start Date: | August 20, 1999 | Projected End Date: March 19, 2002 |
| Project Number: | 99-0058 | |


### Research Objective

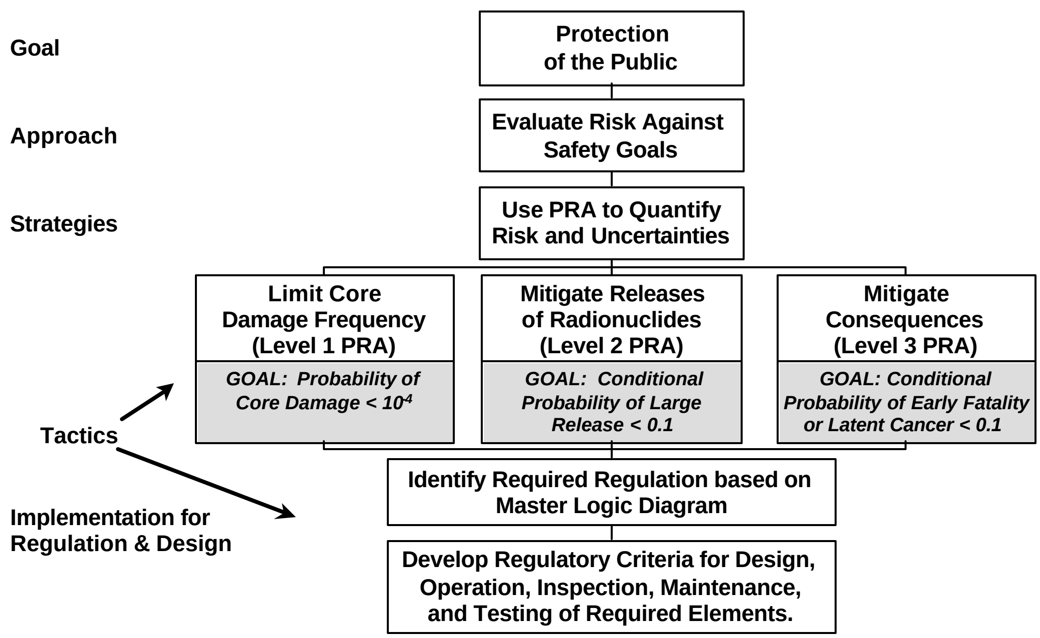
Research for this project addresses the barriers to long-term use of nuclear-generated electricity in the United States. In addition, the Electric Power Research Institute has continued to perform studies on the cost of coal, gas, and nuclear-generated electricity. To be competitive, the cost for the nuclear option would have to decrease to the range of 3 cents/kilowatt-hour over the next two decades. Correspondingly, the total plant capital cost of a typical Advanced Light Water Reactor would have to decrease by about 35 percent to 40 percent, and the construction schedule would have to be shortened to about three years.

In response to the above developments, the Westinghouse Electric Company (formerly ABB Combustion Engineering Nuclear Power) initiated a cooperative proposal with the goal of meeting the above cost reduction targets for new nuclear power plant construction. The vision for this cooperative effort is to meet the cost-reduction goals through implementation of new technology and innovative approaches to the design and licensing of new nuclear power plants. DOE approved three separate projects, which have similar overall objectives of reducing nuclear power plant costs. These three projects are “Risk-Informed Assessment of Regulatory and Design Requirements for Future Nuclear Power Plants” led by Westinghouse, “Smart Nuclear Power Plant Program” led by Sandia National Laboratories, and “Design, Procure, Construct, Install and Test Program” led by Duke Engineering & Services. The Risk-Informed project, covering 2-1/2 years, includes two basic tasks: (1) “Development of Risk-Informed Methodologies” and (2) “Strengthening the Reliability Database.” The primary benefit of this project is the development of innovative methods for an all-new, highly risk-informed design and regulatory process.

### Research Progress

Shortly after initiating this project, team members established the principal strategies required to achieve the project’s cost reduction goals. It was agreed that a very basic and significant change to the current method of design and regulation was needed. That is, it was believed that the cost reduction goal could not be met by fixing the current system (i.e., an evolutionary approach) and a new, more advanced, approach for this project would be needed. It is believed that a completely new design and regulatory process would have to be developed – a "clean sheet of paper" approach. This new approach (figure below) would start with risk-based methods, would establish probabilistic design criteria, and would implement defense-in-depth only when necessary to meet public policy issues (e.g., use of a containment building no matter how low the probability of a large release is) and to address uncertainties in probabilistic methods and equipment performance. This new approach is significantly different from the Nuclear Regulatory Commission's (NRC) current risk-informed program for operating plants. For our new approach, risk-based methods are the primary means for assuring plant safety, whereas in the NRC's current approach, defense-in-depth remains the primary means of assuring safety.

**The New Regulatory Framework Driven by Probabilistic Analyses**




The primary accomplishments in the first year of this project include:

- Development of a new, highly risk-informed design and proposed regulatory framework.
- Establishment of the preliminary version of the new, highly risk-informed design process.
- Core damage frequency predictions showing that, based on new, lower pipe rupture probabilities, the emergency core cooling system equipment can be reduced or eliminated without reducing plant safety.
- The initial development of methods for including uncertainties in a new integrated structures-systems design model.

Under the proposed new regulatory framework, options for the use of "design basis accidents" were evaluated. Whereas, in the current regulatory process, the design basis accidents and their evaluation are primarily deterministic, it is expected that design basis accidents would be an inherent part of the Probabilistic Safety Assessment for the plant and their evaluation would be probabilistic. The change in thinking from deterministic to probabilistic design basis accidents will require a fundamental change in the way accidents are analyzed and evaluated (e.g., if probabilistic criteria are met, then deterministic judgments would not be used to add conservatism or design margin).

Other accomplishments include:

- Conversion of an NRC database for cross-referencing NRC criteria and industry codes and standards to Microsoft 2000 software.
- An assessment of the NRC's hearing process, which concluded that the normal cross-examination during public hearings is not actually required by the U.S. Administrative Procedures Act.
- Identification and listing of reliability data sources.
- Interfacing with other industry groups (e.g., Nuclear Energy Institute and the International Atomic Energy Agency) and the NRC at workshops for risk-informing regulations.

**Planned Activities**

In the remainder of this project, the tasks summarized above will be continued. The primary activities include fuller development of the new design and regulatory process, its demonstration with more cost reduction estimates, refinement of the new risk-informed regulatory framework, integration of the new structures-systems design model into the new design process, evaluation of existing reliability data against needs of the new design process, evaluation of NRC staff's design review process, and continued interactions with NRC and industry.

Westinghouse also expects to set up agreements with one or more Korean organizations for their participation in this project. The purpose of this cooperation would be to bring Korean design and operating experience into the project at the same time they perform additional work scope. These agreements will be reviewed and approved by other project participants as well as the DOE.

The deliverables for this project will not only document the actual work which was done, but will provide a clear description of how the results could be applied to new Generation IV designs (e.g., the Pebble Bed Modular Reactor) as well as current Advanced Light Water Reactor designs. Since the new design and regulatory process starts from a "clean sheet of paper," a completely new set of regulations will have to be developed when the new process is fully implemented. Therefore, the deliverables for this task will also provide a summary or example vision of what the new regulations would look like.

## Standards and Guidelines for Cost Effective Layout and Modularization of Nuclear Reactor Plants

| | | | |
|---|---|---|---|
| PI: | James Winters, Westinghouse Electric Company | | |
| Project Start Date: | April 1999 | Project End Date: | April 2000 |
| Project Number: | 99-0059 | | |

### Research Objective

The objective of this overall task was to develop and promulgate layout and modularization standards and guidelines, which, if followed, will reduce the overall cost of new reactor designs. Layout considerations affect many areas, which, in turn, affect overall cost. These areas include operation, maintenance, and licensing, as well as capital cost. Layout can have a significant effect on how the plant satisfies regulatory issues such as separation, fire and flood control, access control and As Low As Reasonably Achievable (ALARA). Layout can determine the extent of modularization that can be realized, and how it can be used to minimize construction time in the field. Modularization and parallel fabrication of items in the factory and in the field has been shown to significantly reduce schedule and cost in a number of industries. It can also be a significant cost adder if implemented improperly. The objective of integrated plant layout and modularization should be to minimize plant lifetime costs and risks though effective minimization of capital and operating costs.

This one-year program included four tasks with discreet deliverables and the associated management. The first deliverable was a presentation of overall layout standards. It included what Westinghouse believes to be inviolate rules for layout of a nuclear plant. Each of the rules has proven itself to be cost effective. In addition to those which are obvious for reduction of capital and operating expense, the document included those which reduce regulatory review time and expense. The second deliverable contained guidelines for layout with the objective of maximizing effective modularization. If the intent is to prepare large portions of the plant in a factory, such as for the Generation 4 reactors, then there are layout guidelines, which, if followed, will facilitate design, manufacture, and assembly. These guidelines were developed from lessons learned in the modularization of AP600, which is a highly modularized plant. Third was a compilation of module design standards. It presents rules, which maximize the cost-effective implementation of a modularization strategy. It included standards for detail analysis, design and acceptance of modules (both structural and equipment). The fourth was a set of guidelines for design details, which provide for effective fabrication and assembly of modules. It was a set of lessons learned from detailed constructibility studies performed to enhance the cost effectiveness of AP600.

**Research Progress**

The first deliverable was prepared to quantify, streamline, and document explicitly those internal layout rules which have been shown to benefit overall cost or licensability for plants such as AP600. Internal correspondence was reviewed and layout experts were interviewed to assemble a working list of layout rules. These rules were then reviewed, prioritized and quantified to determine which should be included in a list of layout standards. The object of layout standards was that they are rules that should be followed without exception. Layout standards included items such as requiring that separate divisions of safety related Class 1E electrical and control equipment and wiring should be physically separated by flood and fire barriers. Another example was to quantify the maintenance space envelopes required for various pieces of equipment. The quantification included rules for items such as drip pans and drains. It also included guidance on equipment and tool supports. Other good engineering practices for overall layout were identified.

The second deliverable was a documented set of guidelines for modularization. Part of the challenge of realizing the benefits of modularization is to lay out the plant in such a way that modules and parallel manufacture actually do reduce the overall plant cost or schedule. For example, "don't ship air" is a guideline for not creating a module where there is no benefit of factory assembly. Another is "don't ship concrete," which relates to the fact that concrete facilities will exist on site and putting the concrete into a module after landing it is preferable to paying for the weight and difficulty of shipping hardened concrete from the factory. These rules will be of significant value to smaller Generation IV reactor designs, whose modules (or shippable units) will be a larger fraction of the total plant than for larger plants.

The object of the guidelines is that they are rules that should be considered when establishing and implementing selected shippable units. Included in these guidelines are the overall items to consider when deciding on maximum module size and weight, or on the extent of outfitting and test to be done in the factory. It covers both equipment and structural type modules and delineates methods to maximize effective modularization starting from the conceptual design phases.

The third deliverable (module standards) focuses on fabricating self-contained units of a power plant that can be transported to a site and operated for 15 years or more without major maintenance. This deliverable reflects discussions with module fabricators, structural designers, transportation experts, and others, as well as inclusion of lessons learned while developing detail module designs for our AP600 customers. A comprehensive documentation of this experience, enhanced by the lessons learned on AP600, should be very useful in the design of the shippable units (modules) for any reactor, especially those for Generation IV plants, where the module represents a large percentage of the overall plant.

The fourth deliverable (module detail guidelines) documents a number of internal module design detail lessons learned. These detail design lessons learned relate to the best practices for such things as placing and attaching pipe and tray supports, locating and orienting lifting points and supports, methods for structural attachments and joining, and other details. Note that standardization of detail in itself is usually a cost saver, in that no relearning is required of the designer or the fabricator.

**Planned Activities**

All four deliverables are complete and have been submitted. The funded research project is complete.

## Demand-Driven Nuclear Energizer Module

| | | |
|---|---|---|
| PI: | Daniel O'Connor, Oak Ridge National Laboratory | |
| Project Start Date: | August 1, 1999 | Projected End Date: September 30, 2002 |
| Project Number: | 99-0064 | |

### Research Objective

Demand-Driven Nuclear Energizer Module (NEM) is an advanced reactor concept that would take advantage of newly developed materials with enhanced heat transfer characteristics and superb high temperature mechanical properties to provide an inherently safe, self-regulated heat source. The high temperatures achievable make it suitable for a multiplicity of applications. The concept achieves demand-driven heat generation without the need of moving parts or working fluids. The nature of the reactor design makes the concept inherently safe, proliferation resistant, and ideal as a long-term, reliable source of power for harsh, remote, and/or inaccessible environments on Earth and space. Low-cost power generation is envisioned over a wide range of temperature and power.

### Research Progress

Neutronics analyses were initiated to evaluate fuel and reactor design and operating parameters. Materials research was initiated to evaluate how the structural and thermal properties vary with density and radiation exposure. A physical model was built using graphite foam, electric heaters, and a computer model to benchmark computer models, reflect neutronics and materials findings to evaluate reactivity coefficients and reactor configurations, and to simulate performance of reactor safety, stability, and instrumentation and controls. The resulting product will be an initial conceptual design for the reactor concept. More specific details of research accomplishments in the three major activity areas are as follows:

Neutronics Analysis

- Scoping calculations were performed for the design of graphite-foam-uranium cores capable of achieving over 15 years of operation without refueling. Computations of burnup - from 0 to 40,000 MWd/ton (nine steps) - and temperature dependent nuclear parameters - from 300 to 1200 $^{o}$C (four steps) - were performed for a reference core configuration. Collapsed four-group neutronic parameters were also generated using the AMPX code to provide input to the interactive simulator under development.

- The reference core consists of a 77 cm diameter cylindrical core with 12 percent $U_{235}$ enriched fuel embedded in graphite foam of 0.5 g/cc density, with a 15 cm thick reflector made of 1.87 g/cc density graphite.

- Scoping calculations for graphite-reflected graphite-foam-$U_{233}/Th_{232}$ cores with zero reactivity swing with burnup were initiated. The $U_{233}/Th_{232}$ cycle does not have the inconveniences associated with Pu production, however $U_{233}$ can be easily separated from the $Th_{232}$ and according to ORNL TM-13517, a $U_{233}$ enrichment of 12 percent is equivalent to an enrichment of 20 percent in $U_{235}$.

Materials Research

- Critical to the success of this reactor concept is to assess the impact of neutron irradiation on the thermo-mechanical characteristics of the carbon foam. A total of six capsules have been fabricated. The following activities occurred in calendar year 2000: Two capsules with ten specimens each were inserted in the High Flux Isotope Reactor (HFIR) early June. They were extracted in August and are in the cooling off period prior to analysis. Two more capsules, also with ten specimens each, were inserted in the HFIR in August and extracted in early October.

- Methods to impregnate the foams with gelcasting, sol-gel, Chemical Vapor Infiltration (CVI), and other techniques were evaluated. Also, other design ideas for the reactor core were evaluated based on all the novel characteristics of the foam.

Simulation, Prototyping, and Control

- A 12-cm diameter by 16-cm high cylinder of graphite foam mockup of the reactor core was fabricated. Heating rods were obtained that extend the full length of the cylinder. Debugging of the control electronics has continued and building safety enclosures for the electronics and core mockup is ongoing.

- Development of the interactive multi-group, multi-region reactor simulator has continued. The simulator's computed neutronic and power generation compared well with detailed computations of the code used to generate the four-group neutron data inputs. Validation and implementation of the thermal heat transfer and feedback reactivity will follow to yield a coupled neutronic and heat transport simulation.

**Planned Activities**

Neutronics Analysis: Specific applications will be selected which will be used to determine reflector needs, selection of structural materials, and geometric constraints. Integral to this will be determination of the required fissile mass as a function of integral energy output, reactor configurations, and operating and shutdown temperatures.

Materials Research: Graphite foams will be prepared with varying densities, and structural and physical property characterization will be conducted on each foam. Extrusion methods will be studied to determine the effect of manufacturing processes on thermal conductivity. Characterization studies will be conducted on irradiated specimens to determine the effect on structure, dimensional stability, thermal conductivity, thermal expansion, strength modules, and strain to failure.

Simulation, Prototyping, and Control: The NEM model will be updated to reflect neutronics and materials findings. Reactivity coefficients and target configurations will be modeled.

## Development of Advanced Technologies to Reduce Design, Fabrication, and Construction Costs for Future Nuclear Plants

PI: J. Michael O'Connell, Duke Engineering & Services

Collaborators: North Carolina State University, Massachusetts Institute of Technology, Sandia National Laboratory, Westinghouse Electric Company Nuclear Systems

Project Start Date: August 1999 Projected End Date: June 2002

Project Number: 99-0077

**Research Objective**

The objective of this project is to develop technologies to reduce the capital costs and construction schedule time line for future nuclear power plants. Specifically, researchers are aiming to identify those mechanisms that can be applied to reduce the overall cycle time for the Design, Procure, Construction, Installation and Testing (DPCIT) for an advanced nuclear plant by 40 percent. Also, efforts are focused on providing increased confidence in the overall process of ensuring an advanced nuclear project can be built within the cost and schedule targets assumed for a competitive energy marketplace.

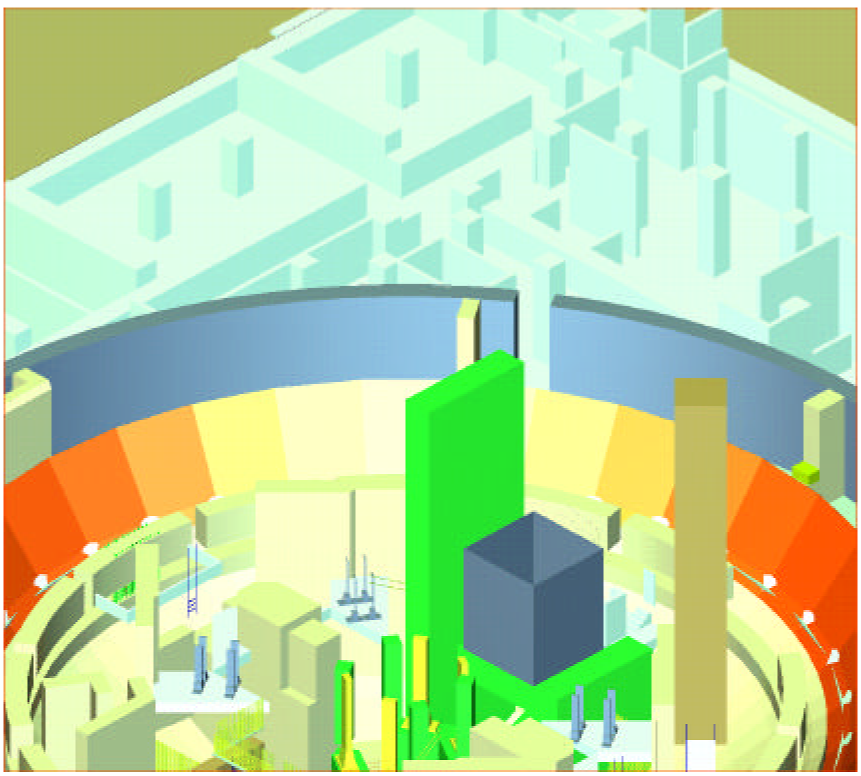
The purchase of an advanced nuclear power plant would initially be based upon the assessment of the total capital cost on a dollar per installed kilowatt electric (KWe) coupled with the planned operations and maintenance costs on an operating cost per installed KWe. Both these metrics are the yardsticks by which nuclear power plants are compared against market alternatives of gas fired generation or coal-fired generation. While the existing fleet of nuclear power plants in the U.S. operates cost effectively and competitively in a partially deregulated market, the decision to invest in new nuclear generation is contingent upon not only the capital cost per KWe installed, but also the confidence with which the schedule of delivery can be completed. The prior work sponsored jointly by the DOE and the Electric Power Research Institute in the Advanced Light Water Reactor (ALWR) program produced reactor plant designs that are optimized for operations and maintenance expenditure, but not for capital cost or schedule as the earlier research initiatives were conducted when the electric power system had not experienced the impact of deregulation.

Thus, delivery of a new reactor plant within the three constraints of quality, cost, and schedule is not currently achievable in a deregulated market. The challenge is therefore to examine those issues that have driven our costs and schedules. Work will be done to link prior industry research that has examined specific incremental improvement strategies with applications of information technology and new thinking on coordination of businesses to produce dramatic reductions in the capital cost of new reactor plants. This project's focal point for keeping score of potential improvements is on the total cost and cycle time associated with the DPCIT cycle. By examining each of these activities in building a plant, project researchers expect to apply new thinking and improvement techniques that have been developed in other industries.

**Research Progress**

The project team has accomplished an initial identification of capital cost and schedule reduction strategies. One key insight into the reduction of capital cost and schedule is that backfitting new technologies into pre-existing designs do not offer as significant a payoff as working with new designs as they are being created. This favors the Generation IV Advanced Nuclear Plants in that these plants are either in the process of incorporating the kinds of improvements this project has examined, or there is the potential to incorporate these insights before finalizing the design.

Another key insight is in how information technologies will be applied to both the design and construction processes to simulate not only the design and its construction sequence, but also to play a role in improving the execution of supporting activities such as procurement and in providing real time status of field construction activities. The use of 4-dimension (3D plus schedule) simulation software has provided insights into examining different sequences of major subassembly installations. These insights have yielded "on paper" savings of several critical path months. The picture below provides a snapshot from the 4D simulation software.



**Examination of Major Module and Equipment Installation Sequences Using 4D Schedule Simulations**

In the domain of risk reduction for the overall management of capital cost and schedule, preliminary work with Systems Dynamics Modeling and Bayesian Belief Networks show promise as effective tools for the management of change in complex projects such as nuclear facilities. In summary, then, the project work has been addressing specific contributors to capital costs and schedules, while also examining the execution of large scale projects using advanced tools that will help address the confidence issues needed to proceed with new nuclear plant construction.

**Planned Activities**

The Year 2 research efforts will incorporate insights gained from Year 1 and focus on the following areas:

- New design technologies to achieve capital cost and cycle time reductions.
- Power uprates made possible through incorporation of risk-informed impact.
- Information technologies that facilitate collaborative engineering.
- Plant fabrication and construction technology advances.
- Evaluation of evolving passive design impacts.
- Reduction in project execution risk with new management assessment tools.

The overall goal for Year 2 is to continue with cost reduction application while at the same time working to identify those strategies that will also reduce the risk and ensure that the proposed shortened schedule can be accomplished.

## Innovative Chemithermal Techniques for Verifying Hydrocarbon Integrity in Nuclear Safety Materials

PI: L. Mason, Pacific-Sierra Research Corporation

Collaborators: University of Virginia, University of Maryland

Project Start Date: August 1999 Projected End Date: September 2002

Project Number: 99-0094

### Research Objective

This research and development program is designed to explore new methods of assessing current condition and predicting remaining life of critical hydrocarbon materials in nuclear power plant environments. Of these materials, Class "1E" safety cable insulation is the primary focus. Additionally, o-ring, seal, and lubricant products designed for nuclear applications round out the materials studied. This three-phase applied research program is providing industry with new innovative methods and reference data to conduct pragmatic material condition-monitoring programs for a wide range of polymer-based products. Key research objectives (products) include a material-condition-monitoring database, optimization and standardization of various testing procedures, implementation of proven engineering development methodologies, and inter-technology correlation analyses. Milestones are defined by a 5-task work-breakdown schedule. Task 1 encompasses front-end R&D program activities and planning of additional tasks. Task 2 concerns identification of subject cable materials, their acquisition, accelerated aging, testing by a suite of chemithermal methods, and results reporting. Tasks 3 and 4 comprise similar objectives for, respectively, o-ring and seal, and lubricant materials. Task 5 concerns required programmatic documentation. Research progress to date under Phase 1 fell mainly within Tasks 1, 2, and 5.

### Research Progress

The greatest fraction of Phase 1 resources for this project was expended during conduct of Task 1, the "Research and Development Plan." The next largest fraction of resources was applied to progress of the first research task, Task 2, "Polymer Cable Insulation," specifically described below. Regarding Task 1, personnel requirements were determined and fulfilled; a new laboratory space was commissioned. Spare parts and routine supplies were acquired for three chemithermal analyzers: a Perkin-Elmer TGA7 (thermogravimetric analyzer); and two Perkin-Elmer DSC7s (differential-scanning calorimeter) instruments, one with an available high-pressure (up to 600 psig) cell accessory. Computer hardware and software upgrades included Perkin-Elmer software upgrades and an operating platform upgrade to Windows NT. These intense activities greatly expanded the laboratory's capability to simultaneously operate its then current suite of analyzers, as well as future additions, which now include a Perkin-Elmer TMA7 (thermomechanical analyzer) and a Perkin-Elmer Fourier transform infrared (FTIR) analyzer, the latter being configured to routinely analyze thermogravimetric analysis (TGA) combustion gasses. Development of three research task plans proceeded as expected. These tasks were, respectively, focused upon the subject materials: 1E electric cable insulation materials; o-ring and seal materials; and lubricants. Development of each task revolved around a template of activities that included the following: identification of critical materials; acquisition; sample preparation; accelerated aging to simulate normal aging over 40 years under combined radiation and thermal stress conditions; chemithermal measurements; and analysis and reduction of data. Specifically regarding the conduct of Task 2, accelerated aging protocols for cables were developed in the context of a rectangular matrix approach. This matrix was called the qualification-aging matrix (QAM), patterned after much previously successful research. Twelve condition points in the QAM correspond to material conditions ranging from unaged to fully aged by multiple stresses throughout a full normal life in-situ. In fully aged condition, operational integrity of these materials is expected to be intact throughout a postulated loss of coolant accident (LOCA). All condition

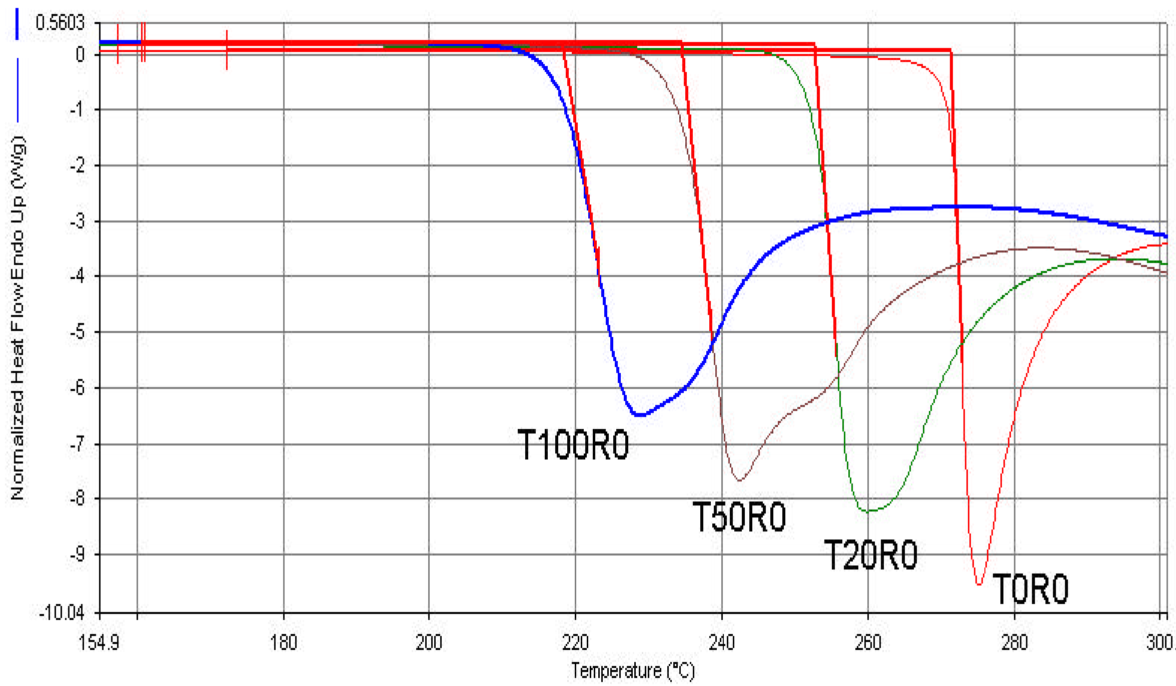



**Illustration of the decrease in oxidation-induction temperature (OITP) onset calculation as a function of increasing thermal 1E qualification aging. Curves labeled "T0R0, T20R0, T50R0, and T100R0" represent bulk Rockbestos green conductor material aged to 0, 20, 50, and 100% of manufacturer-specified thermal-aging protocol. These results show the utility of using chemithermal methods to predict polymer degradation with a high degree of reproducibility.**

points for a given material were planned to be analyzed by chemithermal analytical methods, including: oxidation induction time (OIT), which measures product stability at high temperature – and antioxidant content remaining, hence, remaining life; oxidation-induction temperature (OITP) which is a more rapid measure of stability and structural changes, related to OIT; and, TGA, which measures thermal stability and gives some compositional information. Analytical methods for OIT and OITP tests had previously been standardized by Veridian PSR through funded government research. Standardization of these procedures involved multi-parametric experiments involving popular cable materials then under consideration. Sample mass, particle size, experimental conditions, and analyzer operating parameters and programs were all systematically investigated. Similar experiments were conducted in this research to optimize TGA methodology. Critical cable insulation products were identified through extensive contacts with material suppliers and users. Identification of critical cables for research is an on-going challenge, for installed-product operating data are continually updated, the number of manufacturers declines, virgin supplies of popular cables dwindle, and new products used for selective plant cable replacements become increasingly important. An array of ethylene-propylene rubber (EPR) and cross-linked polyethylene (XLPE) insulated cable products was selected, requested, and gradually amassed for this program. As these materials were being acquired, accelerated thermal aging was conducted, while chemithermal measurements of unaged and thermally aged samples were made. When enough materials had been thermally aged, gamma-irradiations were contracted for at the University of Maryland. Measurements of OIT, OITP, and TGA to-date have been in line with expectations, notably punctuated by some exciting new discoveries, one of which is mentioned below.

**Planned Activities**

The bulk of Phase 2 effort is targeted at the conduct of pilot studies involving o-ring and seal materials, the acquisition of which ran ahead of schedule during Phase 1. Such materials selected include ethylene-propylene (EP), which is similar to but behaves somewhat differently than the cable-type EPR, and butyl and nitrile rubbers of a few formulations. As the remainder of these materials is acquired, final decisions will be made regarding appropriate accelerated aging protocols and chemithermal measurement matrices, based upon exploratory measurements in progress on small samples. In Phase 3, a similar approach will be taken in regard to lubricant products, which are just beginning to arrive in sample quantities. Throughout the remainder of this project, electric cable insulation research will be continued. Efforts will be focused upon full completion of the QAM-based set of OIT, OITP, and TGA measurements (the condition-monitoring database). Correlations of these measurements with each other and with other available and relevant data will be pursued to the greatest extent possible. A fascinating and unexpected discovery from Phase 1, involving a correlation of OITP and TGA data will receive intense scrutiny. From this correlation it is possible (for at least one XLPE insulation material) to extract not only overall-condition data, but also specific indications of thermal history and radiation dose. TGA data interpretation, which was found to be more time-intensive than expected, will receive the additional effort required. One or more blind studies will be conducted in order to fortify confidence in the relatively unintrusive material-condition monitoring and life-assessment methods being developed here, through the chemithermal analysis of safety-critical hydrocarbons in use throughout the nuclear industry.

## Modular and Full Size Simplified Boiling Water Reactor Design with Fully Passive Safety Systems

PI: Mamoru Ishii, Purdue University

Collaborators: Brookhaven National Laboratory

Project Start Date: August 1, 1999 Projected End Date: September 30, 2002

Project Number: 99-0097

**Research Objective**

The main goal of this research project is the scientific design of a compact modular 200 MWe and a full size 1200 MWe, simplified boiling water reactors (SBWR). Specific objectives of this research are to:

- Perform scientific designs of the core neutronics and core thermal-hydraulics for small capacity and full size simplified boiling water reactors;
- Develop passive safety system design;
- Improve and validate safety analysis code;
- Demonstrate experimentally and analytically all design functions of safety systems for design basis accident (DBA); and
- Develop the final scientific design of both SBWR systems, SBWR-200 and SBWR-1200.

**Research Progress**

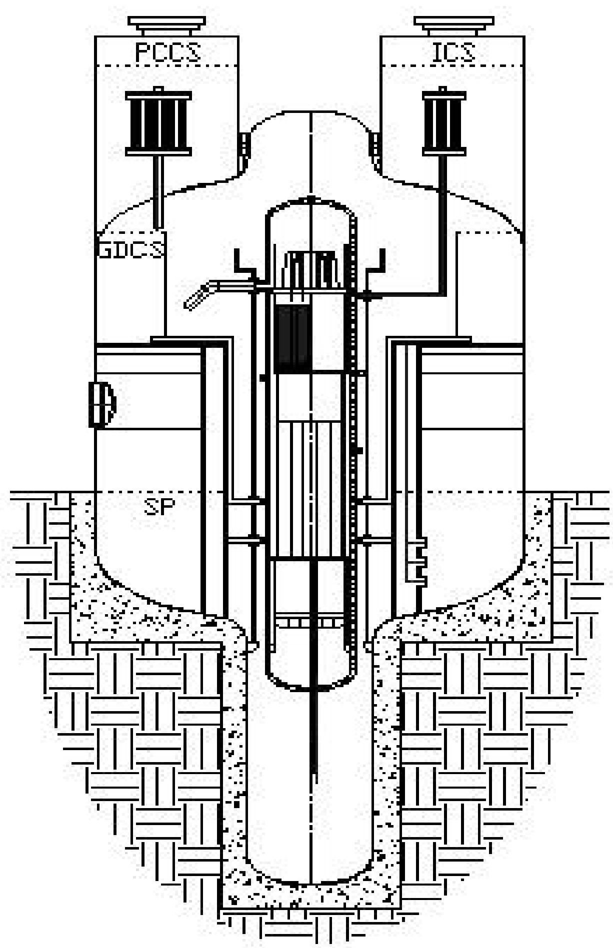
Research conducted on this project over the past year includes:

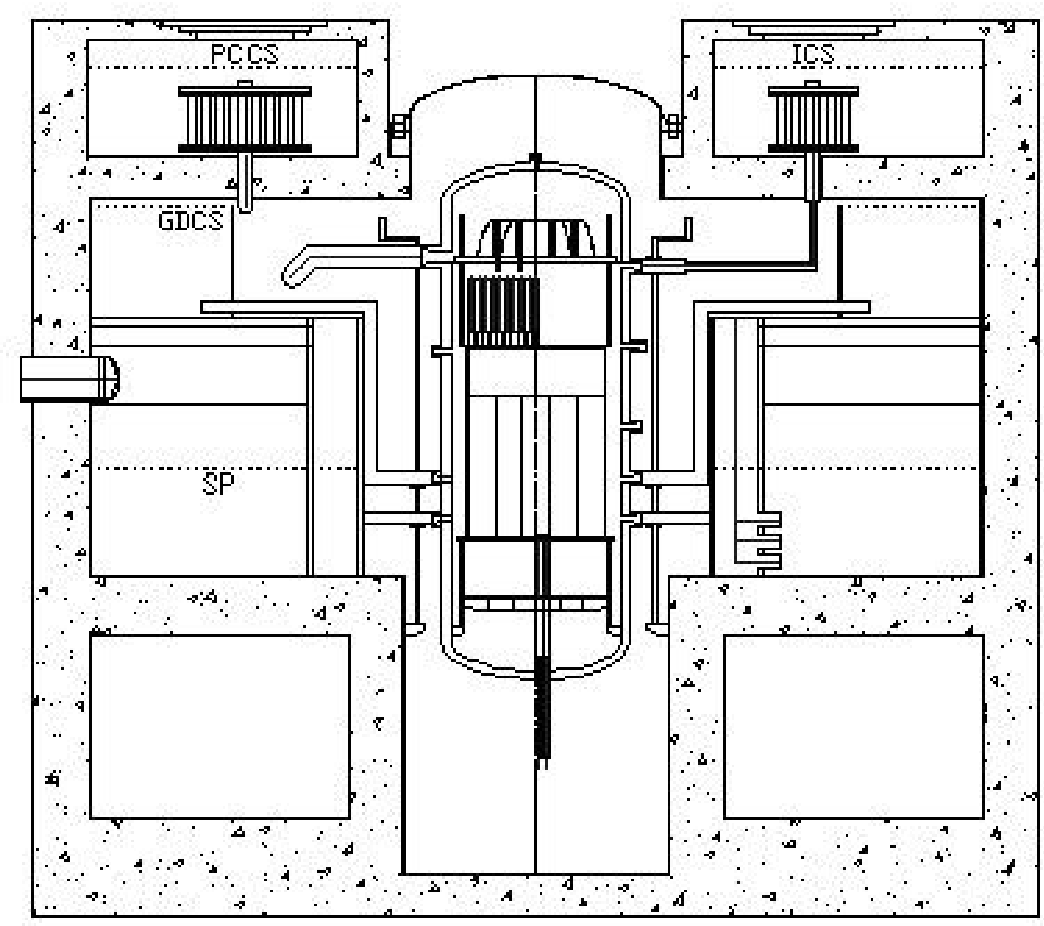
- Development of a preliminary design for the SBWR-200 and SBWR-1200 thermalhydraulic systems. The preliminary design involved identification of principle design criteria dictated by the safe operation of the reactor, identification of coolant requirements, design of the engineered safety, and emergency cooling systems based on passive systems.
- Design of a preliminary reactor engineered safety system including reactor-cooling system and emergency core cooling systems for SBWR-200 and SBWR-1200. These systems were based on natural gravity force. The passive safety system is reliable and safe to operate.
- A detailed scaling analysis was performed. The results of the scaling study were used in the performance of the integral tests and data analysis.
- Large break and a small break loss of coolant accident (LOCA) integral tests for the SBWR-200 were carried out. These integral tests were perfomed to assess the safety systems and the response of the emergency core cooling systems to LOCA in a scaled

facility called PUMA and the results have been used in the analysis of the safety systems. Main steam line break (MSLB) accident test was carried out for large break loss of coolant design basis accident (DBA) analysis while bottom drain line break (BDLB) accident test was carried out for small break loss of coolant DBA.

- RELAP5/MOD3 best estimate reactor thermal hydraulic code was used to model the PUMA MSLB and BDLB integral tests. The analysis was used to demonstrate the safety features of the modular SBWR design and to validate the code applicability in the facility scope. Overall, the code gave a reasonably accurate prediction of the system thermal hydraulic behaviors. This allows for an accurate assessment of the design feature of SBWR-200 safety components. It also indicates some code deficiency that should be improved for a better simulation.
- Performed a preliminary neutronics analysis and core design for SBWR-200 and SBWR-1200. The neutronics work performed during the first year of the project has been: (1) to acquire and validate the computer codes required for the neutronics design and analysis of the SBWR (HELIOS, PARCS, and RELAP5/TRAC); (2) to develop neutronics and thermal-hydraulics models of the SBWR-600 and compare results to the RAMONA-4B predictions; and, (3) to perform preliminary designs of the SBWR-200 and SBWR-1200.
- Performed a preliminary study on stability of the SBWR-200 and SBWR-600 under normal startup and abnormal startup.
- Preliminary design of containment and the internals for the SBWR-200 and SBWR-1200 are shown in the figures below.

**SBWR-200 Reactor Containment**






**SBWR-1200 Reactor Containment**

## Planned Activities

- Development and testing of the passive vacuum break valve for the compact modular SBWR-200 and full size SBWR-1200.
- Development and testing of the passive high-pressure emergency core injection system.
- Performance of detailed neutronic analysis and development of the core design through the core physics calculations for the SBWR-1200.
- Performance of integral tests and code evaluation for DBA.
- Performances of BWR stability analysis for SBWR-1200 reactor for steady state, start-up and other transients.
- Performance of final conceptual scientific design of compact modular SBWR-200 and full size SBWR-1200.

## A New Paradigm for Automatic Development of Highly Reliable Control Architectures for Future Nuclear Plants

PI: Richard Wood, Oak Ridge National Laboratory

Collaborators: North Carolina State University (NCSU), University of Tennessee (UT)

Project Start Date: August 1, 1999 Projected End Date: August 31, 2002

Project Number: 99-0119

### Research Objective

This research focuses on development of methods for automated generation of control systems that can be traced directly to design requirements for the life of the plant. The final goal is to "capture" the design requirements inside a "control engine" during the design phase. This control engine is not only capable of automatically designing the initial implementation of the control system, but it also can confirm that the original design requirements are still met during the life of the plant as conditions change.

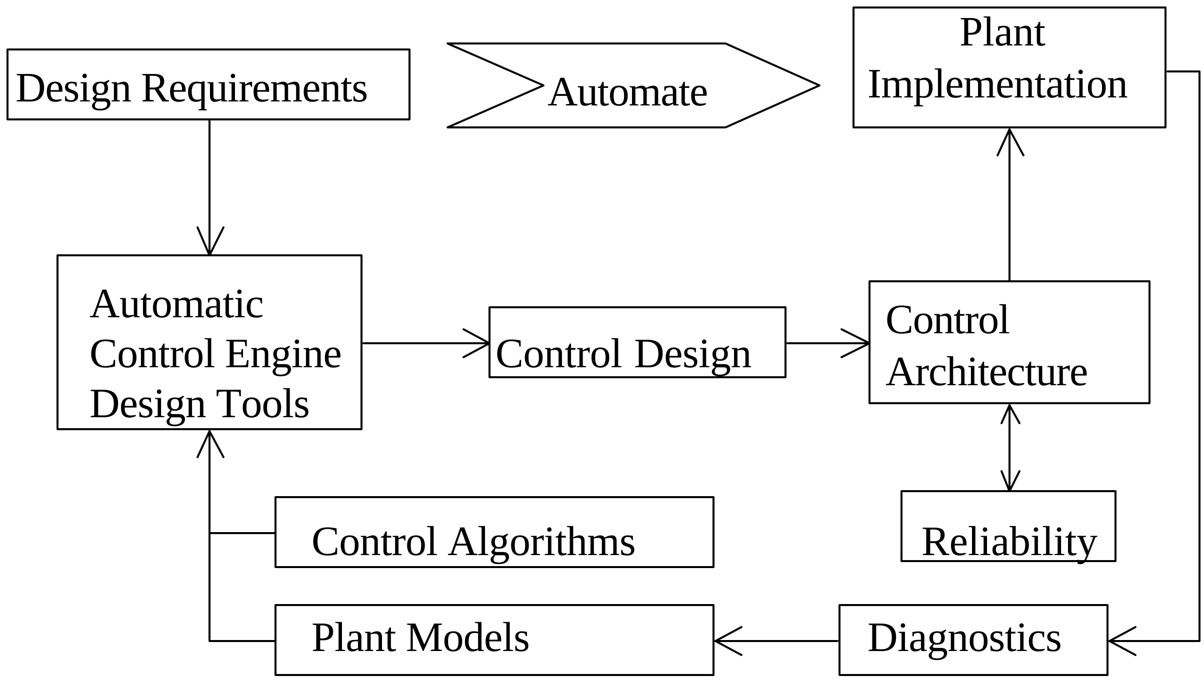
The control engine captures the high-level requirements and stress factors that the control system must survive (e.g., a list of transients, or a requirement to withstand a single failure). Therefore, the control engine is able to generate automatically the control system algorithms and parameters that optimize a design goal and satisfy all requirements. As conditions change during the life of the plant (e.g., component degradation, or subsystem failures) the control engine automatically "flags" that a requirement is not satisfied, and it can even suggest a modified configuration that would satisfy it. This control engine concept is shown schematically in the figure below.

### Research Progress

Phase I accomplishments include:

Advanced Control Tools and Methods: Research in this area is focused on developing and demonstrating the control engine concept. Libraries of control algorithms have been developed, with some of them successfully applied to a prototype control engine problem. A general methodology has been developed for handling the sensor and actuator nonlinearities as piecewise linear functions.

Advanced Monitoring and Diagnostics: The objective of this task is to develop an on-line monitoring system for fault detection and isolation of sensors and field devices in a nuclear power plant. Data-driven models have been developed for the characterization of sub-system dynamics for prediction state variables, control functions, and expected control actions.




Schematic diagram of the automated control design process

Nuclear Power Simulation and Reliability Methods: Since 1996, a full plant engineering simulation code has been under development and in use at NCSU for simulating the dynamic response of pressurized water reactors during normal operational transients as well as design basis events. Work under this task required the addition of a full balance-of-plant model, as well as other improvements, to the plant simulator. Options have been added to the code to allow for degradation in the heat transfer across the steam generator from both fouling and blocked or plugged tubes, as well as the corruption of sensor outputs through step and ramp changes in sensor output with arbitrary levels of random noise.

Nuclear Information System Architecture and Integration: Research addressing the control and information system architecture for future nuclear power plants involve the evolution of the Plant-Control Computing Environment (PCCE) concept and the generation of functional requirements. The following functional requirements have been generated: general design attributes; human-system interface requirements; control application interface requirements; computing platform interface requirements; monitoring and control requirements; fault handling and recovery requirements; system management requirements; and configuration requirements.

**Planned Activities**

In Phases 2 and 3, selected functional elements of the PCCE will be developed to facilitate a proof-of-principle demonstration. Standardized display and communications functional elements will be devised to satisfy the functional requirements generated in Phase 1. Application programming interfaces will be developed for selected control, diagnostic, and communications functions.

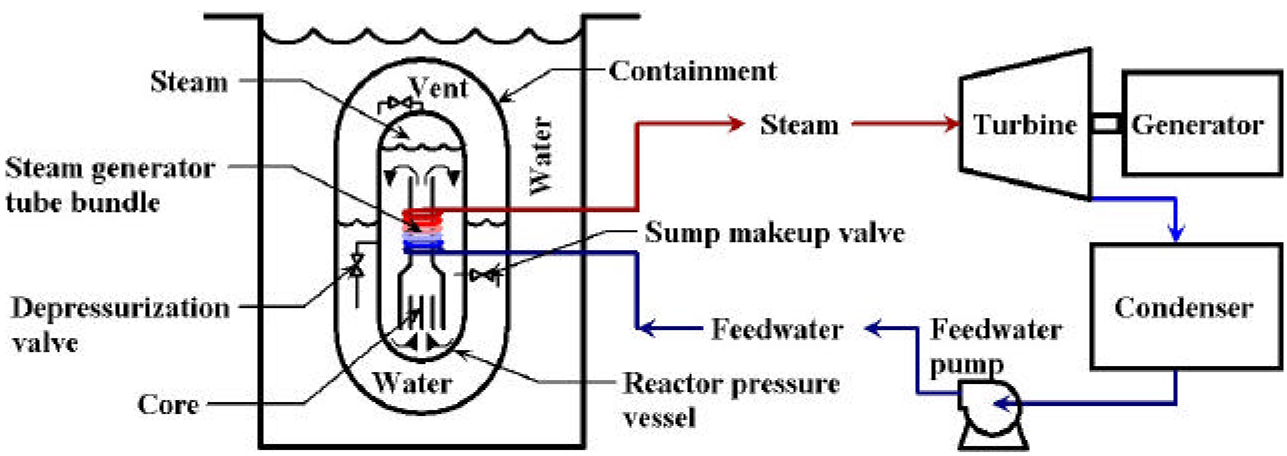
## Multi-Application Small Light Water Reactor

| | | | |
|---|---|---|---|
| PI: | S. Michael Modro, Idaho National Engineering and Environmental Laboratory | | |
| Collaborators: | NEXANT, Inc., Oregon State University (OSU) | | |
| Project Start Date: | October 1999 | Projected End Date: September 2002 | |
| Project Number: | 99-0129 | | |

**Research Objective**

The primary objective of the Multi-Application Small Light Water Reactor (MASLWR) project is to develop the conceptual design for a safe and economic plant, and to test the design feasibility. A small, natural circulation light water reactor is proposed with the goal of various applications, primarily electric power generation, but flexible enough to be used for process heat with deployment in a variety of locations. Through economic and engineering analyses the project will address the design and safety attributes of the concept. This will be coupled with testing in an integral test facility to demonstrate the concept's technical feasibility.

The determination of the requirements and design criteria was based on goals that included: maximizing modularity, a standard plant design, certification before construction, two-year construction schedule, five-year refueling schedule, simplified operation and maintenance, and sixty-year plant life-cycle. All of these goals were focused toward providing a competitive busbar cost of 40 mils/kilowatt hour (kWh). The figure below is a representation of the proposed plant design concept.




**MASLWR Concept**

**Research Progress**

Requirements and Design Criteria Established: The approach to establishing the requirements and design criteria was to invoke the U.S. Code of Federal Regulations "safety specifications" in their entirety. Further, the basic philosophy of the Electrical Power Research Institute (EPRI) project to develop a standardized design and technical requirements applicable to Advanced Light Water Reactors (ALWRs), and the Nuclear Regulatory Commission's (NRC) review thereof, was adopted. However, the EPRI/NRC results, relative to Passive Design Reactors have not been necessarily invoked in their entirety for two reasons: (1) it is believed that reactor design technology has advanced in the six to eight years following the NRC review; and (2) one of the primary elements of the NERI is to "think-out-of-the-box" to develop promising new solutions to nuclear power plant (NPP) design.

The MASLWR team found it convenient to develop and document the requirements and design criteria in a hierarchical manner. That is, except at the highest level (normally a policy type statement), each requirement or criterion can be traced to a more inclusive requirement or criterion at the next higher level.

Baseline Design Concept Developed: A baseline design was developed based on a power level at the upper limit of the power range suggested for small reactors by the NERI program. The initial concept was drafted for 300 Megawatts electric (MWe), however thermal analyses showed that because of natural circulation requirements and overall size constraints the power level had to be reduced to about 250 MWe. Development of the baseline design concept has been sufficiently completed to determine that it complies with the safety requirements and criteria, and satisfies the major goals already noted, except that busbar cost is 57.2 mils/kWh. Therefore it is unlikely to conform to the competitive busbar cost goal of 40 mils/kWh. It was concluded that further cost reduction can be achieved only by smaller units, which would be almost entirely assembled at a factory. Costs for applications such as cogeneration, water desalination or district heating were not addressed since these depend on local conditions, demand and economy and can not be easily generalized.

Scaling Methodology Developed: The initial scaling methodology development has been completed and has confirmed that the baseline design could be well simulated in the OSU Advanced Plant Experiment (APEX) experimental facility with determinable/achievable modifications.

Investigation of Concept Evolution Initiated: The most promising approach appears to be an evolution from the baseline concept to a small reactor (~100 MWt, 20 MWe) that allows a "self-contained" assembly of reactor vessel, steam generators and containment. These units would be manufactured at a single centralized facility, transported by rail, road, and/or ship, and installed as a series of self-contained units. This approach also allows for staged construction of an NPP and "pull and replace" during each five-year refueling cycle.

Preliminary estimates indicate that the evolutionary design concept will approach the competitive busbar cost of 40 mils/kWh.

**Planned Activities**

Recent design performance studies strongly indicate that power in the 100 MWt design can be doubled (i.e., to 200 MWt) and the overall height of the installation can be significantly decreased. These performance studies investigated the viability of operation at saturation conditions, thereby producing a two-phase mixture in the hot leg and a single-phase cold leg, a condition that maximizes the natural circulation driving force for coolant flow. Continuing activities planned for Phase 2 (FY2001) are in four areas as follows:

Pressure Vessel, Primary and Secondary Systems, and Safety Systems Design Optimization: The goal is to further decrease the cost of electricity production while maintaining or increasing safety of plant operation. Activities planned for November and December 2000 and January 2001 include: concept refinement; performance analysis to realize maximum efficiency in electricity production; development of a Phenomenon Identification and Ranking Table (PIRT) followed by appropriate safety analyses as directed by the PIRT; development of nuclear steam supply system and balance of plant system layouts for the optimized design.

Containment Optimization: The containment design (i.e., an individual containment for each reactor) was optimized during November and December 2000. A second containment design option (i.e., a single containment for multiple reactors) will also be examined.

Cost Analysis Refinement: An interim refinement of the existing cost analysis was conducted in November and December 2000 as dictated by the design information evolution of the above efforts.

Experimental Program: Development of the experimental program is planned for completion in January 2001, followed by experimental rig construction/modification and subsequent testing, which will be performed in the remaining part of FY2001.

# STAR: The Secure Transportable Autonomous Reactor System, Encapsulated Fission Heat-Source


| | | |
|---|---|---|
| PI: | Ehud Greenspan, University of California, Berkeley | |
| Collaborators: | Westinghouse, Argonne National Laboratory, Lawrence Livermore National Laboratory. | |
| Project Start Date: | August 1, 1999 | Projected End Date: June, 2001 |
| Project Number: | 99-0154 | |

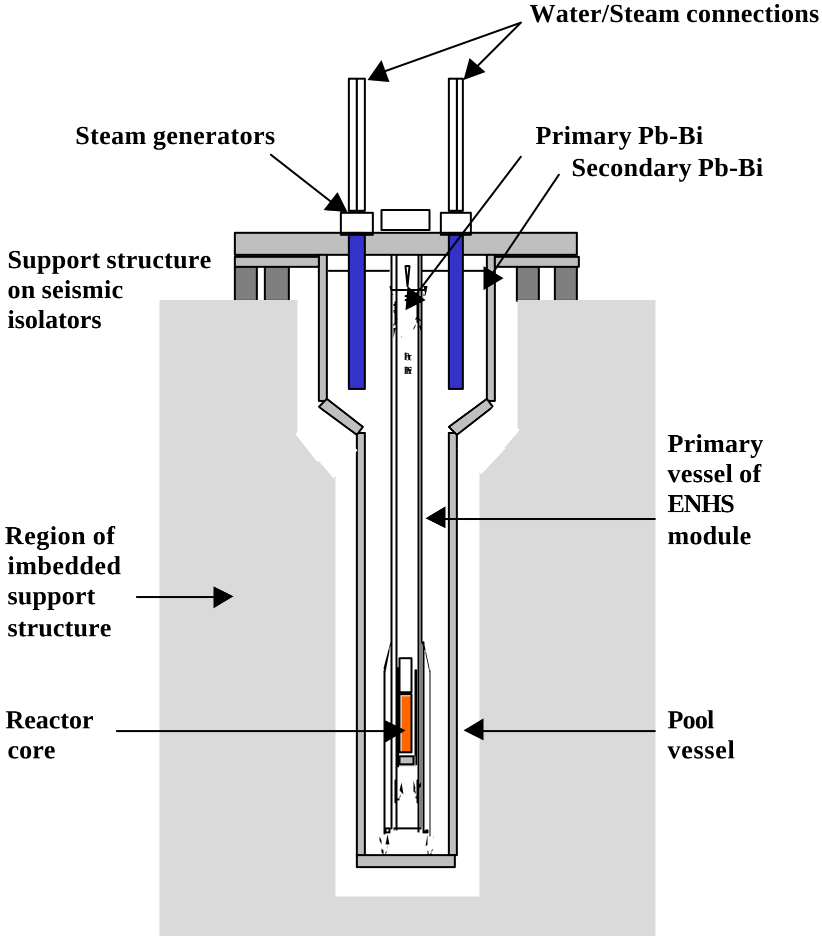

## Research Objective

The Encapsulated Nuclear Heat Source (ENHS) is a new lead (Pb)-bismuth (Bi) or cooled highly modular 125 MWth fast spectrum reactor concept that has a combination of the following features:

- 20 years of full power operation without refueling.
- Nearly constant fissile fuel contents and reactivity coefficient ($k_{eff}$); hence, very small excess reactivity built-in and very simple reactor control system.
- The ENHS modules are factory manufactured and transported already fueled to the site.
- No on-site refueling and fueling hardware.
- No mechanical connections between the ENHS module and the energy conversion plant, making it easy to install and replace.
- A number of ENHS modules may be installed in a single pool of secondary coolant making a power plant of up to several hundred MWe in capacity.
- At end of life, the ENHS module serves as a spent fuel storage cask and, later, as a spent-fuel shipping-cask. That is, the fuel is locked inside the ENHS from cradle to grave.
- 100 percent natural circulation resulting in passive load following capability and autonomous control. After the reactor is brought to full power by removal of the safety rod and radial reflector, the compensation for reactivity changes and for power variations is done via temperature feedback.

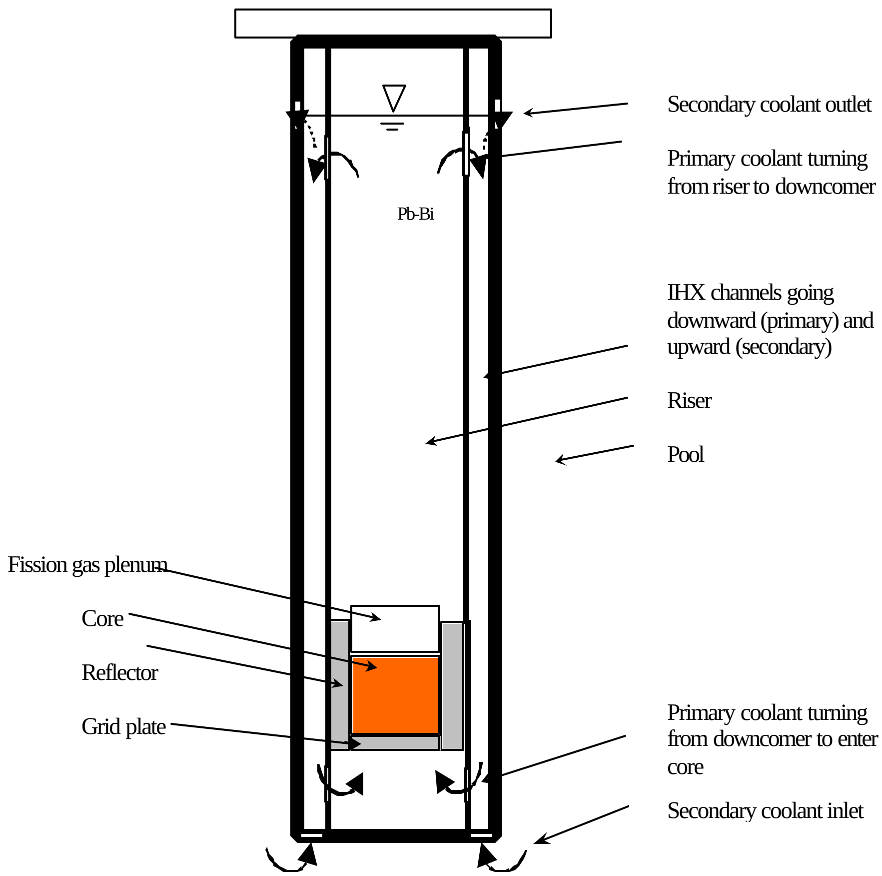
This combination of features offers a highly safe nuclear energy system that is characterized by low waste, exceptionally high proliferation resistance and high uranium utilization.

A description of one of several possible embodiments of a reactor concept having a single ENHS module is depicted in the figures below. The reactor consists of nine modules: one ENHS and eight steam generators. All these modules are factory fabricated and transported to the power plant site completely assembled ready to be inserted into the reactor pool. The primary coolant that is heated in the core flows up the riser, turns over into an Intermediate Heat Exchanger (IHX) of a novel design and flows back into the coolant plenum underneath the core. The IHX is integrated between the inner-, and the outer-structural walls. The secondary coolant flows from the pool outside of the vessel into the bottom of the IHX and exits back to the pool near the top of the IHX.




**A schematic vertical view of a single ENHS reactor (Not to Scale)**

The objectives of the first year study was to assess the feasibility of: 1) designing cores for 20 years of full power operation without refueling and with nearly zero burnup reactivity swing, using either Pu-U or enriched uranium fuel; 2) designing the ENHS to have 100 percent natural circulation with reasonable module dimensions and weight;3) designing the ENHS module to be free of mechanical connections; 4) designing and manufacturing the confinement wall; 5) fueling the ENHS module in the factory, transporting it fuelled to the nuclear power plant site and removing it from the pool unopened; 6) designing the ENHS to have autonomous load-following capability; and 7) removing decay heat passively.




**A schematic vertical cut through an ENHS module (Not to scale)**

## Research Progress

The design domain has been defined for cores that can operate at 125 MWth for 20 years with nearly zero burnup reactivity swing. The core design variables include the core height, lattice pitch-to-diameter ratio and fissile fuel contents. It was found possible to design such cores using either Pu-U fuel having ~11-12 weight percent Pu or uranium enriched to ~13 weight percent. The resulting cores are very simple: they have uniform composition, no blanket or reflector assemblies and a single safety rod assembly. An axially movable annular reflector assembly is used to bring the core from shutdown to full power. Tungsten was found to be an attractive material for the reflector; it can be scrammed by gravity and save 20 cm on the ENHS module diameter.

It was found feasible to design ENHS modules to deliver 125 MWth from the primary coolant to the secondary coolant through a 4 mm thick confinement wall (that separates the two coolants) with maximum primary coolant to maximum secondary coolant temperature drop of 50$^{o}$C and with 100 percent natural circulation. The required reactor vessel height is close to 20 meters. In fact, good synergism was found between the requirement for 100 percent natural circulation and the requirement for primary-to-secondary temperature drop of 50$^{o}$C. The dimensions of approximately a dozen different ENHS modules with 100 percent natural circulation and flat $k_{eff}$ cores have been determined. The total weight of an ENHS module when fueled and when loaded with Pb-Bi up to the upper core level is estimated to be on the order of 300 tons. This is approximately half the weight of steam generators for large pressurized water reactors (PWRs) that have been transported from the factory to nuclear power plant sites. Dimensions of an ENHS module with 100 percent natural circulation are somewhat smaller than dimensions of a large PWR steam generator. Hence it is concluded that the ENHS module can be factory manufactured and fueled.

A significantly more compact and lower weight ENHS module has been conceived and conceptually designed. It uses cover-gas lift-pump for coolant circulation. The gas circulators are located outside of the reactor vessel. The resulting ENHS module need be only approximately 10 m high and have a shipping weight of approximately 100 tons.

An intermediate heat exchanger (IHX) that is integrated within the ENHS module vessel wall and has practically identical heat transfer characteristics to those of the originally proposed confinement wall has been conceived and analyzed. It consists of rectangular channels circumscribing the primary coolant riser in the space between the inner structural wall and the outer structural wall. This integrated IHX was found able to withstand the loads that are expected during transportation, installation and operation.

A preliminary transient and accident analysis was performed for a reference ENHS design. The accidents considered so far include startup accident, loss of heat sink accident, and steam line break without scram accident. It was found that under all accident conditions considered, fuel and clad temperatures will remain significantly below the safety limits and the integrity of all systems will be preserved. It was also found that the ENHS reactor can maintain 100 percent natural circulation over the entire range from nominal power to decay heat power level. It can automatically follow load variations over a wide power range.

In summary, no show-stoppers were encountered so far. In fact, as a result of the first year study the ENHS concept appears more practical and more promising than perceived at the outset of this study. A number of novel design approaches have been conceived during the first year. These include the following: use of a coolant lift pump to reduce module size and weight; several different integrated IHX configurations for carrying the heat across the reactor vessel wall; several different fabrication approaches for the heat transport wall; several approaches for the core mechanical design that feature small pressure drop and enhanced negative reactivity feedback to temperature increase; reduced coolant flow by-passing the core; tungsten-based radial reflector for enhanced safety and reduced volume; elimination of a special radiation shield for the reactor vessel; compact simple and safe tube-in-tube type steam generators; and several approaches for reactor module factory assembly and subsequent shipping as an integral, sealed module.

**Planned Activities**

The activities planned for the second project year include the following:

- Investigate the feasibility of designing the pool to have natural circulation while eliminating excessive mixing of cold and hot coolant as well as flow stagnation.
- Investigate the feasibility of melting the Pb-Bi (or Pb) in which the fuel is embedded for shipment by filling the ENHS module with hot Pb-Bi and by inserting it into a hot Pb-Bi pool. Also, the feasibility of solidifying the Pb-Bi in a reasonable time after removing the ENHS module from the pool.
- Design the overall plant layout, with emphasis on plant components that are affected by the unique features of the ENHS.
- Establish overall life-cycle logistics (from factory to waste storage), including both technical, licensing and proliferation-resistance considerations.
- Investigate the feasibility of using the ENHS module as a shipping and storage cask of fresh and spent fuel.
- Perform a more complete safety assessment of the ENHS.
- Investigate the feasibility of lift-pumps.
- Investigate the feasibility of a steam generator integrated within the ENHS IHX.
- Investigate the feasibility of high-energy conversion efficiency.
- Investigate the feasibility of alternate coolants.

Research efforts are in collaboration with the Central Research Institute of Electric Power Industry (CRIEPI) and with Toshiba of Japan and with Korea Advanced Institute of Science and Technology (KAIST) of Korea. Starting in October 2000 research groups from Korea Atomic Energy Research Institute (KAERI) and from the University of Seoul have joined the collaboration.

## On-Line Intelligent Self-Diagnostic Monitoring for Next Generation Nuclear Power Plants

PI: Leonard J. Bond, Pacific Northwest National Laboratory

Project Start Date: August 1, 1999 Projected End Date: August 31, 2002

Project Number: 99-0168

### Research Objective

Operating experience from U.S. nuclear power plants indicates that degradation of power plant performance in terms of unscheduled shutdowns, extensive maintenance, and operational efficiency occurs predominantly because of vibration, bio-fouling, and erosion/corrosion, and the effect of these mechanisms on the system. The objective of this project is to design and demonstrate the operation of the real-time intelligent self-diagnostic and prognostic monitoring system for next generation nuclear power plant systems. This project provides a proof-of-principle technology demonstration for On-Line Intelligent Self-Diagnostic Monitoring System (SDMS) on a pilot plant scale service water system, where a distributed array of sensors is integrated with active components and passive structures typical of next generation nuclear power reactor and plant systems. This project employs state-of-the-art sensors, instrumentation, and computer processing to improve the monitoring and assessment of the power reactor system and to provide diagnostic and automated prognostics capabilities.

### Research Progress

Design of Experimental Hardware and Software: The project investigative focus was established by utilizing relevant Nuclear Regulatory Commission Nuclear Plant Aging Program data to define which degradation mechanisms have the greatest applicability to tomorrow's nuclear platforms. An open architecture multi-module design SDMS architecture has been completed. System computing hardware has been configured and is operational in the laboratory. Preliminary examination of cavitation from a first principles perspective shows sufficient material exists to commence physics modeling studies. Work on other stressor-degradation correlations must wait for additional phase studies.

Wireless Communication: Radio Frequency Modules and Sensors: Two radio frequency (RF) smart modules were fabricated and successfully deployed on the experimental test loop. A Visual Basic program running on a personal computer (PC) communicated with the reader (RS-232 link). The reader passed the data to the PC where it was displayed in graphical form. Both RF modules have onboard liquid crystal displays for local status and diagnostic presentation. Each module has a unique address allowing for additional sensor modules to be linked to the system.

Fabrication of SDMS Demonstration System and SDMS Test-Bed: The experimental test apparatus was received and the basic loop components and process instrumentation installed to allow component operational ranges (experimental envelope) to be verified as illustrated in the figure below. The test bed will simulate conditions experienced by low temperature reactor auxiliary systems. The "fouling meter" was demonstrated using an ultrasonic pulse-receiver and digital oscilloscope. Initial specifications were developed for the necessary semi-custom transducers that will be procured in Phase II. Initial pilot plant trials were performed. The updated system design and safety review for the Phase I as-built system were completed. A RF-multi-sensor module has been installed and tested using temperature and other system data. A draft standard operating procedure for initial trials has been completed.

**SDMS System with Display**

## Planned Activities

- Complete implementation of SDMS methodology on laboratory test loop.
- Fabricate advanced RF tag/multi-sensor units.
- Fabricate SDMS demonstration system.
- SDMS performance demonstration through a developing program of measurements and data analysis for a pilot plant scale water treatment system.
- Non-destructive degradation and stressor recognition models will be tested and verified on the test loop.

## Nuclear Process Heat for the Clean and Efficient Utilization of the Fossil Resource

PI: Kenneth R. Stroh, Los Alamos National Laboratory

Collaborators: Texas A&M University

Project Start Date: August 1999 Project End Date: August 2001

Project Number: 99-0188

### Research Objective

Nuclear fission has traditionally been used to produce electricity. However, in order to take advantage of the potential of nuclear energy, the areas of applicability of nuclear can be broadened. A brief look at current energy consumption patterns indicates that significant amounts of primary energy are consumed as heat. This suggests that nuclear sources can make contributions to the thermal energy market. In this study, nuclear energy is considered as a primary source for process heat. The design effort is focused on the steam reforming of methane, which is chosen as a surrogate for other candidate chemical processes.

The High Temperature Gas-cooled Reactor (HTGR) has a number of inherent safety characteristics, which make it attractive for this application. The HTGR also can produce high quality, high temperature process heat, which makes it attractive as a primary energy source. In addition, this concept has the potential to be competitive with other sources on the energy market.

The main goal of this study was to explore the options and limitations for coupling nuclear reactor heat to an endothermic chemical process. Important aspects of HTGR design and safety, high temperature fuel performance, and system requirements were taken into consideration. Important aspects of reactor physics of the HTGR were also examined.

### Research Progress

The HTGR has the potential to compete with other systems for primary energy production. The high temperatures which can be achieved in the pebble-bed HTGR lead to high values of thermal efficiency, better thermal dynamic cycles, and a broader range of possibilities for replacing conventional heat sources. A number of new high temperature materials have been developed since the first pebble-bed HTGR design was proposed. With these improvements, outlet temperatures of the order of 850$^o$C to 900$^o$C or even higher may be achievable.

The following areas have been studied:

- Analysis of HTGR reactor physics and important components of the pebble-bed HTGR. Review of existing pebble-bed HTGR designs and the unique characteristics of this core for computational modeling.
- Evaluation of the influence of the HTGR core parameters on neutronics.
- Improvement of HTGR concepts on the basis of efficient utilization of different forms and types of nuclear fuels and new structural materials.
- Determination of the safety characteristics of the HTGR core.

In this study, the detailed modeling of the pebble-bed HTGR core utilized up-to-date basic nuclear data and computational methods. Transport theory and Monte Carlo methods were used to take into account the three-dimensional complexity of the HTGR design. Models of the pebble-bed HTGR core accounted for the double heterogeneity of the core containing fuel pebbles and dispersion fuel. Within the frame of this study, the pebble-bed model has been verified using the low-enriched uranium (LEU)-High Temperature Reactor (HTR) PROTEUS calculation benchmark results obtained through the International Atomic Energy Agency Coordinated Research Program on the "Validation of Safety Related Reactor Physics Calculations for Low-Enriched HTGR's." The investigations focused on core consideration.

The following are the main conclusions based on the analysis of the core design and the safety and fuel performance:

- Replacement of the SiC coating interlayer of the fuel particle by the ZrC coating interlayer does not significantly influence the neutron multiplication level in the pebble-bed core. However, the presence of zirconium (Zr) in the core reduces the multiplication capability, and hence the fuel performance in the pebble-bed system.

- The pebble-bed HTGR core operation capabilities are acceptable at the potential temperatures.

- Performance of dioxide and dicarbide fuels in the pebble-bed HTGR core is compatible and the observed differences are small. However, the rate of depletion for carbide fuel is lower than for oxide.

- In case of the pebble-bed HTGR with LEU, the uranium enrichment can be reduced. The minimum permissible uranium enrichment level is 4-5 percent . Fuel lifetimes for LEU with 10 percent of U-235 is three to four years. It is possible to utilize pure Pu-fuel and mixed U-Pu in the pebble-bed HTGR core instead of uranium fuel. In the case of utilization of Pu-fuel and mixed U-Pu in the pebble-bed core, fuel lifetimes can be increased up to 10 years.

- Uranium (U)-fuel, pure plutonium (Pu)-fuel, and mixed U-Pu fuel have negative temperature reactivity coefficients in the pebble-bed HTGR core.

- The pebble-bed HTGR core can be used to burn weapons grade plutonium. Additional study is needed for fuel performance optimization for plutonium disposition in the pebble-bed core in order to provide the most efficient utilization of the material with maximum depletion.

**Planned Activities**

The following activities planned for the FY 2001 research effort will focus on a 50 MWth pebble bed core building on the Texas A&M study performed to date.

- Retain all of the principal characteristics of the core used in the Texas A&M analysis.
- Perform a thermal and fluid-flow analysis of the entire reactor system.
- Complete a preliminary plant layout integrating all of the major components.
- Produce a final report with the conceptual design and supporting documentation and calculations.

# NUCLEAR ENERGY RESEARCH INITIATIVE

## Novel Integrated Reactor Power Conversion System

| | | |
|---|---|---|
| PI: | Dimitri Paramonov, Westinghouse Electric Company LLC | |
| Collaborators: | University of New Mexico | |
| Project Start Date: | August 1999 | Projected End Date: September 2002 |
| Project Number: | 99-0198 | |

**Research Objective**

The overall objective of this project is to assess the technical and economic feasibility, develop engineering solutions, and determine a range of potential applications for a Novel Integrated Reactor/Energy Conversion System. The near term goal is the design of a power supply for use by developing countries in remote locations that is proliferation resistant, reliable, and economical. The heart of the concept is the use of a single working fluid (liquid metal) to be heated in a fast reactor and energy conversion of heat directly into electricity in an Alkali Metal Thermal to Electric Converter (AMTEC). It is expected that the integration of the nuclear heat source and energy conversion system would result in a power system with:

- A high degree of proliferation resistance due primarily to the use of a long life core (about 15 years without fuel shuffling or refueling).
- Enhanced reliability and safety due to the use of direct energy conversion methods, such as AMTEC and a thermoelectric bottoming cycle.
- Economic power generation using a simple system layout, isothermal operation of the energy conversion devices, operation without refueling, and possibly, disposal without the potential for radioactive releases or material diversion.

The project is being performed by Westinghouse Electric Company LLC, which is responsible for the long life sodium reactor development, the University of New Mexico's Institute for Space Nuclear Power Studies, which is developing a suitable AMTEC energy conversion system, and the University of New Mexico's New Mexico Engineering Research Institute.

**Research Progress**

The first year of the project focused on the feasibility issues associated with a long life, high temperature liquid metal-cooled core, selection of the working fluid, core-to-AMTEC coupling scheme and interface parameters, and energy conversion system design and performance.

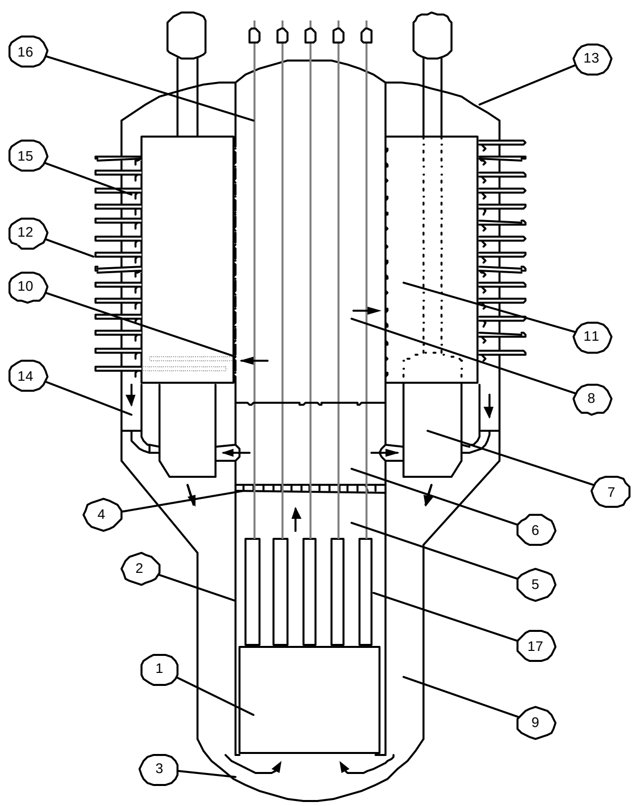
The neutronics calculations for a core design cooled by sodium or potassium were performed with a three dimensional Monte Carlo model and a set of newly developed high temperature cross-sections. The core consists of 60 hexagonal fuel assemblies with each assembly containing 169 fuel rods. It also includes two groups having six control rod assemblies in each and a central control rod assembly to control transients. $B_4C$ is currently considered the control rod absorber material. A flat, pancake core design is adopted (core height-to-diameter ratio of 0.4). Later studies may re-evaluate this ratio and attempt to improve the trade-off between the neutron economy and reactivity control. Simulations of voiding confirmed that the core exhibits a negative void coefficient. Initial evaluation of the control rod reactivity worth indicates that it is appropriate. As a result, the feasibility of a long life sodium-or potassium-cooled core was analytically demonstrated as meeting the neutronic and reactivity control design expectations and requirements.

An extensive evaluation of lithium, sodium, and potassium as the working fluid was performed based on performance (potassium might deliver significantly higher AMTEC efficiency), core thermal-hydraulics and safety, accumulated experience, and implications for a thermoelectric bottoming cycle design. Based on this assessment, lithium was eliminated, sodium was selected as the first choice, and potassium was selected as the second choice. Proven cold trapping techniques are judged adequate to control impurities in the envisioned pumped liquid metal circuit.

Based on the AMTEC performance analyses, fuel cladding and AMTEC structural performance considerations, a mixed mean core outlet temperature of 1000°K was selected as the governing parameter for the core-to-AMTEC interface. Vapor generation outside of the core through flash evaporation was selected as a coupling scheme to generate electricity and optimize AMTEC performance. At an AMTEC electrolyte temperature of 1000°K, a sodium AMTEC has a maximum efficiency of 23.5 percent and optimized condenser temperature of 630°K, versus 29.0 percent and 550°K for a potassium AMTEC. A schematic of an integral vessel housing reactor core, AMTEC converters and coolant pumps is depicted in the figure below.

Because cladding performance is considered to be the limiting design parameter, it was the focus of the thermal-hydraulic analyses. Nominal and maximum (3σ confidence level) cladding temperatures in the hot channel were determined using a semi-statistical uncertainty analysis approach. The resulting nominal and maximum cladding temperatures in the hot channel were found to be 1100°K (1490°F) and 1150°K (1580°F), respectively. These values are well within the limits of the selected Nb-1Zr cladding material.

Selection of Nb-1Zr as the reference cladding material is based on the good performance of the Nb-1Zr and uranium nitride fuel system in extensive irradiation tests for the SP-100 space reactor. The disadvantages and nuclear penalties of using Nb-1Zr as the cladding material are known. For the projected maximum cladding temperatures, selected high temperature alloys could be employed. Austenitic alloys previously used in liquid metal reactor (LMR) fuel rod tests were found to have insufficient creep strength at the maximum cladding temperatures. Precipitation hardened nickel alloys have sufficient creep strength, but loose ductility during irradiation and were previously found to be not suitable as LMR cladding materials. Most of the solution hardened high temperature materials include cobalt as an essential alloying element and are, therefore, also not suitable as cladding material. A suitable nickel alloy cladding with adequate creep strength, post irradiation ductility and without cobalt has not been found. Development of such a material could have application in high temperature gas cooled reactors and is probably forthcoming. However, application of such material as a high temperature fuel rod cladding material requires extensive irradiation testing of the cladding material and fuel rod. Therefore, Nb-1Zr is the reference choice material. A nickel alloy with yet untested irradiated properties is an alternative material.




**The reference reactor vessel and system layout schematic (1 – core, 2 – control rod guides, 3 – vessel, 4 – high pressure drop orifice (flash evaporator), 5 – high temperature, high pressure, subcooled working fluid region, 6 – high temperature, high pressure, saturated working fluid region, 7 – pump/mixer, 8 – high pressure, high temperature, saturated vapor region, 9 – high pressure, low temperature region, 10 – entrance to the AMTEC vapor feed channel, 11 – AMTEC energy conversion module, 12 – heat rejection heat pipe, 13 – low-pressure vessel portion, 13 – low temperature, low pressure region, 14 – low pressure, low temperature region, 15 - AMTEC cell working fluid discharge line, 16 – control rod drive line, and 17 - control rod guide.**

**Planned Activities**

The first year of the program has demonstrated basic technical feasibility of a direct cycle liquid metal reactor – AMTEC power system. Activities planned for the second phase include:

- Complete the burnup calculations for middle and end of core life.
- Finalize the reactor control approach.
- Perform three-dimensional thermal-hydraulic core modeling and select an orificing scheme.
- Design fuel rods for conditions consistent with core neutronics and thermal-hydraulics.
- Assess transient system performance.
- Design AMTEC cells and modules and finalize selection of structural materials.
- Develop an overall system layout.
- Address materials compatibility and mass-transport issues.
- Assess the system potential for co-generation.
- Design the thermoelectric bottoming cycle.
- Assess operation and maintenance issues, spent fuel disposal alternatives, transportation safety and proliferation resistance issues.

## Direct Energy Conversion Fission Reactor

| | |
|---|---|
| PI: | Gary F. Polansky, Sandia National Laboratories |
| Collaborators: | Los Alamos National Laboratory, General Atomics, University of Florida, Texas A&M University |
| Project Start Date: | August 1999      Projected End Date: September 2002 |
| Project Number: | 99-0199 |

### Research Objective

The goal of this project is to use nuclear energy to generate electricity without boiling water. A nuclear fission reaction produces neutrons, electrons, gamma rays, and energetic positively charged heavy atoms with 95 percent recoverable energy. These particles heat the surrounding structure usually generating energy in the form of heated water. The efficiency of follow-on processes, however, tends to limit the amount of generated electrical power. The steam cycle, for example, limits overall efficiencies for current nuclear power plant designs to approximately 33 percent. Direct nuclear energy conversion is any scheme that utilizes the fission energy directly from fissioning nuclear fuel. The intent of this project is to produce a design package that serves as the cornerstone to the process that ends with commercial development of a direct energy conversion device.

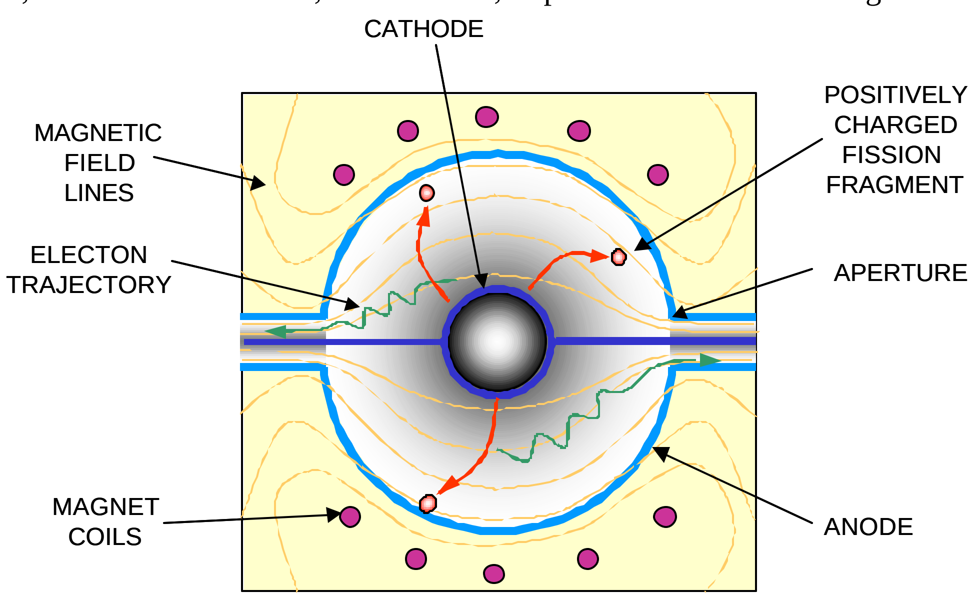
Experiments conducted during the late 1950's and early 1960's demonstrated the viability of the basic physics of direct energy conversion. However, technical challenges then limited practical efficiencies. Since then, dramatic improvements have occurred in such technological disciplines as computational mechanics, reactor pumped lasers, pulsed power, and space nuclear power that are directly applicable to this technology. The objective of this project is to re-examine these concepts and to apply new technology to find new and potentially commercially feasible fission energy alternatives.

### Research Progress

A project team consisting of scientists and engineers from Sandia National Laboratories, General Atomics, Los Alamos National Laboratory, Texas A&M University, and the University of Florida recently completed the first year of this project. After reviewing published literature, and developing additional concepts, schemes employing the physics of electromagnetics, magnetohydrodynamics, photonics, solid-state electronics, and electrostatics have been considered.

Several promising concepts involve a magnetically insulated fission electric cell. In its simplest form, the cell emits charged particles at the cathode and collects them at the anode. An intermediate electrode suppresses the flow of electrons, allowing a voltage to build-up across the electrodes. In a fission electric cell, the cathode is fissioning material. As fission occurs, it emits positively charged heavy atoms and electrons. If the electrons can be separated from the positive charges, a usable voltage can be generated between the two electrodes. Historic designs placed a fine grid of negatively charged wire between the electrodes. This grid forms a barrier to electron flow, but was previously demonstrated to be significantly inefficient. Advances in complex magnetic field modeling and superconductor technology make it possible today to design an efficient magnetic field to replace the wire grid. The magnetic field acts as a force field to separate the electrons from the heavy atoms. The concept of magnetic insulation was developed at Sandia for inertial confinement of fusion. Depending on the configuration, this concept allows devices with high efficiencies and power generation potentials. Two devices have been selected for further study using this principle; Quasi-Spherical Magnetically-Insulated Fission Electric Cell, and Fission Fragment Magnetic Collimator.

<u>Quasi-Spherical Magnetically Insulated Fission Electric Cell</u>: This design uses spherical cells with the fissioning cathode placed at the center as illustrated in the figure below. High-intensity shaped magnetic fields trap the electrons near the cathode allowing the more massive atoms to reach the anode and deposit their charge. Because a spherical geometry maximizes the recovery of fission particles, this scheme could achieve efficiencies theoretically as high as 60 percent. Overall, this device would be very compact, and would be stacked, like batteries, to produce the desired voltage and current.




**Quasi-Spherical Magnetically Insulated Fission Electric Cell**

<u>Fission Fragment Magnetic Collimator</u>: This theoretical device uses magnetic insulation to direct all the positive and negative charges to common collectors. Fissionable material in thin wires is placed in a parallel magnetic field inside a cylinder. As the fuel fissions, the electrons and positive particles remain separated and drift to the ends of the cylinder. At the ends, the particle energy is collected in an electric field insulated collector.

Efficiencies could achieve 35 percent. These devices can be large and have the potential for generating large quantities of power.

Another approach to direct conversion utilizes the physical concept of magnetohydrodynamics to generate electricity. The combination of charged material moving against a magnetic field causes electrons to flow in electrodes. If the charged material is a fluid, there are no moving parts. The higher the charge and the faster the fluid flow, the higher the electrical output. Such fluid devices are called magnetohydrodynamic (MHD) generators. One device, the Gaseous Vapor Core Reactor utilizes this principle.

<u>Gaseous Vapor Core Reactor with MHD Generator</u>: This direct scheme uses a high-temperature gaseous core reactor to generate partially ionized fissioning plasma that passes through an MHD channel to generate electricity. The unprocessed heat in the MHD cycle is transferred to a superheated Brayton cycle (gas turbine) and/or Rankine power cycle (steam turbine) to achieve combined efficiencies on the order of 60-70 percent.

During this year's study, nine different concepts were investigated. These concepts were analyzed and ranked to select the top three concepts. Efficiency was given the most weight with safety, feasibility, academic interest, operability, and proliferation resistance also being considered. Based on this review, the three concepts discussed above were chosen for further study.

**Planned Activities**

In this coming year, the team will concentrate on detailed definition of these three concepts with emphasis on identifying critical technical issues from each and defining experiments or research to refine the issues further. The culmination of the second year will be the selection of one concept. In the last year of this three year project, the team will concentrate on completing research and experiments while concentrating on compiling a preliminary design and defining future experiments for the selected concept. This activity leads to a final report containing the preliminary design; a list of needed critical technological developments and the research and experiments to achieve these developments.

# Novel Investigation of Iron Cross Sections via Spherical Shell Transmission Measurements and Particle Transport Calculations for Material Embrittlement Studies

PI: Steven M. Grimes, Ohio University

Collaborators: Pennsylvania State University, National Institute of Science & Technology

Project Start Date: August 1, 1999 Projected End Date: August 31, 2002

Project Number: 99-0228

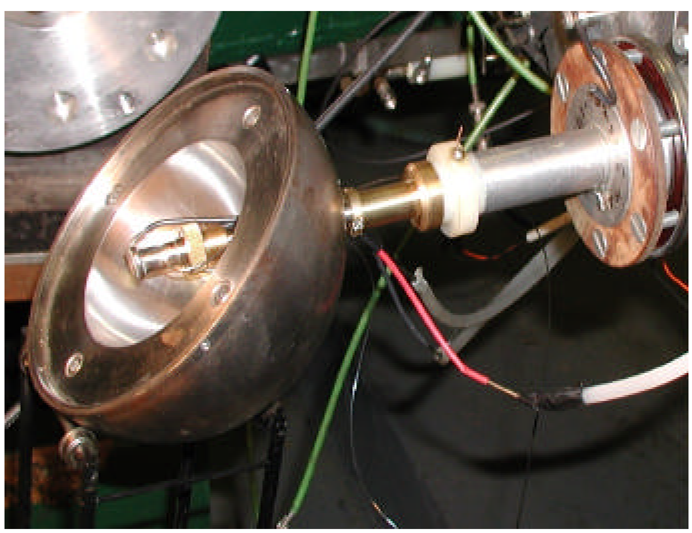
## Research Objective

The objective of this project is to perform precision measurements and detailed neutron transport simulations to accurately determine the iron non-elastic scattering cross sections in order to alleviate the well-known deficiency that exists in reactor pressure vessel (RPV) neutron fluence determinations. Measurements will be performed using accelerator-based neutron sources at energies greater than 1 MeV. Neutron time-of-flight measurements will be made at selected energies with both thin and thick spherical iron shells positioned over the neutron source. Such measurements provide information on the total non-elastic cross section, and various components of the non-elastic cross section for which there are neutrons in the exit channel. The thick shell work retains much of the cross section sensitivity of the thin shell measurements; however, more importantly, this work provides a way of determining the quality of evaluated microscopic cross section data by an application to a macroscopic system through which neutron transport can be determined.

Detailed particle transport calculations are performed to optimize the experiment, to improve the accuracy of the experimental data, and to generate continuous-energy and multigroup cross sections for comparing the measurements to calculations of the neutron transport through the shells. A series of time-dependent Monte Carlo neutron transport calculations will be used to investigate different experimental configurations in order to optimize the experiment. For this task, the $A^3$ (Automated Adjoint Accelerated Monte Carlo Neutron Photon [MCNP]) computer code and the three dimensional Parallel Environment Neutral-particle TRANsport (PENTRAN) code will be utilized. Subsequently, the experimental data will be analyzed using Monte Carlo and deterministic discrete ordinates neutron transport techniques in order to obtain information about energy regions where problems may exist with accepted iron cross section evaluations. It is expected that new methodologies and tools developed from this project may find use in other DOE projects.

**Research Progress**

The design of the experiment has been thoroughly studied, and final plans have been made for performing the experiment. Several hemispherical sections of different dimensions have been obtained for this work. Also, a radius cutter was ordered so that additional hemispheres can be fabricated to give maximum flexibility to adapt to the needs of the spherical shell transmission experiments. High-quality iron has been obtained for making additional hemispheres; in all cases compositional analyses are planned for the iron hemispheres. Nineteen source reactions that are suitable for this work have been studied. The best source for the spherical shell measurements is one that has high intensity and is constant in intensity and energy as a function of angle. The reactions that most closely satisfy these criteria are the $^{15}N(p,n)^{15}O$ and $D(d,n)^{3}He$ reactions, which are appropriate for the low and high energy regions, respectively. Fabrication of the sources has been completed. Measurements were made of source spectra for several reactions that may be appropriate for determining detector efficiency. The Al(d,n) reaction was chosen for this work above 250 KeV, since there is relatively little energy dependent structure in its spectrum. Additional experimental work using the Be(p,n) reaction yielded absolute efficiencies of neutron detectors down to about 80 KeV. Making efficiency measurements with white-spectrum source reactions such as these removes a limitation on previous work by others where the efficiency was determined at a limited number of isolated points necessitating interpolation between those points. The final efficiency determination for the lithium glass and NE-213 neutron detectors will be accomplished at the time of the experiment using the above-described white-spectrum source reactions. The experimental setup for the iron sphere measurements is shown in the figure below.



**Iron Sphere Experimental Setup. The gas cell is located at the center of the sphere with two water cooling lines, one air cooling line, and a gas filling line. The top of the low mass support stand is visible below the lower half of the iron sphere. The upper half of the sphere has been removed to reveal the details of the interior.**

In order to improve the experimental accuracy, new analytical neutron transport methodologies were developed. For example, in selecting an optimal target shape and target-source combination, different target shapes and thicknesses were compared on the basis of particle interaction rates for two available cross-section evaluations. Specifically, a new tallying capability was developed in the MCNP code with which the history (including energy, position, and direction) can be distinguished of those particles that have gone through elastic and/or inelastic scattering interactions. This work impacts both the accuracy and cost of measurements, and it also provides very useful information related to target shape that may be beneficial to this class of measurements. Because of the substantial degree of particle streaming that the experiment exhibits, new methods were developed for generating angular quadrature sets that yield the large number of directions (in excess of the 440 directions available from an S20 level-symmetric quadrature set) necessary for reduction of "ray effects." Also developed was a new methodology that couples PENTRAN forward and adjoint $S_N$ solutions with ray-tracing techniques, which was used to model the experiment. In addition, models were developed for performing sensitivity studies of the effects of variations in the energy dependency of inelastic scattering cross-sections. For this purpose, the PENTRAN code is used, which is very effective for solving deep-penetration problems because of its parallel processing capability and accurate numerical schemes.

**Planned Activities**

Additional work will be done using new tallying capability and $A^3$MCNP and PENTRAN models to further refine the experiment. Additional iron spheres will be fabricated as needed. Work will continue on modeling alternate experimental setups that may yield more accurate results. For example, placement of the detector relative to the target will be examined. Initial measurements will be made of the spectra of neutrons transmitted through a thin iron sphere; inelastic and elastic scattered groups of neutrons will be detected. The new tallying capability of MCNP will be used to estimate similar information. In conjunction, preliminary analysis of the measured data will commence; this will be augmented by appropriate transport simulations. In addition, analytical techniques will be used to compare the results of this work with that obtained with accepted evaluations of the iron cross sections.

## High Efficiency Generation of Hydrogen Fuels Using Nuclear Power

PI: Lloyd Brown, General Atomics

Collaborators: University of Kentucky, Sandia National Laboratory

Project Start Date: August 1, 1999 Projected End Date: August 2002

Project Number: 99-0238

### Research Objective

Hydrogen is an environmentally attractive transportation fuel that has the potential to displace fossil fuels when coupled with fuel cells. Fuel cells are more efficient than conventional battery/internal combustion engine combinations and do not produce nitrogen oxides during low temperature operation. Contemporary hydrogen production is primarily based on fossil fuels—more specifically on natural gas. When hydrogen is produced using energy derived from fossil fuels, there is little or no environmental benefit.

Currently, there is no large scale, cost-effective, environmentally attractive hydrogen production process available for commercialization. The objective of this research is to find an economically feasible process for the production of hydrogen, by nuclear means, using an advanced high-temperature nuclear reactor as the primary energy source. Hydrogen production by thermochemical water splitting, a chemical process that accomplishes the decomposition of water into hydrogen and oxygen using only heat or, in the case of a hybrid thermochemical process, by a combination of heat and electrolysis, could meet these goals.

The essential characteristics of a thermochemical water-splitting process can be seen in the simplified schematic of the sulfur-iodine process illustrated below. Thermal energy drives at least one endothermic high temperature chemical reaction. At least one spontaneous low temperature exothermic chemical reaction delivers waste heat to the environment. Additional chemical reactions, as necessary, balance the overall stoichiometry such that water is the only net reactant and hydrogen and oxygen are the only net products of the process.

### Research Progress

An exhaustive literature search was performed to locate all thermochemical water-splitting cycles. Thermochemical water-splitting is the conversion of water into hydrogen and oxygen by a series of thermally driven chemical reactions. The cycles located were screened using objective criteria, to determine which can benefit, in terms of efficiency and cost, from the high temperature capabilities of advanced nuclear reactors. An important part of the preliminary screening effort dealt with the details of

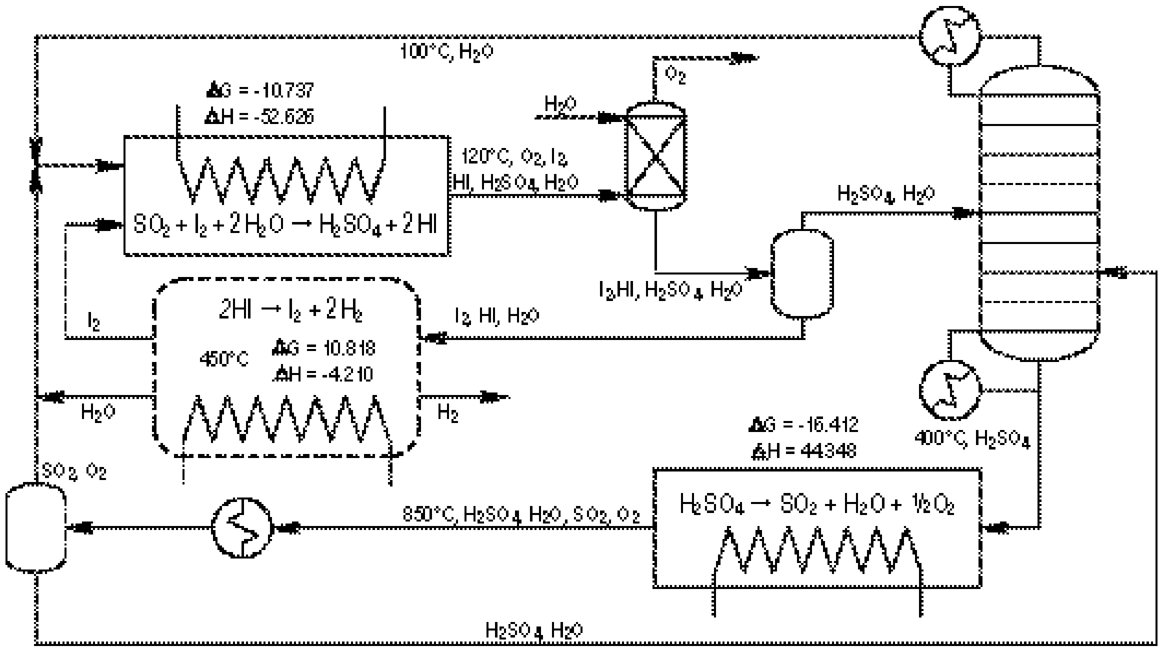
organizing and presenting data in an easy to use form, i.e., the organization of project specific databases.
The literature search turned up far too many cycles (115) to analyze in depth. In order to establish objective screening criteria, with which to reduce the number of cycles to a manageable number, it was necessary to establish meaningful and quantifiable criteria. The desirable cycle characteristics upon which quantifiable metrics were developed and used as screening criteria are as follows. Higher ranked cycles will:

- Have a minimum number of chemical reaction steps in the cycle.
- Have a minimum number of separation steps in the cycle.
- Have a minimum number of elements in the cycle.
- Employ elements, which are abundant in the earth's crust, oceans, and atmosphere.
- Minimize the use of expensive materials of construction by avoiding use of corrosive chemical systems, particularly in heat exchangers.
- Minimize the flow of solids.
- Have maximum heat input temperature compatible with high temperature heat transfer materials.
- Have been the subject of many papers from many authors and institutions.
- Have been tested at a moderate or large scale.
- Have good efficiency and cost data available.

The screening criteria were applied to all 115 cycles and the results were sorted according to the total number of screening points awarded to each process. Using 50 points (out of the total possible of 100) as the cut-off score gave a short list of over 40 cycles. Three additional go/no-go tests were applied to the short list leaving a first stage final short list of 25 cycles. As part of the second stage screening process, detailed investigations were made into the viability of each cycle. The most recent papers were obtained for each cycle, thermodynamic calculations were made over a wide temperature range, and each chemical species was considered in each of its potential forms (gas, liquid, solid, and aqueous solution). As a result of this analysis, two cycles were rated far above the others: Adiabatic UT-3 and sulfur-iodine cycles.

**Planned Activities**

The sulfur-iodine cycle has the highest reported efficiency. Various researchers have pointed out improvements that should increase the already excellent efficiency of this cycle and, in addition, lower the capital cost significantly. During the next phases of this project, improvements that have been proposed to the sulfur-iodine cycle will be investigated and an integrated flowsheet describing a thermochemical hydrogen production plant powered by a high-temperature nuclear reactor will be generated. The detailed flowsheet will allow the process equipment to be sized and calculations to be made on the hydrogen production efficiency. Calculations on the capital cost of equipment will be conducted along with an estimate of the cost of the hydrogen produced as a function of nuclear power costs.




It would be advantageous, but not essential, if some form of joint collaboration can be established with the Japanese (the basic UT-3 cycle was first described at the University of Tokyo and essentially all work on the cycle has been performed in Japan). Although effort for this project is concentrated on the sulfur-iodine cycle, interest in the UT-3 cycle remains. The work proposed here, and which will be carried out for the sulfur-iodine cycle has, to a large part, already been performed in Japan for the Adiabatic UT-3 process. The Japanese are encouraged to perform the required non-steady state analysis. After both the Japanese tasks and the research proposed here are complete, there will be two processes from which to select a means of producing hydrogen using nuclear power.

## "Smart" Equipment and Systems to Improve Reliability and Safety in Future Nuclear Power Plant Operations (SMART-NPP)

| | | |
|---|---|---|
| PI: | Felicia A. Durán, Sandia National Laboratories | |
| Collaborators: | Pennsylvania State University, Massachusetts Institute of Technology, ABB-Combustion Engineering, Duke Engineering & Services | |
| Project Start Date: | August 1, 1999 | Projected End Date: September 2002 |
| Project Number | 99-0306 | |

**Research Objective**

The goal of this research is to design, develop, and evaluate an integrated set of tools and methodologies that can improve the reliability and safety of advanced nuclear power plants through the introduction of 'smart' equipment and predictive maintenance technology. This will ultimately aide in the reduction of construction, maintenance, and operational costs.

To accomplish the goal the "Smart" Equipment program is:

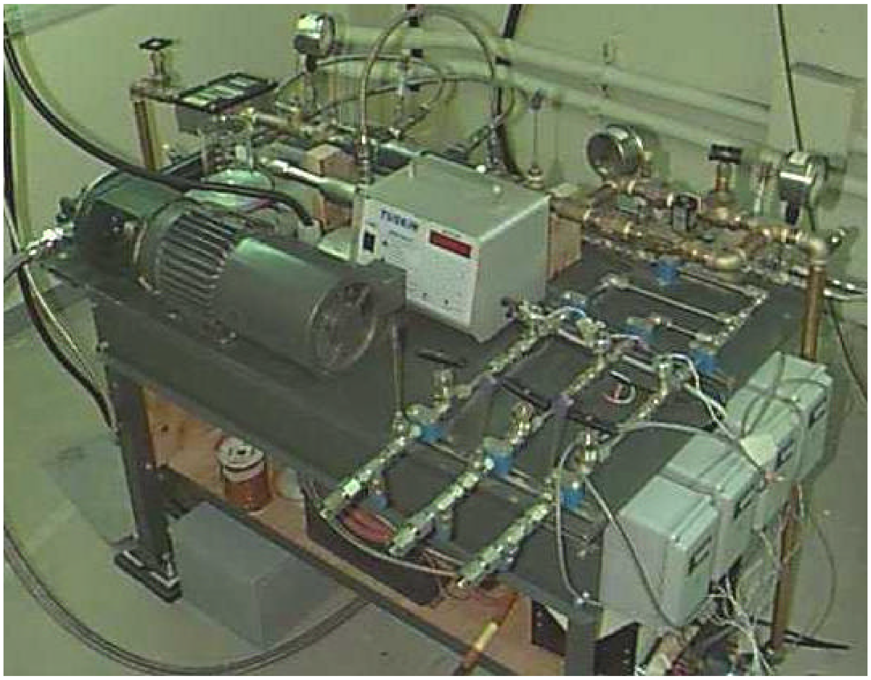
- Identifying and prioritizing nuclear plant equipment that would most likely benefit from adding 'smart' features.
- Developing a methodology for systematically monitoring the health of individual pieces of equipment implemented with 'smart' features (i.e., 'smart' equipment).
- Developing a methodology to provide plant operators with real-time information through 'smart' equipment Man-Machine Interface (MMI) to support their decision-making.
- Demonstrating the methodology on a selected component.
- Expanding the concept to system and plant levels that allow communication and integration of data among 'smart' equipment.

The SMART-NPP team established the following working definition of "Smart Equipment": Smart equipment embodies elemental components (e.g. sensor, data transmission devices, computer hardware and software, MMI devices) that continuously monitor the state of health of the equipment in terms of failure modes and remaining useful life, in order to predict degradation and potential failure and inform end-users of the need for maintenance or system-level operational adjustments.

**Research Progress**

Research accomplishments to date include:

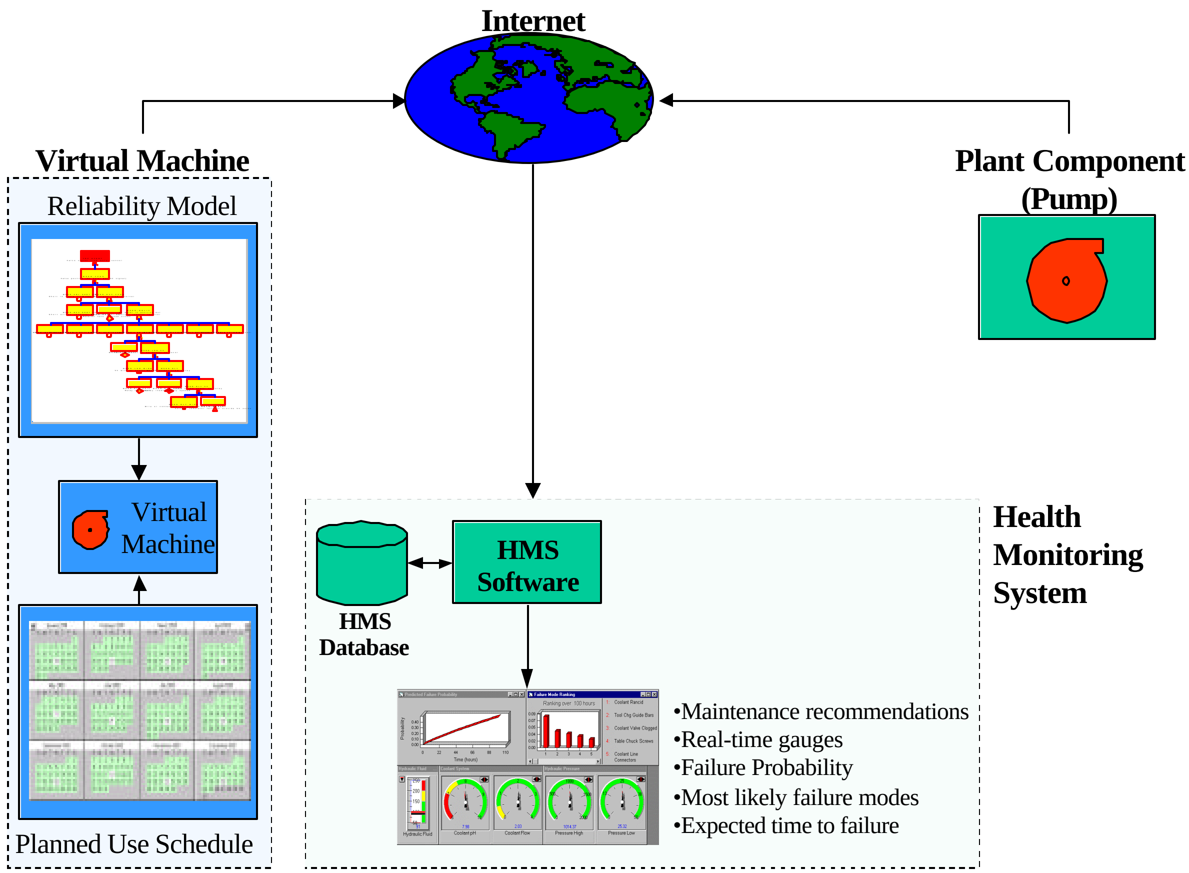
- Developed system/component criteria to establish priorities for 'smart' equipment application and used it to prioritize both pressurized water reactors (PWR) and boiling water reactors (BWR) systems.
- Based on the prioritization, selected a high energy, horizontal centrifugal pump as a demonstration component for a Health Monitoring System (HMS). A demonstration test-bed of the pump lube system has been built at Penn State University. The test-bed, which is illustrated in the picture below, has been instrumented with sensors, including a PC104 smart sensor, and will provide real-world data over the internet to the Health Monitoring System.



**Demonstration test-bed of the pump lube system**

- Developed HMS architecture using Bayesian Belief Networks to determine failure probability information based on sensor data and conditional probabilities.
- Procured the use of a pump lube oil system to supply real-world data to the HMS.
- Created the design for a 'virtual machine' (VM) for the selected pump to supply simulated reliability and sensor data to the HMS. (Figure below.)
- Assessed failure modes for the pump and established an optimum health monitoring plan.
- Reviewed and assessed sensor technology to develop criteria for sensor element selection and sensor system architecture.

- Reviewed 'smart' equipment MMI technology currently being used in other industries to support creation of an MMI prototype.
- Established industry contacts for potential cooperative working arrangements.




**Schematic of the Health Monitoring System linked via the internet to the Virtual Machine and a 'smart' physical plant component**

## Planned Activities

The team has high expectations of realizing a demonstration HMS tied to both a physical, real-world system and a VM simulation by the end of FY 2002. The major deliverables for Project Year Two (October 2000-September 2001) are: 1) Lube System Sensor Installation Report; 2) 'Virtual Machine' (VM) Alpha User's Manual; and, 3) Smart System Demonstration Status Report.

# Continuous-Wave Radar to Detect Defects within Heat Exchanger & Steam Generator Tubes


| | | |
|---|---|---|
| PI: | Thurlow W.H. Caffey, Sandia National Laboratories | |
| Collaborators: | New Mexico State University, Electric Power Research Institute | |
| Project Start Date: | August 1999 | Projected End Date: June 2002 |
| Project Number: | 99-0308 | |


## Research Objective

The overall objective of this three-year program is to design, fabricate, and demonstrate a complete defect-detection system using an in-tube radar (ITR) within a variety of steam-generator tubing typically found in nuclear-electric power plants. The ITR is fundamentally different from the eddy-current methods now in use because it is based on backscatter from a defect rather than the disturbance of current flow in the tube wall. An electric field, parallel to the axis of the tube, is transmitted into the tube wall, reflected from a defect, and returned to an internal receiver all operating in the near field. The fundamental premise is that the change in axial electric field caused by the defect will be distinguishable from the null field present in the absence of defects.

This first year's work had the following research objectives:

- Defect Modeling: Three-dimensional (3D) electromagnetic codes in cylindrical coordinates, including the transmitter, were needed to determine the backscatter from defects of different geometries, orientations, and wall locations.

- Alignment Sensitivity: Preliminary modeling showed that there would be no transmission from the transmitter to the receiver if both were located exactly on the centerline of the tube. However, further modeling was needed to show that slight departures from the ideal coaxial geometry, consistent with mechanical tolerances, would still allow acceptable performance.

- Prototype Design: Mechanical packaging, centering provisions, fiber-optic links, on-board power, antennas, amplifiers, and translation system designs were started both to provide some parameters needed for the above modeling codes, and to ensure timely completion of the project.

**Research Progress**

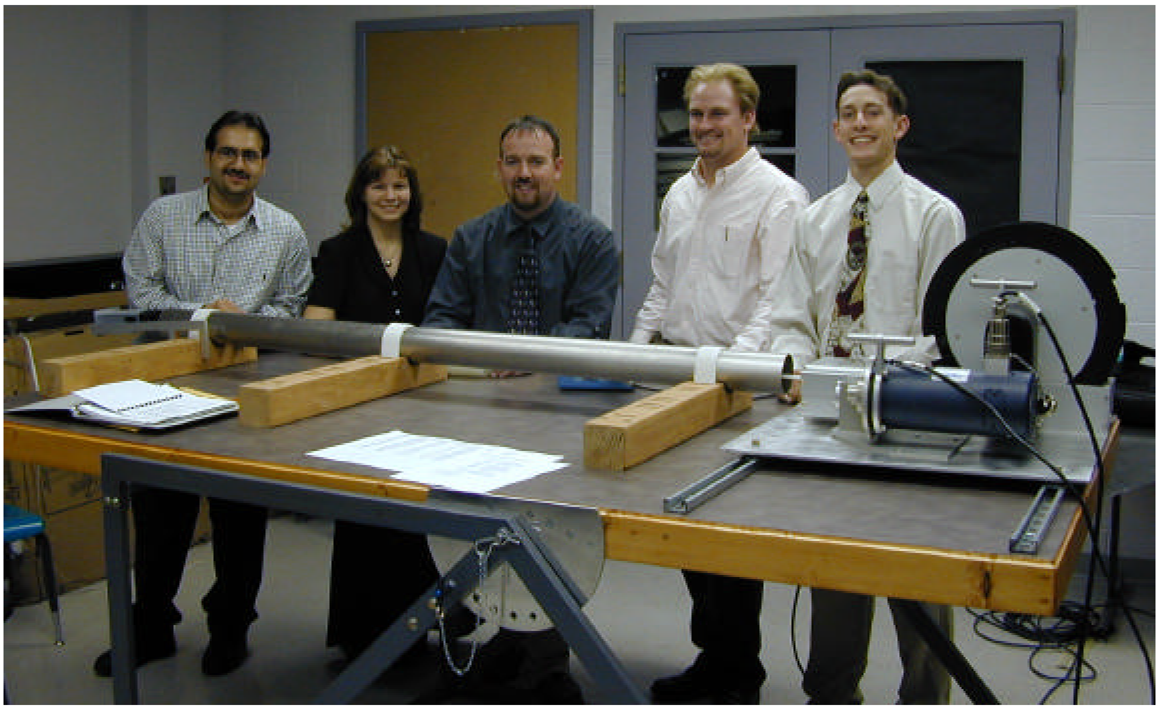
Although the research objectives are presented separately they are actually interrelated. For example, centering provisions have a direct effect upon the amount of direct transmission, or 'clutter', from the source to receiver. First year accomplishments are presented below in the same order as the objectives listed above.

Defect Modeling: Originally, these computations were to be done by scaling the 3D code GEMC at Sandia. It was apparent, by the January project meeting, that the modifications to GEMC would be very time-consuming. An improved version, named HELM, became available from another program but was not successfully used because of platform incompatibilities. In mid-June, a New Mexico State University (NMSU) researcher began development of a cylindrical, finite element 3D code called FEMTUBE. By early September, using a coarse mesh with only 1176 solid elements, this researcher showed that a defect on the outside of the tube wall does cause a corresponding change in the electric field.

This result established the basic premise but only in principle for one fracture model. The milestone report for this task has been delayed pending the computation of a suite of fracture geometries, location, size, and orientation.

Alignment Sensitivity: A theoretical code called CTUBE was further developed at Sandia to compute clutter due to non-ideal geometry. The present design of centering provisions predict that the instrument axis will be maintained within a circle, centered on the tube centerline, with a radius of 5 percent of the inner radius of the tube. CTUBE, however, becomes unstable when the transmitter and receiver are separated by the design value (less than one inch). Preliminary results from CTUBE, at slightly greater distances, predict that the effect of clutter will be acceptably small. This is encouraging, but the milestone report for this task has been delayed pending the solution of the stability problem within the design separation limits.

Prototype Design: The mechanical design of the probe and the testing fixture was assigned as a problem for the nine senior students in a capstone, mechanical engineering design class at NMSU. An early conclusion was to build a scaled-up version of the instrument and measure its performance in a large metal tube. Two different sizes were examined, namely 3.4-inch and 12-inch ID, together with three materials: aluminum, cast iron, and Inconel 600. An electromagnetic analysis showed that a low conductivity metal was required in order to keep the wall thickness from becoming too thin. Accordingly, a six-foot length of Inconel 600, with an ID of 3.438 inches and a 0.2-inch wall thickness was obtained. A three-team design contest was held for the test fixture, and fabrication drawings of the best option are now nearly complete. A commercial source for the translation system with a position encoder has been located (shown in the figure below). The design of the centering system for the scaled-up prototype is complete. Prototype units for the power amplifier for the transmitter as well as the ferrite rod antenna have been designed and fabricated. On the receiver side, a monopole antenna and amplifier have been designed and a prototype unit fabricated. These designs can be finalized once they are integrated with the two-way fiber-optic link guided by the results of calculations with FEMTUBE. Electrical design has received a great deal of attention, not only because of the small volume of the probe. The chief difficulty is that the receiver must be connected to the outside world by a two-way fiber-optic link with two diodes in the receiver that must operate on the micropower delivered by a hearing aid or watch battery.



**In-Tube Radar Project, Student Design Team with 5x demonstration and test model**

## Planned Activities

A recently developed basis system will be incorporated into FEMTUBE to permit the use of small meshes for only the representation of the defect, and not for the entire model tube. This will reduce both computational time and memory requirements. Work on a pattern recognition code has already begun, and will accelerate as different defect responses are provided from FEMTUBE. Three different approaches have been identified to eliminate the stability problems with CTUBE at small separation distances.

These computational efforts and the on-going development and manufacture of the scaled-up prototype should enable the milestone hand-pull-through system tests at NMSU to take place during the summer of 2001 as planned.

## 5. ADVANCED NUCLEAR FUELS

R&D in the advanced fuels area is needed to provide measurable improvements in the understanding and performance of nuclear fuel with respect to safety, waste production, proliferation resistance, and economics in order to enhance the long-term viability of nuclear energy systems. This program element addresses the long-term R&D goal to develop improved performance and advanced fuel designs for existing light water reactors and advanced fuel designs and related fuel cycle requirements for advanced Generation IV reactor designs.

The scope of this long-term R&D includes a variety of thermal and fast spectrum power reactor fuel forms, including ceramic, metal, hybrid, (e.g., cermet, cercet), and liquid, as well as fuel types including 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. The R&D scope also includes development of higher density LEU (<20 percent U-235) fuels for research and development reactors.

Currently selected projects include innovative concepts for material preparation and production of nuclear fuels; inherently safe fuel designs and core response; understanding 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 five percent; and innovation in fuel design, composition, or other attributes that maximize energy production, optimize fissile material utilization, or reduce production costs.

# NUCLEAR ENERGY RESEARCH INITIATIVE

# Development of Improved Burnable Poisons for Commercial Nuclear Power Reactors

PI: M.L. Grossbeck, Oak Ridge National Laboratory

Project Start Date: August 1, 1999 Projected End Date: August 31, 2002

Project Number: 99-0074

## Research Objective

Burnable poisons are used in nuclear reactors to aid in reactivity control and to reduce power peaking. The materials used at the present time suffer from two common disadvantages. The first is that the elements currently used, such as gadolinium and boron result in a small residual negative reactivity. Ideally, the burnable poison should be entirely depleted by the time the fuel is depleted. In fact, some burnable poison or isotopes that result from neutron absorption in the burnable poison remain at the time of fuel depletion and serve to limit the amount of fuel that can be used. The second is that boron transmutes to helium, which creates undesirable internal fuel pin pressures. Elimination or reduction of these two effects will lead to higher fuel burnup and longer core life resulting in lower cost of operation.

For many absorbing elements, such as gadolinium, it is isotopes other than the primary absorber that lead to residual reactivity. A goal of this research is to investigate the possibility of separating isotopes to isolate the absorbing isotope of interest, thus reducing or eliminating the residual reactivity. Absorbing elements such as samarium, gadolinium, dysprosium, and other identified candidates are being considered. State of the art two-dimensional computer codes will be used to determine the effects of the new burnable poisons, in both homogeneous and self-shielded configurations, on reactivity and core safety parameters. The second phase of the project will investigate isotope separation by the plasma separation process, and test separations will be attempted. In the final phase of the project, product forms determined from phase one will be fabricated using techniques of ceramic processing.

## Research Progress

The project is in the first phase where isotopes of strongly absorbing elements are examined. The main thrust of the project uses state of the art computer codes. Three-dimensional calculations are being performed using TALLY, MCNP4B, and ORIGEN2. Two-dimensional calculations are being performed with HELIOS. The core models use 8, 16, and in some cases, 64 burnable poison pins per fuel assembly in a PWR. Values of the reactivity coefficient ($k_{eff}$), normalized pin powers, and fuel and burnable poison burnup, as a function of time are calculated. Then reactivity of the burnable poison is calculated as a function of burnup. This residual reactivity due to the burnable poison is what is expected to be reduced through the isotope separation.

In conjunction with the detailed calculations, ORIGEN2 calculations are being performed on combinations of separated isotopes to examine their time behavior graphically. This series of calculations is used as a check on the Monte Carlo calculations and to point future directions. One group cross sections generated for the spectrum resulting from the burnable poison configuration are used in ORIGEN2. Reasonable agreement has been obtained for the case of homogeneous burnable poisons. Such calculations have demonstrated that removal of $^{154}Gd$ and $^{156}Gd$ results in about a factor of ten reduction in residual reactivity.

At the present time, Gd, Eu, Sm, Dy, Er, Yb, Hf, and Nd have been analyzed for the case of homogeneous burnable poison in the fuel. All have been found to have a self-shielding effect that extends the life of the burnable poison. Although this is usually a beneficial effect, it results in increased residual burnable poison. However, calculations are being done to evaluate burnable poisons in the form of coatings on the fuel pellets. In this configuration, several isotopes show promise if they are separated from the naturally occurring element. The isotopes $^{151}Eu$, $^{164}Dy$, $^{167}Er$, $^{149}Sm$, and $^{177}Hf$ have demonstrated improvement by placing them in a thin layer and enriching them isotopically. The residual reactivity as a function of layer thickness and burnable poison material density is also being investigated.

Calculational techniques have been refined to shorten the run time by a factor of ten. This has permitted rapid progress, and as a result, it is expected that the project will be completed within the time of the extension of phase one, by the end of January 2001. It must be remembered that isotopes cannot be developed. The isotopes provided by nature are all that can be used, making the project a high-risk endeavor. However, small improvements in fuel lifetime can result in large savings in fuel cost and reduction in waste.

**Planned Activities**

The above investigation has lead to exploration of incorporating burnable poison in the fuel cladding. This achieves reduced self-shielding. It also changes the chemistry and compatibility issue to one of cladding rather than fuel. This is being explored at the present time, although results remain preliminary. The concept of incorporating burnable poison in the cladding has led to the production of a cladding/burnable poison alloy, which is now being examined.

Technical discussions have been initiated with a private company that is constructing a facility for separation of isotopes by plasma separation. This method promises to be significantly less expensive than methods used at the present time for isotope separation. In the second phase, it is expected to do a separation run of one or more isotopes identified in the first phase.

# Fuel for a Once-Through Cycle $(Th,U)O_2$ in a Metal Matrix

PI: Sean M. McDeavitt, Argonne National Laboratory

Collaborators: Purdue University

Project Start Date: August 1, 1999 Projected End Date: August 31, 2002

Project Number: 99-0095

## Research Objective

Metal-matrix cermet nuclear fuels have potential for use in a once through, high-burnup, proliferation resistant fuel cycle. This project combines the advantages to be gained from cermet fuel with the resources extension potential of the thorium oxide fuel cycle and the inherent proliferation resistance of mixed oxide ceramics. These advantages fit well with the DOE's focus on the development of Generation IV nuclear power systems and proliferation resistant fuel cycles. The goal of this project is to demonstrate the feasibility of a metal-matrix fuel comprising $(Th,U)O_2$ microspheres in a zirconium matrix that can achieve high-burnup and be directly disposed as nuclear waste.

## Research Progress

For Task 1, Processing and Characterization of $(Th,U)O_2$ Microspheres, spray drying and sintering methods are being developed to fabricate the $(Th,U)O_2$ microspheres. The first year has been spent in obtaining authorization, setting up equipment, and establishing approved procedures. Approvals were obtained from the U.S. Nuclear Regulatory Commission and from the Purdue Radiological Control Committee to receive and use thoria. Using a surrogate alumina powder, slurry dispersion methods were studied and slurry viscosities were measured as a function of shear rate, dispersion methods, and pH. Spray drying procedures were developed using alumina powder and spray dried alumina microspheres were characterized. In addition, the facility and space for performing the spray drying of $(Th,U)O_2$ has been prepared, and the bioassay methods have been established.

In Task 2, Metal Matrix Development and Fuel Fabrication Development, fabrication experiments were completed to investigate processing factors such as surrogate oxide particle size, metal matrix particle size, minimum and/or optimum metal matrix content, mechanical mixing techniques, and drawing methodology. The powder-in-tube drawing techniques appear appropriate for consolidation and forming of the fuel pins. Microscopic analyses of finished parts show a sufficient degree of oxide and metal mixing can be achieved mechanically. However, the use of similar sized oxide and metal precursors seems to preclude the desired phase distribution of isolated oxide particles within a continuous metal matrix. Efforts are focused on methods to coat the oxide particles with metal prior to in-tube processing.

For Task 3, Neutronics and Thermal Design Analysis, research has focused on code acquisition and benchmarking, on preliminary fuel pin neutronics design, and on fuel thermal performance modeling. The fuel lattice code HELIOS was acquired and successfully benchmarked with a Monte Carlo burnup code. Preliminary neutronics design of a thorium metal matrix fuel pin was then performed with the HELIOS code. A tight pitch, "fat" fuel pin was designed with 60 percent heavy metal and 40 percent Zirconium. Slightly different pin designs were developed for pressurized and boiling water reactors, but both designs produced a burnup of greater than 100 GWd/t for a 3-batch core. The fuel thermal performance modeling work involved developing an effective conductivity model for metal matrix composite fuel types. A computer code was developed and was used to perform fuel temperature profiles for use with the HELIOS neutronics code.

## Planned Activities

Regarding Task 3 efforts, neutronics design work will continue and will include detailed fuel assembly and equilibrium cycle core burnup calculations. Task 4, Property, Behavior, and Performance Assessment, preliminary activities are underway to prepare for the measurement of fuel pin properties and performance modeling. Purdue University has obtained a metal matrix version of the fuel performance code, DART, and will begin adapting the code for the proposed fuel type. In addition, an examination of the literature related to interactions of uranium and thorium dioxides with zirconium and Zircaloy is being conducted to guide future investigations into the potential interaction between the $(Th,U)O_2$ microspheres and the zirconium matrix.

## Fundamental Mechanisms of Corrosion of Advanced Zirconium-Based Alloys at High Burn-up

PI: Randy G. Lott, Westinghouse Electric Company LLC

Collaborators: The Pennsylvania State University; Argonne National Laboratory – West; Idaho National Engineering and Environmental Laboratory

Project Start Date: August 1999 Projected End Date: September 2002

Project Number: 99-0128

**Research Objective**

The corrosion behavior of nuclear fuel cladding is a key factor limiting the performance of nuclear fuel elements. Improved cladding alloys, which resist corrosion and radiation damage, will facilitate higher burnup core designs. The objective of this project is to understand the mechanisms by which alloy composition, heat treatment and microstructure affect corrosion rate. This knowledge will be used to predict the behavior of existing alloys outside the current experience base (for example, at high burnup) and predict the effects of changes in operating conditions on zirconium alloy behavior.

Zirconium alloys corrode by the formation of a highly adherent protective oxide layer. The working hypothesis of this project is that alloy composition, microstructure and heat treatment affect corrosion rates through their effect on the protective oxide structure and ion transport properties. Therefore, particular emphasis has been placed on detailed characterizations of the oxides formed on a series of experimental alloys. The goal of this project is to identify these differences and understand how they affect corrosion behavior. To do this, several microstructural examination techniques including transmission electron microscopy (TEM), electrochemical impedance spectroscopy (EIS) and a selection of fluorescence and diffraction techniques using synchrotron radiation at the Advanced Photon Source (APS) are being employed.

Detailed characterizations of oxides are only useful if the observations can be linked to the corrosion behavior of the alloy. That link requires a model of the corrosion mechanism. The modeling effort is designed to organize the data from the characterization studies in a self-consistent manner and link those observations to the corrosion behavior. The ultimate objective of this project is to link the characterization and theoretical modeling efforts to yield improved alloy specifications.

**Research Progress**

The effort in the first year of the project has focused primarily on developing the procedures, tools, and expertise required to accomplish the project objectives. The microstructural examination studies have pioneered new techniques for characterizing corrosion oxides. An experimental facility for studying radiolysis has been designed and is being fabricated. A structure for a comprehensive corrosion model has been developed and the base model is operational. These efforts provide the basis for successful completion of this three year project.

A unique aspect of the project is the development and use of novel techniques. Project researchers from Pennsylvania State University and Westinghouse are leading an effort to characterize oxides on zirconium alloys using synchrotron radiation. Interfaces at the Advanced Photon Source at Argonne were established along with the completion of a key milestone when the project was granted use of a critical beamline following a competitive peer review of the proposed work. An initial micro-diffraction run was completed. In that run, a narrowly focused 0.25? by 2? beam was scanned across a cross-sectioned oxide to characterize the crystal structure as a function of depth. The studies indicate that the oxide is predominantly monoclinic with a small amount of tetragonal oxide also present. The tetragonal oxide is concentrated near the metal/oxide interface.

Corrosion oxides have also been characterized using EIS. There is a direct relationship between the electrical properties of the oxide and the corrosion process. The EIS studies indicate the presence of both a continuous layer of highly insulating oxide at the inner surface and a more porous deteriorated oxide on the outer surface. The project is now positioned to characterize the corrosion oxide of different zirconium-based alloys with varying corrosion resistance using this technique and the work has been initiated.

The physical structure of the corrosion oxides can be examined by TEM. However, preparation of appropriate TEM specimens of these oxides requires carefully developed procedures. To reveal the structure of the oxide, TEM specimens must be prepared in cross-section with the extent of the thin area in a plane perpendicular to the corroding surface. Techniques for successfully preparing cross-sectional specimens were developed. Preliminary studies reveal an extremely fine grain structure with a combination of equi-axed and columnar grains.

The effect of radiolysis on zirconium corrosion is characterized by the local environment rather than the bulk water conditions. The pores and microcracks that form in the oxide layer provide a pathway for water intrusion that create a local aqueous environment. A conceptual design for an experiment facility that simulates the local aqueous environment within the porous oxide film was completed.

A modeling effort was undertaken to provide a framework for relating the results of the characterization work to their impact on corrosion. The basic structure of the corrosion model has been implemented and tested. The modular structure of the model provides flexibility to incorporate individual effects, such as heat flux and continuous oxide growth on corrosion behavior.

**Planned Activities**

Progress during the first year of the program has provided the technology to conduct detailed characterizations of corrosion oxides. The primary objective of the second year will be to utilize this technology to characterize oxides on a variety of Zr alloys. Experience with preliminary studies indicates that it is important to understand both the effects of alloy type and the corrosion environment on the type of oxide that forms. APS, EIS and TEM techniques developed in the first year will be employed to characterize oxides grown in both pure water, steam and Li doped water. Characterizations of existing alloys will be completed and the number of materials under consideration expanded. Where required, additional autoclave exposures will be initiated to provide appropriate sources of oxide specimens.

The current model considers growth of the continuous oxide and breakdown of the oxide in separate modules. The primary outputs of these modules are the continuous oxide growth rate and the critical oxide thickness for breakdown. Emphasis in the second year will shift to modeling of the critical oxide thickness. As data on the oxide structures is accumulated, the model will be adjusted to match the observations.

The oxide characterization and theoretical modeling efforts will eventually produce improved alloy specifications. The project is designed to be evolutionary—lessons learned in the initial phases will be applied in the later phases. This evolutionary process is embodied in the alloy selection and development portion of the project. As the project proceeds, alloy specifications for improved corrosion resistance will be identified.

# Advanced Proliferation Resistant, Lower Cost, Uranium-Thorium Dioxide Fuels for Light Water Reactors

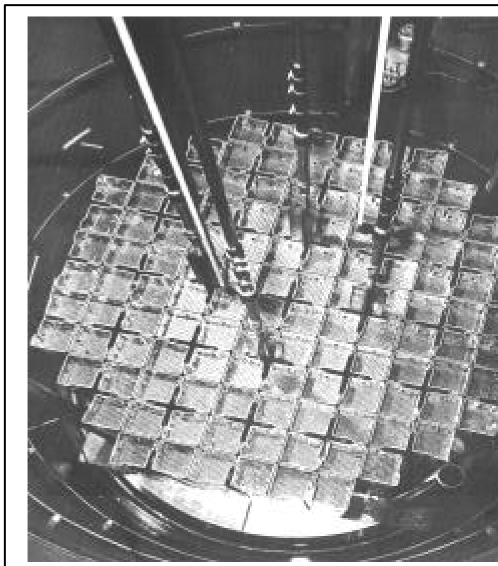

| | | |
|---|---|---|
| PI: | Philip E. MacDonald, Idaho National Engineering and Environmental Laboratory | |
| Collaborators: | Argonne National Laboratory, University of Florida, Purdue University, Massachusetts Institute of Technology, ABB-Combustion Engineering Inc., Westinghouse Electric Corp., Framatome Technologies, Siemens Power Corp. | |
| Project Start Date: | August 1, 1999 | Projected End Date: August 31, 2002 |
| Project Number: | 99-0153 | |


## Research Objective

The overall object of this project is to evaluate the efficacy of high burnup mixed thorium-uranium dioxide ($ThO_2$-$UO_2$) fuels for light water reactors (LWRs). A mixed thoria-urania fuel that can be operated to a relatively high burnup level in current and future LWRs may have the potential to:

- improve fuel cycle economics (allow higher sustainable plant capacity factors);
- improve fuel performance;
- increase proliferation resistance; and
- be a more stable and insoluble waste product than $UO_2$.

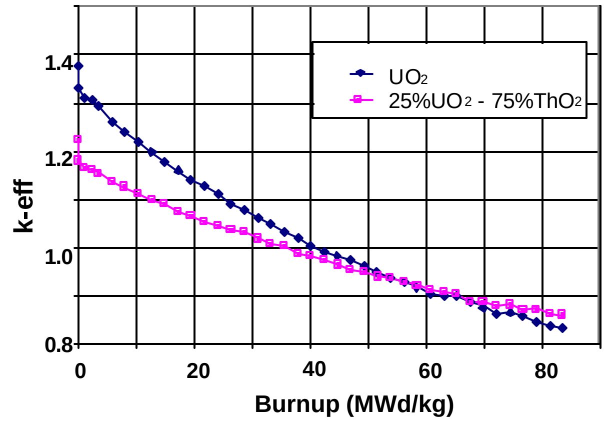
One of the important goals of this project is to study fuels that would be assembly-for-assembly compatible with the fuel in current LWRs. This implies that both utilities and vendors would find this fuel acceptable for manufacturing and use in current LWRs, if the economics prove to be desirable.



**$ThO_2$-$UO_2$ Critical Experiment**

## Research Progress

Reactor Core Neutronic Analysis and Fuel Cycle Design: Fuel cycle analysis performed during Phase I included benchmarking several computer models against available critical data (one of the critical experiments is shown to the right) and then analysis to determine the neutronic and economic viability of using a homogeneously mixed, thorium-uranium dioxide fuel. Several mixed thoria-urania fuel cases, ranging from a 75 percent $ThO_2$-25 percent $UO_2$ base case to a 65 percent $ThO_2$-35 percent $UO_2$ case, were evaluated for reactivity swing with burnup and isotopic concentrations. These cases were compared to all uranium cases with similar U-235 enrichments in the heavy metal (thorium + uranium, see figure to the right). Preliminary analyses of the enrichment and fabrication costs of the homogeneous thorium-uranium fuels have resulted in a cost per MW-hr about 20-25 percent higher than the all-uranium fuel. While the economics do not favor the homogeneous thorium-uranium fuels that have been studied thus far, other indicators do favor thorium-uranium fuel. For instance, the end-of-life isotopic concentrations strongly favor the thorium-uranium fuel based on total plutonium and minor actinide content, leading to a more proliferation resistant fuel as compared to uranium fuel. Also of interest is the reduction (or elimination) of burnable and soluble poisons needed with a thorium-uranium fuel due to the smaller reactivity swing with burnup. Other factors also show an advantage to using thorium-uranium fuel, such as better fuel performance and waste characteristics, and less coolant corrosion control problems due to the minimal use of soluble poisons. In addition, the preliminary studies on the use of a micro-heterogeneous $ThO_2$-$UO_2$ fuel in LWRs show that this fuel type appears to increase the burnup by 15 percent to 25 percent for the same fissile loading. This increase in burnup is significant enough to close the economic gap, and may show that thorium-uranium fuel can be economically competitive with current all-uranium fuels.



**Burnup vs. reactivity of a 25%$UO_2$-75%$ThO_2$ pin cell, and an all $UO_2$ pin cell.**

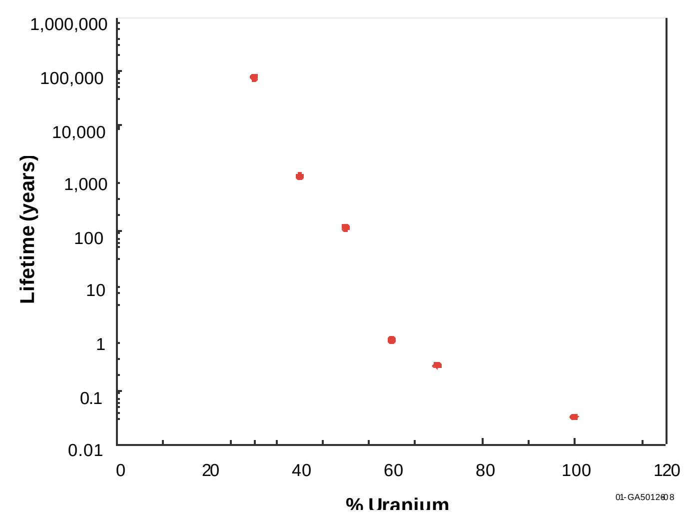
<u>Fuel Manufacturing Costs</u>: First year conclusions are as follows:

- Current uranium-only nuclear fuel manufacturing facilities can be used to manufacture mixed thorium/uranium fuels.
- Extensive changes are required in the wet conversion areas that manufacture the $ThO_2$ and the $UO_2$ to account for the possibility that 20 percent U-235 could be accidentally sent through the conversion line. Due to this rather conservative approach, the resulting facility will be able to handle any fuel composition up to a pure U-235 enrichment of 20 percent.
- Moderate changes will be required in the powder and pelleting areas of the manufacturing facility. The main changes will be in the size of the bulk powder containers. All equipment is currently able to accept powder of any composition up to a pure 20 percent U-235 enrichment level.
- Changes in monitoring for airborne contaminants will be required to account for the much lower Th limit and for the high U activity.

- There are adequate supplies of thorium available on the commercial markets to support use of a mixed $ThO_2$ -$UO_2$ fuel cycle.

Fuel Performance: The thermal, mechanical, and chemical aspects of the behavior of $ThO_2$-$UO_2$ fuel rods during normal, off normal, and design basis accident conditions are being evaluated. During normal operation, $ThO_2$-$UO_2$ fuel may operate with somewhat lower fuel temperatures and internal gas pressures than $UO_2$ fuel at corresponding powers and burnups. During an accident such as a large break loss-of-coolant accident (LOCA), $ThO_2$-$UO_2$ fuel will have less stored energy but a slightly higher internal heat generation rate than $UO_2$ fuel at similar power levels. Correlations, as a function of temperature, thoria and urania concentration, burnup, and other appropriate parameters have been developed from the existing literature for the following material properties: thermal conductivity, specific heat, thermal expansion, emissivity, modulus of elasticity, and melting temperature.

Long Term Stability of $ThO_2$-$UO_2$ Waste: The first year work focused on measuring the kinetic parameters for the air oxidation of $Th_xU_yO_2$ where x + y = 1 and x had values of 1.0, 0.7, 0.6, 0.5, 0.4, 0.3, and 0. A non-isothermal thermogravimetric analysis method was used to determine the kinetic parameters. The research showed that air oxidation rates of the solid solution $UO_2$ and $ThO_2$ samples were much lower than for pure $UO_2$. An example of the results for a 5 percent conversion of various thoria-urania compositions is shown to the right. Note that material with less than about 50 percent $UO_2$ lasts for a relatively long time. This reduction in oxidation rate has advantageous storage implications, if air oxidation is the rate-controlling step in transport of spent fuels into the environment.




**Lifetime of (U,Th)$O_2$ solid solution at room temperature**

**Planned Activities**

- Optimize the fuel form to increase the economic competitiveness of thorium-uranium fuel.
- Determine the projected capital and operating costs of fuel manufacturing.
- Evaluate fuel fabrication issues associated with co-precipitation of the powder and with pressing, sintering, and grinding $ThO_2$-$UO_2$ fuel pellets.

- Evaluate the behavior of $ThO_2$-$UO_2$ fuel during both normal operation and accident conditions, and compare the results with the behavior of current $UO_2$ fuel and USNRC licensing standards.
- Determine the corrosion and dissolution rates of both fresh and previously irradiated $ThO_2$-$UO_2$ fuel in synthetic ground water.

# A Proliferation Resistant Hexagonal Tight Lattice BWR Fuel Core Design for Increased Burnup and Reduced Fuel Storage Requirements


| | | |
|---|---|---|
| PI: | Hiroshi Takahashi, Brookhaven National Laboratory | |
| Collaborators: | Purdue University, Hitachi, Ltd. | |
| Project Start Date: | August 1, 1999 | Projected End Date: August 31, 2002 |
| Project Number: | 99-0164 | |


## Research Objective

The objective of this research is to advance the well-developed water-cooled reactor technology in order to make efficient use of the abundant thorium resources and enhance the proliferation resistance of the nuclear fuel cycle. Considerable effort has been invested in development of the sodium cooled fast reactor to breed fissionable Pu-239 from natural uranium. Much less effort has been expended in development of alternative technologies that take advantage of the considerable experience with light water reactors (LWR) to provide a hard neutron spectrum for converting thorium into the fissile U-233 isotope.

This project investigates the feasibility of a plutonium-thorium (Pu-Th) fuel cycle for a new type of proliferation resistant, economically competitive, high conversion, boiling water reactor (HCBWR). The technology will be developed to burn existing stocks of plutonium, while converting the fertile thorium to fissile U-233. The high conversion will take place in a fast neutron spectrum, which results from minimizing the volume of water in very tight fuel assembly lattices. High fuel burnup will be possible as a result of the continuous generation and fission of U-233 as the plutonium is consumed. Inherent safety will be designed into the reactor because of the favorable feedback neutronics characteristics of thorium and by the use of innovative core heterogeneities. This will insure a negative void coefficient for those accident sequences, which result in off-normal coolant boiling.

The major technical objective of the proposed project is to develop a reactor design that will:

- Minimize the potential for proliferation of weapons grade materials.
- Maximize the inherent safety features of the reactor.
- Maximize the achievable fuel burnup and plant capacity factor.
- Minimize the cost of electricity generation.

## Research Progress

The light water reactor with a hard neutron energy spectrum has been studied in the past, both in the U.S. and in Europe. More recently, there has been considerable interest in the Japanese nuclear industry and research organizations. This research project has evaluated several of the reactor designs proposed by the Japanese industry and research institutes. These designs included: (1) high conversion BWR, (2) long burnup cycle BWR (LBBWR), (3) BWR without blanket, (4) high conversion pressurized water reactor (PWR), and (5) PWR with Pu multi-cycle.

Detailed analysis of high conversion cores have been carried out in Japan over the last two years and the general conclusions were that in order to achieve high burnup, a reactor with a hard neutron energy spectrum is required. A tight lattice BWR core can provide the hard neutron energy spectrum; however, the coolant void coefficient tended to be positive. In order to achieve safe core operation, the analysis showed that a negative void coefficient could be achieved by enhancing neutron leakage during coolant heat up.

From this research project's preliminary analysis of the above reactors, the LBBWR type reactor has been selected for the initial design study. Because nonproliferation is one of the key factors in the NERI program, thorium will be used as fertile material instead of the U-238 which is used in the Japanese study. Use of thorium as the fertile material can also eliminate fissile plutonium more efficiently. In addition, the thorium fuel cycle does not accumulate a significant inventory of minor actinides that have very long half-lives and as such does not exacerbate the high level waste disposal problem.

Code acquisition and benchmarking work has been completed. Both stochastic and deterministic analysis codes are being used in the effort. The Brookhaven National Laboratory Monte Carlo burnup code MCBURN has been benchmarked for high conversion lattices. The collision probability lattice codes HELIOS was purchased from Studsvik/Scandpower and also benchmarked for thorium depletion with hexagonal lattices. A basic neutronics study was performed comparing performance of thorium and uranium fuels in both standard LWR and high conversion lattices. Preliminary design of the HCBWR fuel pin and fuel lattice was then completed using HELIOS and MCNP. Initial results show very favorable fuel burnup performance as well as good safety characteristics. The void coefficient was negative for all cases examined with thorium/plutonium fuel. Preliminary thermal-hydraulics analysis was also performed for the tight pitch channel using the RELAP5 code. Preliminary results are encouraging but there are concerns about adequacy of constitutive relationships for the tight lattice cores.

## Planned Activities

Work has progressed on schedule and some of the tasks on the second year have been initiated during the first year in order to facilitate the analysis. Specifically, the development of a hexagonal lattice capability in the nodal code PARCS was begun in the fourth quarter so that core burnup studies and core safety analysis could be started at the beginning of the second year.

To study the reactor safety of tight lattice Pu-Th reactor the reactor parameters associated with transient kinetic behavior will be calculated with the MCBURN code and provided in the PARCS code calculation.

# Development of a Stabilized Light Water Reactor (LWR) Fuel Matrix for Extended Burnup


| | | |
|---|---|---|
| PI: | Brady D. Hanson, Pacific Northwest National Laboratory | |
| Collaborators: | University of California - Berkeley | |
| Project Start Date: | August 1, 1999 | Projected End Date: September 2002 |
| Project Number: | 99-0197 | |


## Research Objective

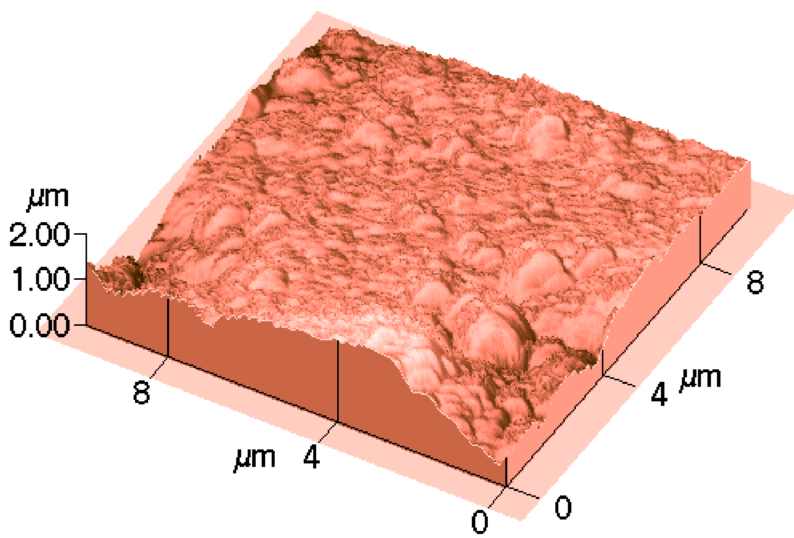
The main objective of this project is to develop an advanced fuel matrix based on the currently licensed $UO_2$ structure capable of achieving extended burnup while improving safety margins and reliability for present operations. Burnup is currently limited by the fission gas release and associated increase in fuel rod internal pressure, fuel swelling, and by cladding degradation. Once fuels exceed a threshold burnup, a "rim" or high burnup structure (HBS) forms. The HBS is characterized by the development of a subgrain microstructure having high porosity and low thermal conductivity. It is believed that the lower thermal conductivity results in larger temperature gradients and contributes to subsequent fission gas release. Fuel designs that decrease the centerline temperature while limiting the HBS restructuring, thereby decreasing the fission gas release should be able to achieve higher burnup and even allow higher operating power for increased efficiency.

Research at Pacific Northwest National Laboratory (PNNL) has demonstrated that the soluble fission products and actinides present in the matrix of irradiated (spent) fuels stabilized the fuel matrix with respect to oxidation to $U_3O_8$. The higher the soluble dopant concentration, the more resistant the fuel has been to undergoing the restructuring of the matrix from the cubic phase of $UO_2$ to the orthorhombic $U_3O_8$ phase. In this project, the attempt is to utilize the changes in fuel chemistry that result from doping the fuel to design a fuel that minimized HBS formation. The use of dopants that can act as getters of free oxygen and fission products to minimize fuel-side corrosion of the cladding is also being studied.

In addition to the use of dopants, project researchers are studying techniques such as the use of large grain sizes and radial variations in enrichment to minimize HBS formation and fission gas release. In this project, a combination of modeling and experimental studies is being used to determine the optimum design.

**Research Progress**

Task 1 (Understand and Model HBS Formation) focused on performing a comprehensive literature review to guide future efforts. Five different high burnup fuels, including two MOX fuels, were sectioned and prepared for examination of the HBS. Atomic force microscopy (AFM) has been used and appears to be able to map the HBS as a function of radius. An example of the morphology of the HBS as viewed using AFM is seen in the figure below.




**3-D AFM Image (10 x 10 µm) of LWR Spent Fuel Showing Restructured Grains in the HBS Region**

The successful use of AFM on these highly radioactive samples is believed to be the first such effort. A scanning electron microscope (SEM) and x-ray diffractometer (XRD) were both readied for examination of these spent fuel samples. Modifications to the Resonance Absorption Burnup (RABURN) model, used to calculate the radial concentrations of fission products and actinides, have been made to incorporate true cylindrical geometry.

Task 2 (Develop Matrix Stabilization Model) efforts went into preparing the SEM and XRD units for testing of the spent fuels and candidate fuels. The SEM is now fully operational and project researchers are waiting for their turn to use the equipment. All of the necessary paperwork to adhere to administrative regulations governing the use of fuel enriched in $^{235}U$ has been completed.

Task 3 (Design and Test Advanced Fuel Matrix) work involved an extensive literature review on the effect of dopants on the $UO_2$ lattice. This review was aimed at guiding the fuel design efforts. All of the equipment necessary to fabricate pellets based on the "recipes" of dopants developed in the other two tasks has been purchased. Most items, including the high temperature tube furnace (for grain growth experiments and sintering of pellets) and the pellet press have been installed. Commercial samples of gadolinia-doped fuels have been ordered for use in baseline tests of physical and chemical properties. The fuels developed for this project will be compared against these baselines. Finally, discussions with Argonne National Laboratory on the use of the Advanced Photon Source or Transmission Electron Microscopy (TEM) facilities to determine the location of dopants in the fuel matrix have been initiated.

## Continuous Fiber Ceramic Composite Cladding for Commercial Water Reactor Fuel

| | |
|---|---|
| PI: | Herbert Feinroth, Gamma Engineering Corporation |
| Collaborators: | Massachusetts Institute of Technology (MIT), McDermott Technology, Inc., Northwestern University, Swales Aerospace, Inc. |
| Project Start Date: | August 1, 1999     Projected End Date: June, 2001 |
| Project Number: | 99-0224 |

**Research Objective**

The objective of this project is to study the use of advanced ceramic materials as cladding for water reactor fuel elements, and to determine, via engineering type tests, the feasibility of substituting such advanced ceramic materials for the Zircaloy cladding now in use. The ceramic materials to be developed and tested in this research program are known as oxide-based continuous fiber ceramic composites (CFCCs).

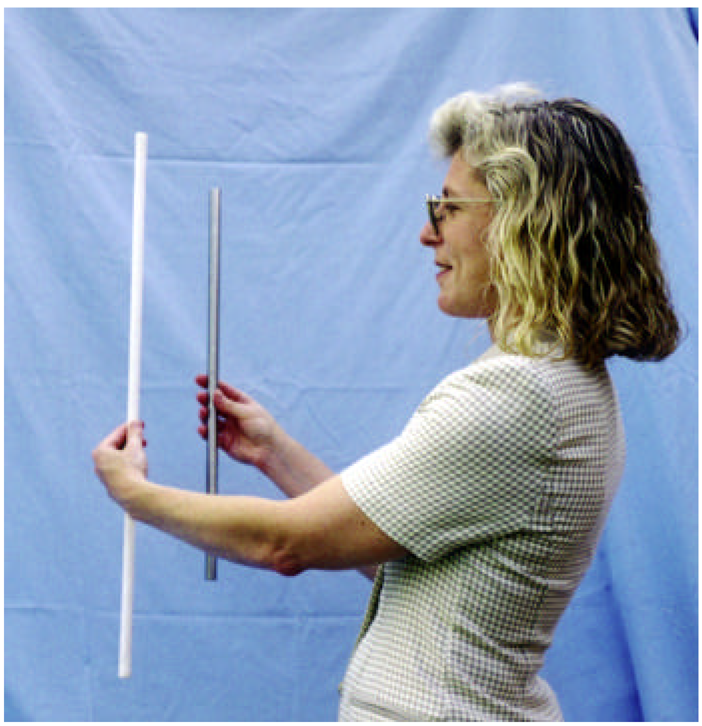
Oxide-based CFCCs have three main characteristics that recommend them for water reactor nuclear fuel cladding application. First, because CFCCs consist of very strong, micron sized fibers in a dense ceramic matrix, they do not behave in a brittle manner. Instead they have a failure mode that is non-catastrophic and similar to metals. Second, CFCCs retain their strength to much higher temperatures (e.g. >2000$^o$F) as compared to metals such as zircaloy, which lose much of their strength above 1000$^o$F. And third, oxide-based CFCCs (as opposed to carbide and nitride based CFCCs) remain chemically passive in high temperature steam. Thus, they do not react violently with water during a hypothetical Loss of Coolant Accident (LOCA), they do not produce heat during such an accident, and they do not produce hydrogen gas. Such characteristics, if applied to cladding in commercial water reactors, would lead to significant reductions in the consequences of low probability core overheating accidents, such as LOCAs. This could lead to improved and simplified reactor plant designs, simplified regulatory criteria, and improved public acceptance of nuclear power resulting from real reduction in residual risk.

This project seeks to address the feasibility of using CFCCs as reliable fuel cladding. Its aim is to determine the feasibility of providing an improved water reactor fuel element, which is significantly more resistant to damage during a LOCA accident than is the current water reactor fuel element. Specifically, the goals for the project are to (1) evaluate and select two or three specific oxide based CFCC materials which have the potential to meet LWR fuel cladding requirements, (2) fabricate LWR fuel clad test specimens from such materials using advanced CFCC fabrication techniques, (3) conduct in-pile corrosion tests on these specimens, along with standard zircaloy specimens, and

(4) expose such specimens to simulated LOCA test conditions to confirm their superior performance during LOCA accident conditions.

**Research Progress**

Approximately sixteen feet of high-density alumina-yttria ceramic composite cladding has been fabricated and delivered to Gamma Engineering Corporation for final sectioning and assembly into the test fixtures at Swales Aerospace and Massachusetts Institute of Technology. A portion of these test samples will be reserved for further characterization and archival storage. The tubes are a composite of high-density alumina fibers (Nextel 610 by 3M), embedded in a matrix of dense yttria-alumina. Some of the tubes (about 4 feet) are then chemical vapor infiltration (CVI)-coated by Northwestern University with either pure alumina, or a mixture of 90 percent alumina, 10 percent chromia to enhance the surface condition and performance of the CFCC material.



**Clad Test Samples**

MIT completed the design of a test fixture for reliable mounting of ten 3-inch long specimens in a special loop to be inserted in their test reactor. The hardware for the fixture is currently under procurement, and assembly of the fixture with the test specimens was planned during the month of August 2000. Swales has completed the assembly and trial use of a special LOCA test rig designed to quench typical clad specimens (3 inches in length) from high temperature (up to 2500$^{o}$F) into room temperature water.

**Planned Activities**

Phase 2 of this project involves two test programs, and further characterization of the fabricated tubes.

Irradiation Test Program: Ten clad specimens (each about 3 inches long) will be irradiated in a special high temperature (600 $^{o}$F) flow loop in MIT's 5 MW nuclear reactor.

LOCA - Thermal Shock Test: Three inch long test specimens will be heated in a special furnace to three different "accident" temperatures: 1000$^{o}$F, 1800$^{o}$F, 2500$^{o}$F. After stabilization at these temperatures, each specimen will be quenched in room temperature water in a special apparatus.

Further Characterization Tests: Visual and microstructure examination will be conducted after the irradiation and thermal shock tests. In addition, permeability tests will be performed on some of the pre-irradiated coated specimens to compare with pre-irradiated uncoated specimens.

Thus far, the project has addressed many of the technical issues associated with the use of CFCCs as cladding in commercial reactors. Some of the issues have been resolved, and others remain for further development. A key factor in determining whether further work is warranted on applying this promising new material to nuclear fuel cladding use will be the results of the planned thermal shock and irradiation testing.

# An Innovative Ceramic Corrosion Protection System for Zircaloy Cladding

PI: Ronald H. Baney, University of Florida

Project Start Date: August 1, 1999 Projected End Date: August 31, 2002

Project Number: 99-0229

## Research Objective

The operational lifetime of current Light Water Reactor (LWR) fuel is limited by thermal, chemical, and mechanical constraints associated with the fuel rods being used to generate nuclear heat. A primary limiting factor of this fuel is the waterside corrosion of the zirconium based alloy cladding surrounding the uranium pellet. This research project intends to develop thin ceramic films with adhesive properties to the metal cladding in order to eliminate the oxidation and hydriding of Zircaloy cladding. The corrosion protection system will allow fuel to operate safely at significantly higher burnups resulting in major benefits to plant safety and plant economics.

A major technical challenge for coating a metal with a ceramic protection system is to develop a cohesive bond between the two materials. The differences between the thermal expansion of the ceramic coating and the thermal expanding metal can, if not properly addressed, interfere with the ceramic's ability to maintain a bond and thus maintain a protective layer.

## Research Progress

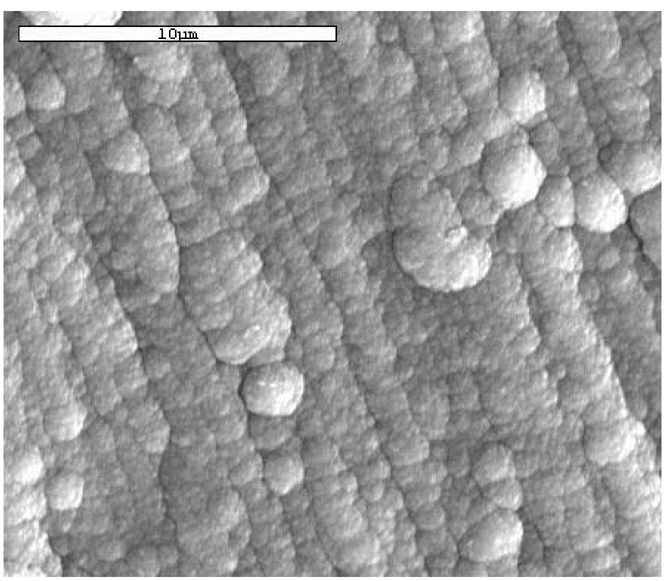
The following ceramics were investigated: alumina, boron carbide, graphite, mullite, silicon carbide, spinel, tungsten carbide, zirconia, and zirconium carbide. A background search was performed to identify their current uses in industry, processing methods, potential cost, their availability, and their suitability as a protective coating material for Zircaloy cladding in a LWR.

The mechanical properties of the coatings, such as coefficient of thermal expansion (CTE) and thermal conductivity, were compared with that of zirconium (Zircaloy) in order to determine the best candidate. A hand-calculated thermal analysis was performed to show temperature changes owing to the different coatings as a function of coating thickness and the validity of these calculations was established by a comparison with the thermal hydraulic computer program COBRA. A neutronic analysis was also performed using the Monte Carlo N-Particle Transport Code (MCNP) to show reactivity changes and unit fuel cell thermal flux changes caused by the different coatings as a function of thickness. The CASMO computer code was utilized to show burnup effects and changes in plutonium concentrations owing to an alumina coating of 50 to 100 microns. As a result of these studies, the two best coating options were identified as alumina and silicon carbide and initial samples were placed in an autoclave to simulate upper limit reactor conditions (water that was at 700F and 3000 PSIA pressure) in order to observe the coatings' corrosive and chemical stability.

Alumina's CTE is within 12 percent of zirconium's throughout the entire temperature range, while silicon carbide has the highest thermal conductivity of 78.8 W/m-K. All of the materials were analyzed thermally in order to calculate the rise in temperature of the fuel centerline, pellet surface, and outer and inner clad surfaces. At 50 microns, none of the coatings caused more than a 0.13 percent rise in cladding temperature and 0.05 percent rise in fuel centerline temperature. Even with a thickness of 500 microns, none of the materials caused more than a 1.5 percent increase in temperatures in any of the regions. Due to the extensive computation time required, only silicon carbide, alumina, zirconium carbide, and zirconia were analyzed neutronically. At the most likely coating thickness between 10 and 50 microns, there was less than a 0.09 percent decrease in reactivity and a 0.5 percent decrease in the thermal flux in the fuel and a 1.7 percent decrease in the thermal flux in the water.

Owing to the displacement of water caused by the coating, there was a hardening of the spectrum and therefore an increase in plutonium production as the fuel is being used. With a coating of 50 microns of alumina, there was as 1.9 percent increase in Pu-239 at 60 GWD/MTU. This increase in plutonium production has the added benefit of extending the reactivity lifetime of the fuel as plutonium becomes used as fuel.

A variety of coating processes for coating carbon, silicon carbide and alumina onto Zircaloy were explored. Carbon, diamond like carbon (DLC), and silicon carbide (SiC) were coated onto Zirc-4 coupons by plasmas-assisted chemical vapor deposition (PACVD). The figure below shows a SEM image of one such coating.




**SEM image of SiC thin films on unpolished Zircalloy deposited at 400C using Silacyclobutane by electron cyclotron resonance (ECR) plasma assisted (PA) chemical vapor deposition (CVD)**

Silicon carbide was also coated by a laser ablation deposition (LAD) process. Alumina was coated by an ultraviolet assisted chemical vapor (UVCVD) process. Alumina was also coated by a spin coating sol-gel process. A thick layer of alumina was coated onto a sheet of Zirc-4 by physical vapor deposition (PVD) using a plasma spray technique.

The quality of the coatings were assessed by visible inspection for uniformity and physical adherence of the coating and by Auger Electron Spectrographic (AES). The quality of the ceramic coating was assessed by the depth of the coating and the thickness of the coating.

**Planned Activities**

The corrosion testing of alumina and other promising coatings will be studied in detail. Further autoclave testing and accelerated corrosion testing will be required in order to complete a performance analysis of the ceramic coatings applied to zirconium alloy. Further investigation is also required to verify bonding throughout the fuel lifetime for the various coating materials. Coating processes will be optimized to give the highest quality coatings.

## 5. ADVANCED NUCLEAR FUELS

R&D in the advanced fuels area is needed to provide measurable improvements in the understanding and performance of nuclear fuel with respect to safety, waste production, proliferation resistance, and economics in order to enhance the long-term viability of nuclear energy systems. This program element addresses the long-term R&D goal to develop improved performance and advanced fuel designs for existing light water reactors and advanced fuel designs and related fuel cycle requirements for advanced Generation IV reactor designs.

The scope of this long-term R&D includes a variety of thermal and fast spectrum power reactor fuel forms, including ceramic, metal, hybrid, (e.g., cermet, cercet), and liquid, as well as fuel types including 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. The R&D scope also includes development of higher density LEU (<20 percent U-235) fuels for research and development reactors.

Currently selected projects include innovative concepts for material preparation and production of nuclear fuels; inherently safe fuel designs and core response; understanding 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 five percent; and innovation in fuel design, composition, or other attributes that maximize energy production, optimize fissile material utilization, or reduce production costs.

# NUCLEAR ENERGY RESEARCH INITIATIVE

# Development of Improved Burnable Poisons for Commercial Nuclear Power Reactors

PI: M.L. Grossbeck, Oak Ridge National Laboratory

Project Start Date: August 1, 1999 Projected End Date: August 31, 2002

Project Number: 99-0074

## Research Objective

Burnable poisons are used in nuclear reactors to aid in reactivity control and to reduce power peaking. The materials used at the present time suffer from two common disadvantages. The first is that the elements currently used, such as gadolinium and boron result in a small residual negative reactivity. Ideally, the burnable poison should be entirely depleted by the time the fuel is depleted. In fact, some burnable poison or isotopes that result from neutron absorption in the burnable poison remain at the time of fuel depletion and serve to limit the amount of fuel that can be used. The second is that boron transmutes to helium, which creates undesirable internal fuel pin pressures. Elimination or reduction of these two effects will lead to higher fuel burnup and longer core life resulting in lower cost of operation.

For many absorbing elements, such as gadolinium, it is isotopes other than the primary absorber that lead to residual reactivity. A goal of this research is to investigate the possibility of separating isotopes to isolate the absorbing isotope of interest, thus reducing or eliminating the residual reactivity. Absorbing elements such as samarium, gadolinium, dysprosium, and other identified candidates are being considered. State of the art two-dimensional computer codes will be used to determine the effects of the new burnable poisons, in both homogeneous and self-shielded configurations, on reactivity and core safety parameters. The second phase of the project will investigate isotope separation by the plasma separation process, and test separations will be attempted. In the final phase of the project, product forms determined from phase one will be fabricated using techniques of ceramic processing.

## Research Progress

The project is in the first phase where isotopes of strongly absorbing elements are examined. The main thrust of the project uses state of the art computer codes. Three-dimensional calculations are being performed using TALLY, MCNP4B, and ORIGEN2. Two-dimensional calculations are being performed with HELIOS. The core models use 8, 16, and in some cases, 64 burnable poison pins per fuel assembly in a PWR. Values of the reactivity coefficient ($k_{eff}$), normalized pin powers, and fuel and burnable poison burnup, as a function of time are calculated. Then reactivity of the burnable poison is calculated as a function of burnup. This residual reactivity due to the burnable poison is what is expected to be reduced through the isotope separation.

In conjunction with the detailed calculations, ORIGEN2 calculations are being performed on combinations of separated isotopes to examine their time behavior graphically. This series of calculations is used as a check on the Monte Carlo calculations and to point future directions. One group cross sections generated for the spectrum resulting from the burnable poison configuration are used in ORIGEN2. Reasonable agreement has been obtained for the case of homogeneous burnable poisons. Such calculations have demonstrated that removal of $^{154}$Gd and $^{156}$Gd results in about a factor of ten reduction in residual reactivity.

At the present time, Gd, Eu, Sm, Dy, Er, Yb, Hf, and Nd have been analyzed for the case of homogeneous burnable poison in the fuel. All have been found to have a self-shielding effect that extends the life of the burnable poison. Although this is usually a beneficial effect, it results in increased residual burnable poison. However, calculations are being done to evaluate burnable poisons in the form of coatings on the fuel pellets. In this configuration, several isotopes show promise if they are separated from the naturally occurring element. The isotopes $^{151}$Eu, $^{164}$Dy, $^{167}$Er, $^{149}$Sm, and $^{177}$Hf have demonstrated improvement by placing them in a thin layer and enriching them isotopically. The residual reactivity as a function of layer thickness and burnable poison material density is also being investigated.

Calculational techniques have been refined to shorten the run time by a factor of ten. This has permitted rapid progress, and as a result, it is expected that the project will be completed within the time of the extension of phase one, by the end of January 2001. It must be remembered that isotopes cannot be developed. The isotopes provided by nature are all that can be used, making the project a high-risk endeavor. However, small improvements in fuel lifetime can result in large savings in fuel cost and reduction in waste.

**Planned Activities**

The above investigation has lead to exploration of incorporating burnable poison in the fuel cladding. This achieves reduced self-shielding. It also changes the chemistry and compatibility issue to one of cladding rather than fuel. This is being explored at the present time, although results remain preliminary. The concept of incorporating burnable poison in the cladding has led to the production of a cladding/burnable poison alloy, which is now being examined.

Technical discussions have been initiated with a private company that is constructing a facility for separation of isotopes by plasma separation. This method promises to be significantly less expensive than methods used at the present time for isotope separation. In the second phase, it is expected to do a separation run of one or more isotopes identified in the first phase.

# Fuel for a Once-Through Cycle $(Th,U)O_2$ in a Metal Matrix

PI: Sean M. McDeavitt, Argonne National Laboratory

Collaborators: Purdue University

Project Start Date: August 1, 1999    Projected End Date: August 31, 2002

Project Number: 99-0095

## Research Objective

Metal-matrix cermet nuclear fuels have potential for use in a once through, high-burnup, proliferation resistant fuel cycle. This project combines the advantages to be gained from cermet fuel with the resources extension potential of the thorium oxide fuel cycle and the inherent proliferation resistance of mixed oxide ceramics. These advantages fit well with the DOE's focus on the development of Generation IV nuclear power systems and proliferation resistant fuel cycles. The goal of this project is to demonstrate the feasibility of a metal-matrix fuel comprising $(Th,U)O_2$ microspheres in a zirconium matrix that can achieve high-burnup and be directly disposed as nuclear waste.

## Research Progress

For Task 1, Processing and Characterization of $(Th,U)O_2$ Microspheres, spray drying and sintering methods are being developed to fabricate the $(Th,U)O_2$ microspheres. The first year has been spent in obtaining authorization, setting up equipment, and establishing approved procedures. Approvals were obtained from the U.S. Nuclear Regulatory Commission and from the Purdue Radiological Control Committee to receive and use thoria. Using a surrogate alumina powder, slurry dispersion methods were studied and slurry viscosities were measured as a function of shear rate, dispersion methods, and pH. Spray drying procedures were developed using alumina powder and spray dried alumina microspheres were characterized. In addition, the facility and space for performing the spray drying of $(Th,U)O_2$ has been prepared, and the bioassay methods have been established.

In Task 2, Metal Matrix Development and Fuel Fabrication Development, fabrication experiments were completed to investigate processing factors such as surrogate oxide particle size, metal matrix particle size, minimum and/or optimum metal matrix content, mechanical mixing techniques, and drawing methodology. The powder-in-tube drawing techniques appear appropriate for consolidation and forming of the fuel pins. Microscopic analyses of finished parts show a sufficient degree of oxide and metal mixing can be achieved mechanically. However, the use of similar sized oxide and metal precursors seems to preclude the desired phase distribution of isolated oxide particles within a continuous metal matrix. Efforts are focused on methods to coat the oxide particles with metal prior to in-tube processing.

For Task 3, Neutronics and Thermal Design Analysis, research has focused on code acquisition and benchmarking, on preliminary fuel pin neutronics design, and on fuel thermal performance modeling. The fuel lattice code HELIOS was acquired and successfully benchmarked with a Monte Carlo burnup code. Preliminary neutronics design of a thorium metal matrix fuel pin was then performed with the HELIOS code. A tight pitch, “fat” fuel pin was designed with 60 percent heavy metal and 40 percent Zirconium. Slightly different pin designs were developed for pressurized and boiling water reactors, but both designs produced a burnup of greater than 100 GWd/t for a 3-batch core. The fuel thermal performance modeling work involved developing an effective conductivity model for metal matrix composite fuel types. A computer code was developed and was used to perform fuel temperature profiles for use with the HELIOS neutronics code.

**Planned Activities**

Regarding Task 3 efforts, neutronics design work will continue and will include detailed fuel assembly and equilibrium cycle core burnup calculations. Task 4, Property, Behavior, and Performance Assessment, preliminary activities are underway to prepare for the measurement of fuel pin properties and performance modeling. Purdue University has obtained a metal matrix version of the fuel performance code, DART, and will begin adapting the code for the proposed fuel type. In addition, an examination of the literature related to interactions of uranium and thorium dioxides with zirconium and Zircaloy is being conducted to guide future investigations into the potential interaction between the $(Th,U)O_2$ microspheres and the zirconium matrix.

# Fundamental Mechanisms of Corrosion of Advanced Zirconium-Based Alloys at High Burn-up

PI: Randy G. Lott, Westinghouse Electric Company LLC

Collaborators: The Pennsylvania State University; Argonne National Laboratory – West; Idaho National Engineering and Environmental Laboratory

Project Start Date: August 1999 Projected End Date: September 2002

Project Number: 99-0128

## Research Objective

The corrosion behavior of nuclear fuel cladding is a key factor limiting the performance of nuclear fuel elements. Improved cladding alloys, which resist corrosion and radiation damage, will facilitate higher burnup core designs. The objective of this project is to understand the mechanisms by which alloy composition, heat treatment and microstructure affect corrosion rate. This knowledge will be used to predict the behavior of existing alloys outside the current experience base (for example, at high burnup) and predict the effects of changes in operating conditions on zirconium alloy behavior.

Zirconium alloys corrode by the formation of a highly adherent protective oxide layer. The working hypothesis of this project is that alloy composition, microstructure and heat treatment affect corrosion rates through their effect on the protective oxide structure and ion transport properties. Therefore, particular emphasis has been placed on detailed characterizations of the oxides formed on a series of experimental alloys. The goal of this project is to identify these differences and understand how they affect corrosion behavior. To do this, several microstructural examination techniques including transmission electron microscopy (TEM), electrochemical impedance spectroscopy (EIS) and a selection of fluorescence and diffraction techniques using synchrotron radiation at the Advanced Photon Source (APS) are being employed.

Detailed characterizations of oxides are only useful if the observations can be linked to the corrosion behavior of the alloy. That link requires a model of the corrosion mechanism. The modeling effort is designed to organize the data from the characterization studies in a self-consistent manner and link those observations to the corrosion behavior. The ultimate objective of this project is to link the characterization and theoretical modeling efforts to yield improved alloy specifications.

**Research Progress**

The effort in the first year of the project has focused primarily on developing the procedures, tools, and expertise required to accomplish the project objectives. The microstructural examination studies have pioneered new techniques for characterizing corrosion oxides. An experimental facility for studying radiolysis has been designed and is being fabricated. A structure for a comprehensive corrosion model has been developed and the base model is operational. These efforts provide the basis for successful completion of this three year project.

A unique aspect of the project is the development and use of novel techniques. Project researchers from Pennsylvania State University and Westinghouse are leading an effort to characterize oxides on zirconium alloys using synchrotron radiation. Interfaces at the Advanced Photon Source at Argonne were established along with the completion of a key milestone when the project was granted use of a critical beamline following a competitive peer review of the proposed work. An initial micro-diffraction run was completed. In that run, a narrowly focused 0.25? by 2? beam was scanned across a cross-sectioned oxide to characterize the crystal structure as a function of depth. The studies indicate that the oxide is predominantly monoclinic with a small amount of tetragonal oxide also present. The tetragonal oxide is concentrated near the metal/oxide interface.

Corrosion oxides have also been characterized using EIS. There is a direct relationship between the electrical properties of the oxide and the corrosion process. The EIS studies indicate the presence of both a continuous layer of highly insulating oxide at the inner surface and a more porous deteriorated oxide on the outer surface. The project is now positioned to characterize the corrosion oxide of different zirconium-based alloys with varying corrosion resistance using this technique and the work has been initiated.

The physical structure of the corrosion oxides can be examined by TEM. However, preparation of appropriate TEM specimens of these oxides requires carefully developed procedures. To reveal the structure of the oxide, TEM specimens must be prepared in cross-section with the extent of the thin area in a plane perpendicular to the corroding surface. Techniques for successfully preparing cross-sectional specimens were developed. Preliminary studies reveal an extremely fine grain structure with a combination of equi-axed and columnar grains.

The effect of radiolysis on zirconium corrosion is characterized by the local environment rather than the bulk water conditions. The pores and microcracks that form in the oxide layer provide a pathway for water intrusion that create a local aqueous environment. A conceptual design for an experiment facility that simulates the local aqueous environment within the porous oxide film was completed.

A modeling effort was undertaken to provide a framework for relating the results of the characterization work to their impact on corrosion. The basic structure of the corrosion model has been implemented and tested. The modular structure of the model provides flexibility to incorporate individual effects, such as heat flux and continuous oxide growth on corrosion behavior.

**Planned Activities**

Progress during the first year of the program has provided the technology to conduct detailed characterizations of corrosion oxides. The primary objective of the second year will be to utilize this technology to characterize oxides on a variety of Zr alloys. Experience with preliminary studies indicates that it is important to understand both the effects of alloy type and the corrosion environment on the type of oxide that forms. APS, EIS and TEM techniques developed in the first year will be employed to characterize oxides grown in both pure water, steam and Li doped water. Characterizations of existing alloys will be completed and the number of materials under consideration expanded. Where required, additional autoclave exposures will be initiated to provide appropriate sources of oxide specimens.

The current model considers growth of the continuous oxide and breakdown of the oxide in separate modules. The primary outputs of these modules are the continuous oxide growth rate and the critical oxide thickness for breakdown. Emphasis in the second year will shift to modeling of the critical oxide thickness. As data on the oxide structures is accumulated, the model will be adjusted to match the observations.

The oxide characterization and theoretical modeling efforts will eventually produce improved alloy specifications. The project is designed to be evolutionary—lessons learned in the initial phases will be applied in the later phases. This evolutionary process is embodied in the alloy selection and development portion of the project. As the project proceeds, alloy specifications for improved corrosion resistance will be identified.

# Advanced Proliferation Resistant, Lower Cost, Uranium-Thorium Dioxide Fuels for Light Water Reactors

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

Collaborators: Argonne National Laboratory, University of Florida, Purdue University, Massachusetts Institute of Technology, ABB-Combustion Engineering Inc., Westinghouse Electric Corp., Framatome Technologies, Siemens Power Corp.

Project Start Date: August 1, 1999 Projected End Date: August 31, 2002

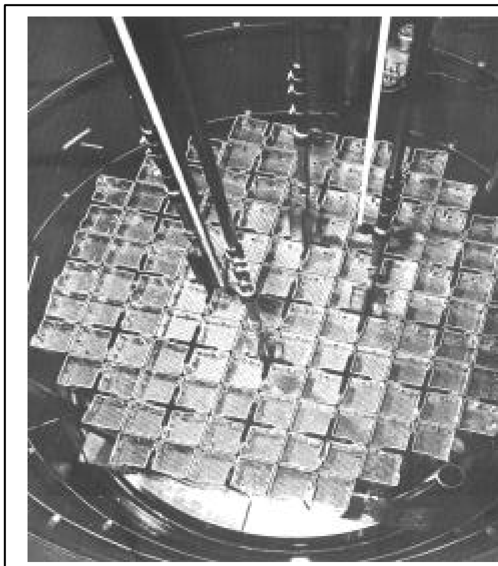
Project Number: 99-0153

## Research Objective

The overall object of this project is to evaluate the efficacy of high burnup mixed thorium-uranium dioxide ($ThO_2$-$UO_2$) fuels for light water reactors (LWRs). A mixed thoria-urania fuel that can be operated to a relatively high burnup level in current and future LWRs may have the potential to:

- improve fuel cycle economics (allow higher sustainable plant capacity factors);
- improve fuel performance;
- increase proliferation resistance; and
- be a more stable and insoluble waste product than $UO_2$.

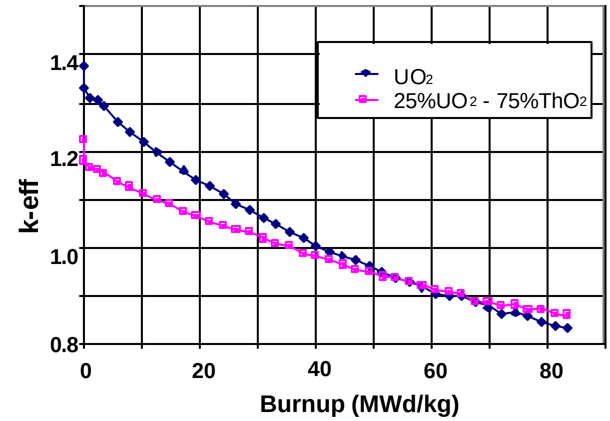
One of the important goals of this project is to study fuels that would be assembly-for-assembly compatible with the fuel in current LWRs. This implies that both utilities and vendors would find this fuel acceptable for manufacturing and use in current LWRs, if the economics prove to be desirable.



**$ThO_2$-$UO_2$ Critical Experiment**

## Research Progress

Reactor Core Neutronic Analysis and Fuel Cycle Design: Fuel cycle analysis performed during Phase I included benchmarking several computer models against available critical data (one of the critical experiments is shown to the right) and then analysis to determine the neutronic and economic viability of using a homogeneously mixed, thorium-uranium dioxide fuel. Several mixed thoria-urania fuel cases, ranging from a 75 percent $ThO_2$-25 percent $UO_2$ base case to a 65 percent $ThO_2$-35 percent $UO_2$ case, were evaluated for reactivity swing with burnup and isotopic concentrations. These cases were compared to all uranium cases with similar U-235 enrichments in the heavy metal (thorium + uranium, see figure to the right). Preliminary analyses of the enrichment and fabrication costs of the homogeneous thorium-uranium fuels have resulted in a cost per MW-hr about 20-25 percent higher than the all-uranium fuel. While the economics do not favor the homogeneous thorium-uranium fuels that have been studied thus far, other indicators do favor thorium-uranium fuel. For instance, the end-of-life isotopic concentrations strongly favor the thorium-uranium fuel based on total plutonium and minor actinide content, leading to a more proliferation resistant fuel as compared to uranium fuel. Also of interest is the reduction (or elimination) of burnable and soluble poisons needed with a thorium-uranium fuel due to the smaller reactivity swing with burnup. Other factors also show an advantage to using thorium-uranium fuel, such as better fuel performance and waste characteristics, and less coolant corrosion control problems due to the minimal use of soluble poisons. In addition, the preliminary studies on the use of a micro-heterogeneous $ThO_2$-$UO_2$ fuel in LWRs show that this fuel type appears to increase the burnup by 15 percent to 25 percent for the same fissile loading. This increase in burnup is significant enough to close the economic gap, and may show that thorium-uranium fuel can be economically competitive with current all-uranium fuels.




**Burnup vs. reactivity of a 25%$UO_2$-75%$ThO_2$ pin cell, and an all $UO_2$ pin cell.**

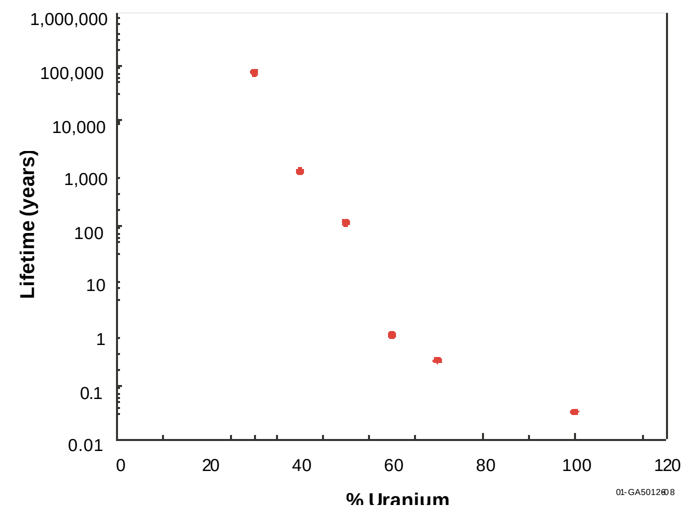
<u>Fuel Manufacturing Costs</u>: First year conclusions are as follows:

- Current uranium-only nuclear fuel manufacturing facilities can be used to manufacture mixed thorium/uranium fuels.
- Extensive changes are required in the wet conversion areas that manufacture the $ThO_2$ and the $UO_2$ to account for the possibility that 20 percent U-235 could be accidentally sent through the conversion line. Due to this rather conservative approach, the resulting facility will be able to handle any fuel composition up to a pure U-235 enrichment of 20 percent.
- Moderate changes will be required in the powder and pelleting areas of the manufacturing facility. The main changes will be in the size of the bulk powder containers. All equipment is currently able to accept powder of any composition up to a pure 20 percent U-235 enrichment level.
- Changes in monitoring for airborne contaminants will be required to account for the much lower Th limit and for the high U activity.

- There are adequate supplies of thorium available on the commercial markets to support use of a mixed $ThO_2$ -$UO_2$ fuel cycle.

Fuel Performance: The thermal, mechanical, and chemical aspects of the behavior of $ThO_2$-$UO_2$ fuel rods during normal, off normal, and design basis accident conditions are being evaluated. During normal operation, $ThO_2$-$UO_2$ fuel may operate with somewhat lower fuel temperatures and internal gas pressures than $UO_2$ fuel at corresponding powers and burnups. During an accident such as a large break loss-of-coolant accident (LOCA), $ThO_2$-$UO_2$ fuel will have less stored energy but a slightly higher internal heat generation rate than $UO_2$ fuel at similar power levels. Correlations, as a function of temperature, thoria and urania concentration, burnup, and other appropriate parameters have been developed from the existing literature for the following material properties: thermal conductivity, specific heat, thermal expansion, emissivity, modulus of elasticity, and melting temperature.

Long Term Stability of $ThO_2$-$UO_2$ Waste: The first year work focused on measuring the kinetic parameters for the air oxidation of $Th_xU_yO_2$ where x + y = 1 and x had values of 1.0, 0.7, 0.6, 0.5, 0.4, 0.3, and 0. A non-isothermal thermogravimetric analysis method was used to determine the kinetic parameters. The research showed that air oxidation rates of the solid solution $UO_2$ and $ThO_2$ samples were much lower than for pure $UO_2$. An example of the results for a 5 percent conversion of various thoria-urania compositions is shown to the right. Note that material with less than about 50 percent $UO_2$ lasts for a relatively long time. This reduction in oxidation rate has advantageous storage implications, if air oxidation is the rate-controlling step in transport of spent fuels into the environment.




**Lifetime of (U,Th)$O_2$ solid solution at room temperature**

### Planned Activities

- Optimize the fuel form to increase the economic competitiveness of thorium-uranium fuel.
- Determine the projected capital and operating costs of fuel manufacturing.
- Evaluate fuel fabrication issues associated with co-precipitation of the powder and with pressing, sintering, and grinding $ThO_2$-$UO_2$ fuel pellets.

- Evaluate the behavior of $ThO_2$-$UO_2$ fuel during both normal operation and accident conditions, and compare the results with the behavior of current $UO_2$ fuel and USNRC licensing standards.
- Determine the corrosion and dissolution rates of both fresh and previously irradiated $ThO_2$-$UO_2$ fuel in synthetic ground water.

# A Proliferation Resistant Hexagonal Tight Lattice BWR Fuel Core Design for Increased Burnup and Reduced Fuel Storage Requirements

PI: Hiroshi Takahashi, Brookhaven National Laboratory

Collaborators: Purdue University, Hitachi, Ltd.

Project Start Date: August 1, 1999 Projected End Date: August 31, 2002

Project Number: 99-0164

## Research Objective

The objective of this research is to advance the well-developed water-cooled reactor technology in order to make efficient use of the abundant thorium resources and enhance the proliferation resistance of the nuclear fuel cycle. Considerable effort has been invested in development of the sodium cooled fast reactor to breed fissionable Pu-239 from natural uranium. Much less effort has been expended in development of alternative technologies that take advantage of the considerable experience with light water reactors (LWR) to provide a hard neutron spectrum for converting thorium into the fissile U-233 isotope.

This project investigates the feasibility of a plutonium-thorium (Pu-Th) fuel cycle for a new type of proliferation resistant, economically competitive, high conversion, boiling water reactor (HCBWR). The technology will be developed to burn existing stocks of plutonium, while converting the fertile thorium to fissile U-233. The high conversion will take place in a fast neutron spectrum, which results from minimizing the volume of water in very tight fuel assembly lattices. High fuel burnup will be possible as a result of the continuous generation and fission of U-233 as the plutonium is consumed. Inherent safety will be designed into the reactor because of the favorable feedback neutronics characteristics of thorium and by the use of innovative core heterogeneities. This will insure a negative void coefficient for those accident sequences, which result in off-normal coolant boiling.

The major technical objective of the proposed project is to develop a reactor design that will:

- Minimize the potential for proliferation of weapons grade materials.
- Maximize the inherent safety features of the reactor.
- Maximize the achievable fuel burnup and plant capacity factor.
- Minimize the cost of electricity generation.

## Research Progress

The light water reactor with a hard neutron energy spectrum has been studied in the past, both in the U.S. and in Europe. More recently, there has been considerable interest in the Japanese nuclear industry and research organizations. This research project has evaluated several of the reactor designs proposed by the Japanese industry and research institutes. These designs included: (1) high conversion BWR, (2) long burnup cycle BWR (LBBWR), (3) BWR without blanket, (4) high conversion pressurized water reactor (PWR), and (5) PWR with Pu multi-cycle.

Detailed analysis of high conversion cores have been carried out in Japan over the last two years and the general conclusions were that in order to achieve high burnup, a reactor with a hard neutron energy spectrum is required. A tight lattice BWR core can provide the hard neutron energy spectrum; however, the coolant void coefficient tended to be positive. In order to achieve safe core operation, the analysis showed that a negative void coefficient could be achieved by enhancing neutron leakage during coolant heat up.

From this research project's preliminary analysis of the above reactors, the LBBWR type reactor has been selected for the initial design study. Because nonproliferation is one of the key factors in the NERI program, thorium will be used as fertile material instead of the U-238 which is used in the Japanese study. Use of thorium as the fertile material can also eliminate fissile plutonium more efficiently. In addition, the thorium fuel cycle does not accumulate a significant inventory of minor actinides that have very long half-lives and as such does not exacerbate the high level waste disposal problem.

Code acquisition and benchmarking work has been completed. Both stochastic and deterministic analysis codes are being used in the effort. The Brookhaven National Laboratory Monte Carlo burnup code MCBURN has been benchmarked for high conversion lattices. The collision probability lattice codes HELIOS was purchased from Studsvik/Scandpower and also benchmarked for thorium depletion with hexagonal lattices. A basic neutronics study was performed comparing performance of thorium and uranium fuels in both standard LWR and high conversion lattices. Preliminary design of the HCBWR fuel pin and fuel lattice was then completed using HELIOS and MCNP. Initial results show very favorable fuel burnup performance as well as good safety characteristics. The void coefficient was negative for all cases examined with thorium/plutonium fuel. Preliminary thermal-hydraulics analysis was also performed for the tight pitch channel using the RELAP5 code. Preliminary results are encouraging but there are concerns about adequacy of constitutive relationships for the tight lattice cores.

## Planned Activities

Work has progressed on schedule and some of the tasks on the second year have been initiated during the first year in order to facilitate the analysis. Specifically, the development of a hexagonal lattice capability in the nodal code PARCS was begun in the fourth quarter so that core burnup studies and core safety analysis could be started at the beginning of the second year.

To study the reactor safety of tight lattice Pu-Th reactor the reactor parameters associated with transient kinetic behavior will be calculated with the MCBURN code and provided in the PARCS code calculation.

# NUCLEAR ENERGY RESEARCH INITIATIVE

## Development of a Stabilized Light Water Reactor (LWR) Fuel Matrix for Extended Burnup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| PI: | Brady D. Hanson, Pacific Northwest National Laboratory | |
| Collaborators: | University of California - Berkeley | |
| Project Start Date: | August 1, 1999 | Projected End Date: September 2002 |
| Project Number: | 99-0197 | |


**Research Objective**

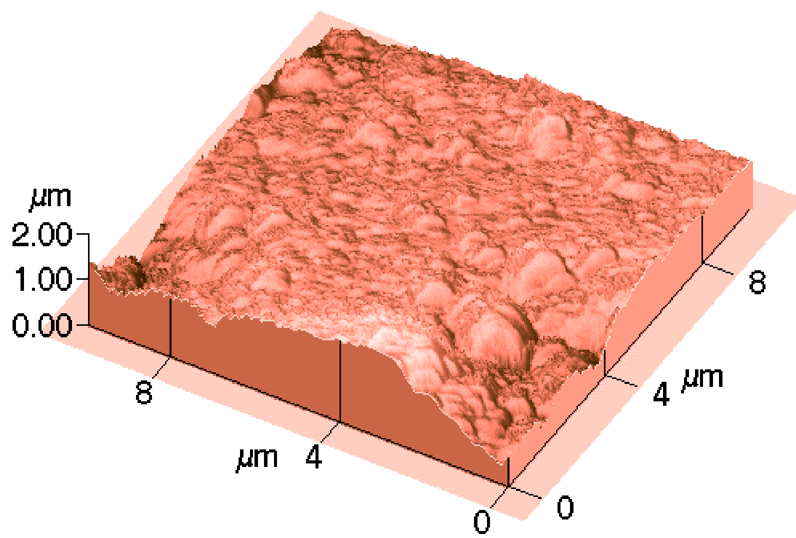
The main objective of this project is to develop an advanced fuel matrix based on the currently licensed $UO_2$ structure capable of achieving extended burnup while improving safety margins and reliability for present operations. Burnup is currently limited by the fission gas release and associated increase in fuel rod internal pressure, fuel swelling, and by cladding degradation. Once fuels exceed a threshold burnup, a "rim" or high burnup structure (HBS) forms. The HBS is characterized by the development of a subgrain microstructure having high porosity and low thermal conductivity. It is believed that the lower thermal conductivity results in larger temperature gradients and contributes to subsequent fission gas release. Fuel designs that decrease the centerline temperature while limiting the HBS restructuring, thereby decreasing the fission gas release should be able to achieve higher burnup and even allow higher operating power for increased efficiency.

Research at Pacific Northwest National Laboratory (PNNL) has demonstrated that the soluble fission products and actinides present in the matrix of irradiated (spent) fuels stabilized the fuel matrix with respect to oxidation to $U_3O_8$. The higher the soluble dopant concentration, the more resistant the fuel has been to undergoing the restructuring of the matrix from the cubic phase of $UO_2$ to the orthorhombic $U_3O_8$ phase. In this project, the attempt is to utilize the changes in fuel chemistry that result from doping the fuel to design a fuel that minimized HBS formation. The use of dopants that can act as getters of free oxygen and fission products to minimize fuel-side corrosion of the cladding is also being studied.

In addition to the use of dopants, project researchers are studying techniques such as the use of large grain sizes and radial variations in enrichment to minimize HBS formation and fission gas release. In this project, a combination of modeling and experimental studies is being used to determine the optimum design.

**Research Progress**

Task 1 (Understand and Model HBS Formation) focused on performing a comprehensive literature review to guide future efforts. Five different high burnup fuels, including two MOX fuels, were sectioned and prepared for examination of the HBS. Atomic force microscopy (AFM) has been used and appears to be able to map the HBS as a function of radius. An example of the morphology of the HBS as viewed using AFM is seen in the figure below.




**3-D AFM Image (10 x 10 mm) of LWR Spent Fuel Showing Restructured Grains in the HBS Region**

The successful use of AFM on these highly radioactive samples is believed to be the first such effort. A scanning electron microscope (SEM) and x-ray diffractometer (XRD) were both readied for examination of these spent fuel samples. Modifications to the Resonance Absorption Burnup (RABURN) model, used to calculate the radial concentrations of fission products and actinides, have been made to incorporate true cylindrical geometry.

Task 2 (Develop Matrix Stabilization Model) efforts went into preparing the SEM and XRD units for testing of the spent fuels and candidate fuels. The SEM is now fully operational and project researchers are waiting for their turn to use the equipment. All of the necessary paperwork to adhere to administrative regulations governing the use of fuel enriched in $^{235}U$ has been completed.

Task 3 (Design and Test Advanced Fuel Matrix) work involved an extensive literature review on the effect of dopants on the $UO_2$ lattice. This review was aimed at guiding the fuel design efforts. All of the equipment necessary to fabricate pellets based on the "recipes" of dopants developed in the other two tasks has been purchased. Most items, including the high temperature tube furnace (for grain growth experiments and sintering of pellets) and the pellet press have been installed. Commercial samples of gadolinia-doped fuels have been ordered for use in baseline tests of physical and chemical properties. The fuels developed for this project will be compared against these baselines. Finally, discussions with Argonne National Laboratory on the use of the Advanced Photon Source or Transmission Electron Microscopy (TEM) facilities to determine the location of dopants in the fuel matrix have been initiated.

# Continuous Fiber Ceramic Composite Cladding for Commercial Water Reactor Fuel

PI: Herbert Feinroth, Gamma Engineering Corporation

Collaborators: Massachusetts Institute of Technology (MIT), McDermott Technology, Inc., Northwestern University, Swales Aerospace, Inc.

Project Start Date: August 1, 1999 Projected End Date: June, 2001

Project Number: 99-0224

## Research Objective

The objective of this project is to study the use of advanced ceramic materials as cladding for water reactor fuel elements, and to determine, via engineering type tests, the feasibility of substituting such advanced ceramic materials for the Zircaloy cladding now in use. The ceramic materials to be developed and tested in this research program are known as oxide-based continuous fiber ceramic composites (CFCCs).

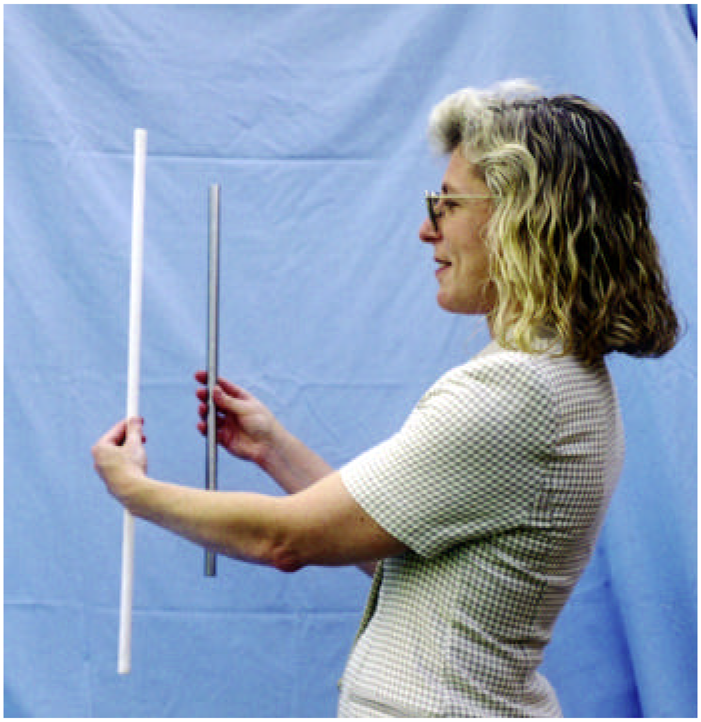
Oxide-based CFCCs have three main characteristics that recommend them for water reactor nuclear fuel cladding application. First, because CFCCs consist of very strong, micron sized fibers in a dense ceramic matrix, they do not behave in a brittle manner. Instead they have a failure mode that is non-catastrophic and similar to metals. Second, CFCCs retain their strength to much higher temperatures (e.g. >2000$^{o}$F) as compared to metals such as zircaloy, which lose much of their strength above 1000$^{o}$F. And third, oxide-based CFCCs (as opposed to carbide and nitride based CFCCs) remain chemically passive in high temperature steam. Thus, they do not react violently with water during a hypothetical Loss of Coolant Accident (LOCA), they do not produce heat during such an accident, and they do not produce hydrogen gas. Such characteristics, if applied to cladding in commercial water reactors, would lead to significant reductions in the consequences of low probability core overheating accidents, such as LOCAs. This could lead to improved and simplified reactor plant designs, simplified regulatory criteria, and improved public acceptance of nuclear power resulting from real reduction in residual risk.

This project seeks to address the feasibility of using CFCCs as reliable fuel cladding. Its aim is to determine the feasibility of providing an improved water reactor fuel element, which is significantly more resistant to damage during a LOCA accident than is the current water reactor fuel element. Specifically, the goals for the project are to (1) evaluate and select two or three specific oxide based CFCC materials which have the potential to meet LWR fuel cladding requirements, (2) fabricate LWR fuel clad test specimens from such materials using advanced CFCC fabrication techniques, (3) conduct in-pile corrosion tests on these specimens, along with standard zircaloy specimens, and

(4) expose such specimens to simulated LOCA test conditions to confirm their superior performance during LOCA accident conditions.

**Research Progress**

Approximately sixteen feet of high-density alumina-yttria ceramic composite cladding has been fabricated and delivered to Gamma Engineering Corporation for final sectioning and assembly into the test fixtures at Swales Aerospace and Massachusetts Institute of Technology. A portion of these test samples will be reserved for further characterization and archival storage. The tubes are a composite of high-density alumina fibers (Nextel 610 by 3M), embedded in a matrix of dense yttria-alumina. Some of the tubes (about 4 feet) are then chemical vapor infiltration (CVI)-coated by Northwestern University with either pure alumina, or a mixture of 90 percent alumina, 10 percent chromia to enhance the surface condition and performance of the CFCC material.



**Clad Test Samples**

MIT completed the design of a test fixture for reliable mounting of ten 3-inch long specimens in a special loop to be inserted in their test reactor. The hardware for the fixture is currently under procurement, and assembly of the fixture with the test specimens was planned during the month of August 2000. Swales has completed the assembly and trial use of a special LOCA test rig designed to quench typical clad specimens (3 inches in length) from high temperature (up to 2500$^{o}$F) into room temperature water.

**Planned Activities**

Phase 2 of this project involves two test programs, and further characterization of the fabricated tubes.

Irradiation Test Program: Ten clad specimens (each about 3 inches long) will be irradiated in a special high temperature (600 $^oF$) flow loop in MIT's 5 MW nuclear reactor.

LOCA - Thermal Shock Test: Three inch long test specimens will be heated in a special furnace to three different "accident" temperatures: 1000$^o$F, 1800$^o$F, 2500$^o$F. After stabilization at these temperatures, each specimen will be quenched in room temperature water in a special apparatus.

Further Characterization Tests: Visual and microstructure examination will be conducted after the irradiation and thermal shock tests. In addition, permeability tests will be performed on some of the pre-irradiated coated specimens to compare with pre-irradiated uncoated specimens.

Thus far, the project has addressed many of the technical issues associated with the use of CFCCs as cladding in commercial reactors. Some of the issues have been resolved, and others remain for further development. A key factor in determining whether further work is warranted on applying this promising new material to nuclear fuel cladding use will be the results of the planned thermal shock and irradiation testing.

# An Innovative Ceramic Corrosion Protection System for Zircaloy Cladding

PI: Ronald H. Baney, University of Florida

Project Start Date: August 1, 1999 Projected End Date: August 31, 2002

Project Number: 99-0229

## Research Objective

The operational lifetime of current Light Water Reactor (LWR) fuel is limited by thermal, chemical, and mechanical constraints associated with the fuel rods being used to generate nuclear heat. A primary limiting factor of this fuel is the waterside corrosion of the zirconium based alloy cladding surrounding the uranium pellet. This research project intends to develop thin ceramic films with adhesive properties to the metal cladding in order to eliminate the oxidation and hydriding of Zircaloy cladding. The corrosion protection system will allow fuel to operate safely at significantly higher burnups resulting in major benefits to plant safety and plant economics.

A major technical challenge for coating a metal with a ceramic protection system is to develop a cohesive bond between the two materials. The differences between the thermal expansion of the ceramic coating and the thermal expanding metal can, if not properly addressed, interfere with the ceramic's ability to maintain a bond and thus maintain a protective layer.

## Research Progress

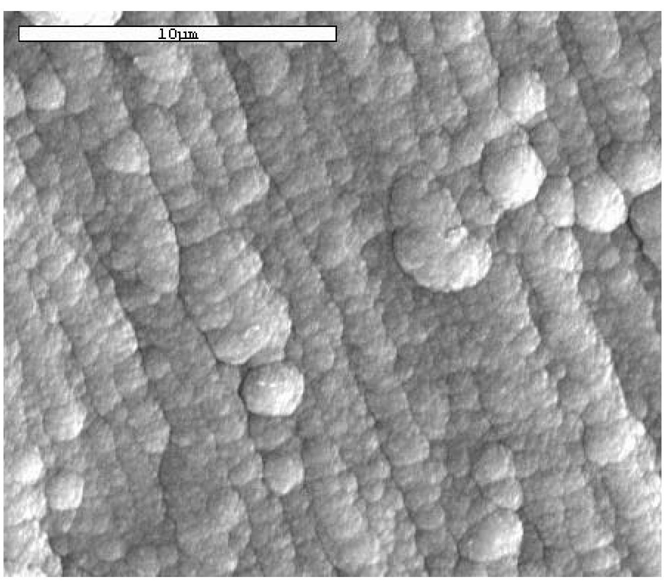
The following ceramics were investigated: alumina, boron carbide, graphite, mullite, silicon carbide, spinel, tungsten carbide, zirconia, and zirconium carbide. A background search was performed to identify their current uses in industry, processing methods, potential cost, their availability, and their suitability as a protective coating material for Zircaloy cladding in a LWR.

The mechanical properties of the coatings, such as coefficient of thermal expansion (CTE) and thermal conductivity, were compared with that of zirconium (Zircaloy) in order to determine the best candidate. A hand-calculated thermal analysis was performed to show temperature changes owing to the different coatings as a function of coating thickness and the validity of these calculations was established by a comparison with the thermal hydraulic computer program COBRA. A neutronic analysis was also performed using the Monte Carlo N-Particle Transport Code (MCNP) to show reactivity changes and unit fuel cell thermal flux changes caused by the different coatings as a function of thickness. The CASMO computer code was utilized to show burnup effects and changes in plutonium concentrations owing to an alumina coating of 50 to 100 microns. As a result of these studies, the two best coating options were identified as alumina and silicon carbide and initial samples were placed in an autoclave to simulate upper limit reactor conditions (water that was at 700F and 3000 PSIA pressure) in order to observe the coatings' corrosive and chemical stability.

Alumina's CTE is within 12 percent of zirconium's throughout the entire temperature range, while silicon carbide has the highest thermal conductivity of 78.8 W/m-K. All of the materials were analyzed thermally in order to calculate the rise in temperature of the fuel centerline, pellet surface, and outer and inner clad surfaces. At 50 microns, none of the coatings caused more than a 0.13 percent rise in cladding temperature and 0.05 percent rise in fuel centerline temperature. Even with a thickness of 500 microns, none of the materials caused more than a 1.5 percent increase in temperatures in any of the regions. Due to the extensive computation time required, only silicon carbide, alumina, zirconium carbide, and zirconia were analyzed neutronically. At the most likely coating thickness between 10 and 50 microns, there was less than a 0.09 percent decrease in reactivity and a 0.5 percent decrease in the thermal flux in the fuel and a 1.7 percent decrease in the thermal flux in the water.

Owing to the displacement of water caused by the coating, there was a hardening of the spectrum and therefore an increase in plutonium production as the fuel is being used. With a coating of 50 microns of alumina, there was as 1.9 percent increase in Pu-239 at 60 GWD/MTU. This increase in plutonium production has the added benefit of extending the reactivity lifetime of the fuel as plutonium becomes used as fuel.

A variety of coating processes for coating carbon, silicon carbide and alumina onto Zircaloy were explored. Carbon, diamond like carbon (DLC), and silicon carbide (SiC) were coated onto Zirc-4 coupons by plasmas-assisted chemical vapor deposition (PACVD). The figure below shows a SEM image of one such coating.




**SEM image of SiC thin films on unpolished Zircalloy deposited at 400C using Silacyclobutane by electron cyclotron resonance (ECR) plasma assisted (PA) chemical vapor deposition (CVD)**

Silicon carbide was also coated by a laser ablation deposition (LAD) process. Alumina was coated by an ultraviolet assisted chemical vapor (UVCVD) process. Alumina was also coated by a spin coating sol-gel process. A thick layer of alumina was coated onto a sheet of Zirc-4 by physical vapor deposition (PVD) using a plasma spray technique.

The quality of the coatings were assessed by visible inspection for uniformity and physical adherence of the coating and by Auger Electron Spectrographic (AES). The quality of the ceramic coating was assessed by the depth of the coating and the thickness of the coating.

**Planned Activities**

The corrosion testing of alumina and other promising coatings will be studied in detail. Further autoclave testing and accelerated corrosion testing will be required in order to complete a performance analysis of the ceramic coatings applied to zirconium alloy. Further investigation is also required to verify bonding throughout the fuel lifetime for the various coating materials. Coating processes will be optimized to give the highest quality coatings.

## 6. NUCLEAR WASTE MANAGEMENT

This program area addresses the long-term R&D goal related to fuel cycle research which considers the impact of fuel cycle options on waste generation, waste form, and waste storage and disposal.

Projects currently funded include R&D that address nuclear waste technological improvements to the back end fuel cycle process. Novel approaches are proposed to reduce the physical volume of spent nuclear fuel and to recycle or reuse spent nuclear fuel without reprocessing in a manner that maintains the highest degree of proliferation resistance. Additional R&D is being performed in the use of concrete in nuclear waste containment.

# NUCLEAR ENERGY RESEARCH INITIATIVE

## Monitoring the Durability Performance of Concrete in Nuclear Waste Containment

PI: Franz-Josef Ulm, Massachusetts Institute of Technology

Collaborators: Commissariat a l'Energie Atomique (French Atomic Energy Commission)

Project Start Date: August 1, 1999 Projected End Date: August 31, 2002

Project Number: 99-0126

### Research Objective

Concrete is commonly employed in radioactive waste disposal as an effective construction material for containment barriers, liners, and encasement of containers. The objective of this research is to develop the scientific knowledge and the appropriate engineering tools required to evaluate and quantify the durability performance of nuclear waste concrete containment subjected to the pessimistic chemical degradation scenario of calcium leaching. Monitoring the durability performance means here the quantitative assessment, in time and space, of the integrity of the containment during the entire storage period and requires the consideration of the multiple couplings between diffusion-dissolution of calcium and deformation and cracking.

With regard to the time-scale, the durability design of waste containers needs to consider some reference scenario of chemical degradation, in particular the pessimistic one of calcium leaching by pure water. This design scenario refers to the risk of water intrusion in the storage system. For the reference scenario at hand, it is generally assumed that concrete is subject to leaching by permanently renewed deionized water acting as a solvent. The calcium ion concentration in the interstitial pore solution leads to dissolution of the calcium bound in the skeleton of Portlandite Crystals, $Ca(OH)_2$, and calcium-silica-hydrates (C-S-H), with sharp dissolution fronts. This calcium leaching leads to a degradation of the mechanical properties of concrete (material strength, Young's modulus). Cracks increase the diffusivity of the calcium ions through the structure, and can lead to an acceleration of the chemical degradation, and hence to an acceleration of the overall structural aging kinetics. This process can lead to a closed loop of accelerated structural degradation.

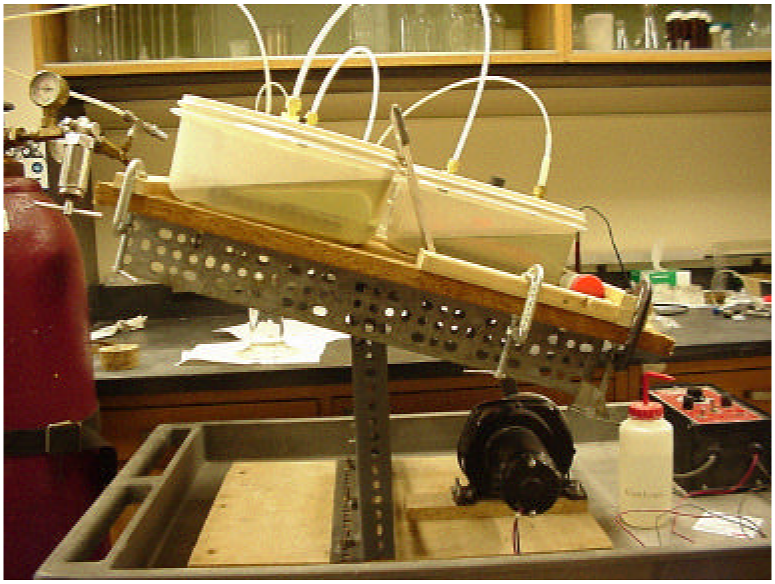
### Research Progress

After the first year of research, the important scientific findings that will translate into industrial benefits in the field of concrete durability in nuclear waste storage are as follows:

- The chemical process of calcium leaching involving kinetics and mineral composition were studied, including the use of alternative leaching agents. State-of-the-art material tests were employed.
- The consequences of calcium leaching on the mechanical behavior of cement paste were identified in mechanical tests, invoking three dimensional (3-D) stress states. For the first time, the governing mechanical parameters were identified in 3-D.
- The role of cracks on demineralization of porous materials was the object of an extensive study. By means of dimensional analysis, the governing similarity properties of calcium leaching and degradation of concrete were identified in an unprecedented completeness.
- In particular, making use of similarity properties of the governing equations of ‘real’ calcium leaching in concrete, it was shown that a pure diffusive mass transport through a crack or fracture will not significantly affect the overall degradation kinetics of a concrete structure, while advective transport may accelerate the degradation process.

The resulting industrial benefits can be summarized as follows:

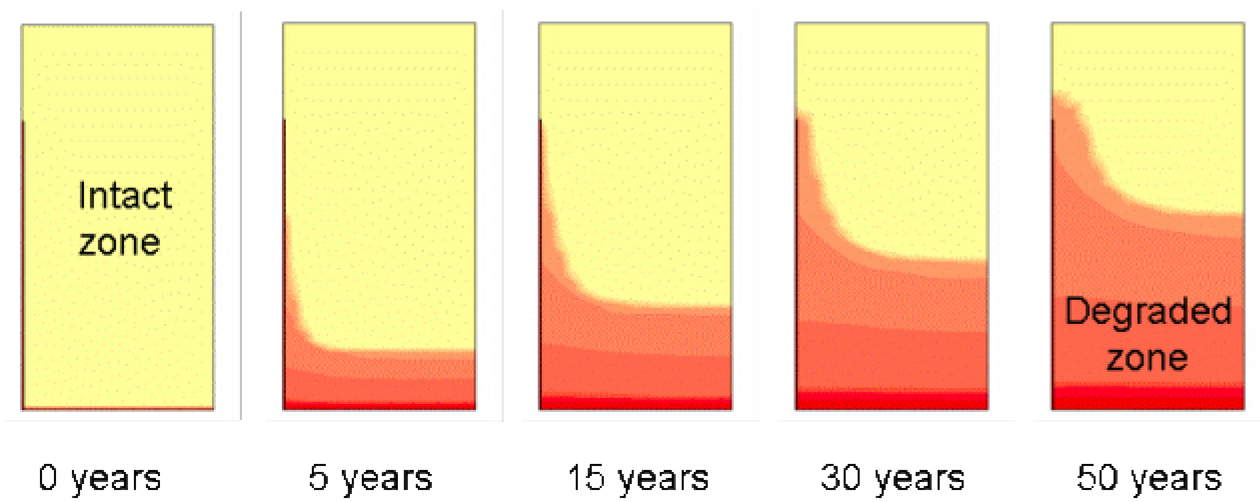
- Based on the scientific analysis of the calcium leaching process, an accelerated material leaching test was conceived and put into practice, allowing for 300-fold accelerated calcium leaching. The developed test setup is illustrated in the picture below. This makes it possible to test different kinds of cementitious materials with regard to their leaching characteristics before being utilized in industrial applications.
- Changes in mineral composition due to calcium leaching are now predictable and can be implemented in industrial planning and design tools. For instance, the thickness of



**Experimental setup for accelerated calcium leaching of cement-based materials: Material samples are immersed in a 6M ammonium nitrate solution for accelerated leaching. In order to obtain good mixing of the ammonium nitrate solution and most homogeneous leaching conditions possible, tanks containing the ammonium nitrate bath are mounted on a slowly oscillating table.**

containment structures can be adopted with regard to the demineralization design scenario.

- The results of mechanical testing are a key element for the mechanical modeling of calcium leaching, needed for industrial monitoring and decision support systems for safe storage systems.
- The evolution of a calcium-leaching front was implemented successfully in a commercial finite element code. This is a necessary condition for transfer of the research results into engineering practice. The figure below shows a typical example of the propagation of a dissolution front around a fracture that can be obtained by means of the developed program. This model can be readily employed for long-term structural leaching analysis.
- The profound analysis of influential parameters concerning cracks in cementitious materials and their consequences on leaching have immediate industrial application. For example, it makes it possible to analyze the suitability for industrial applications of a given cementitious material or structure at any given moment during its life span. This can improve the decision quality compared with a decision that solely considers the crack size, as is common practice in parts of industry today.
- The issue of nuclear waste storage and the corresponding initiatives of the U.S. government through DOE's NERI program are brought to a large audience consisting of both the scientific-engineering community and the broader public.




**Propagation of the dissolution front around a crack (left of the figure) obtained by model-based simulations. This type of results indicate that small fractures do not significantly increase the overall deterioration kinetics of calcium leaching.**

**Planned Activities**

The next steps of the project will include the completion of the experimental studies on the material and structural level. In addition, the computational mechanics approach will be extended, developing the mechanical model accounting for the chemo-hygral-mechanical cross effects. Focus of this combined experimental-theoretical approach will be on bridging scales from the microscale of the experimentally assessed material deterioration to the macroscale of engineering prediction of the performance of concrete employed in nuclear waste repositories.

# Chemical Speciation of Neptunium in Spent Fuel

PI: Ken R. Czerwinski, Massachusetts Institute of Technology

Collaborators: Argonne National Laboratory

Project Start Date: August 1, 1999 Projected End Date: August 31, 2002

Project Number: 99-0127

## Research Objective

This project will examine the chemical speciation of neptunium in spent nuclear fuel. Neptunium has been identified as a radionuclide of concern and information on the chemical form of neptunium in spent fuel is lacking. The identification of the neptunium species in spent fuel would allow a greater scientific based understanding of its long-term fate and behavior in waste forms.

The chemical species and oxidation state of neptunium will be determined in spent fuel and alteration phases. Different types of spent fuel will be examined. Once characterized, the chemical behavior of the identified neptunium species will be evaluated if it is not present in the literature. Special attention will be given to the behavior of the neptunium species under typical repository near-field conditions (elevated temperature, high pH, varying Eh). This will permit a timely inclusion of project results into near-field geochemical models. Additionally, project results and methodologies have applications to neptunium in the environment, or treatment of neptunium containing waste.

## Research Progress

Speciation of Neptunium in Spent Fuel and Alteration Products: The application of synchrotron-based methods, X-ray absorption near edge spectroscopy (XANES) and extended X-ray absorption fine structure (EXAFS), to the identification and characterization of environmentally relevant solids is well established. The application of synchrotron methods to establish the oxidation states of actinides in precipitated, altered, and unaltered neptunium phases has also been demonstrated. Progress continues with the characterization of carefully prepared neptunium standards to build a library of spectra that will help establish the nature of the unknowns. Preparations for synchrotron studies of neptunium-bearing solids were also completed.

Analyze Np Solid Phases and Information of Np Alteration Phases: Progress in these areas involved examining two separate efforts; the subsurface chemistry of neptunium when organics are present and the effects of microbiological activity on neptunium speciation and phase alteration. The reactivity of Np(VI) with citrate was investigated as a model system to understand the role of complexation and redox conditions in defining the oxidation state distribution under subsurface conditions. It was established that citrate reduces Np(VI) to Np(V) within days under all conditions investigated. The disappearance of Np(VI) was first-order under all conditions investigated but the pseudo first order rate constant was not proportional to the concentration of citrate due to changes in the reaction mechanism.

Research was also initiated to establish the effects of microbiological activity on the speciation of neptunium. Emphasis is on a *Shewanella* strain that is an anaerobic metal-reducing bacterium common to many subsurface aquifers. The methodology for growing and studying this isolate was established. Interaction experiments with neptunium are planned for the early part of the second year in the project.

Behavior of Np Species with Ligands: The sorption and precipitation of Np(V) on goethite, montmorillonite, and tuff was studied. The first experiment was done in 0.1 M $NaClO_4$, at room temperature, and in a nitrogen glove box. The second experiment was done in 0.1M $NaClO_4$, at room temperature, and under an air atmosphere. The third experiment was done in J-13 groundwater, at room temperature, and under an air atmosphere. Supernate concentrations were measured and the solid phase was analyzed at the Advanced Photon Source at ANL. Current results show sorption of Np(V) to goethite, montmorillonite, and tuff. The proton exchange capacity was found to be 0.228±0.018 meq OH/g for FeOOH and 0.770±0.016 meq OH/g for montmorillonite. This data will be used to model Np(V) sorption.

In further studies under inert atmosphere the supernate concentrations in the goethite samples dropped to approximately 60 percent of the original Np concentration at low pH, and decreased to very low concentrations by pH 7.5. The Np concentrations in the tuff samples were slightly higher than those in the goethite samples at low pH. This trend continued until approximately pH 9.5, which is the pH were hydrolysis is predicted to begin. At this point, Np concentration decreased dramatically until pH 11. After pH 11, Np concentration increased again. This suggests a pH dependent precipitation of Np within the tuff system or a pH dependent sorption effect. Previous studies elsewhere found sorption within the pH range of 6.5 to 8.5, but also found that some tuff samples exhibited negligible sorption. Further studies are necessary to better understand the change in supernate concentration as a function of pH.

Data for Modeling: Modeling of Np under Yucca Mountain conditions from pH 5 to pH 12, Eh from 0 V to 1.5 V and temperature from 25 °C to 100 °C was performed with CHESS 2.4. Seven different main Np species were observed in the calculations. In conditions below 0.5 V the tetravalent $NpO_2$ is formed. Three pentavalent Np species, $NpO_2^+$, $NpO_2CO_3^-$, $NpO_2OH_{(aq)}$ are dominant in the potential ranging from 0.5 V to 1.15 V. Three hexavalent Np species: $NpO_2(CO_3)_3^{4-}$, $NpO_2(CO_3)_2^{2-}$, $NpO_2OH^+$, are in the oxidizing conditions above 1.15 V. Other species with fluoride, sulfate and phosphate are calculated to exist but at very low concentrations. The database lack mixed ligand species or possible Np mineral type phases that may be found in spent fuel. In addition, the predicted behavior of $NpO_2$ indicates future efforts need to examine the dissolution kinetics.

Electrodeposition system for alpha spectroscopy: Electrodeposition has been shown to be the most effective method of actinide sample preparation for alpha spectroscopy. An electrodeposition apparatus was made in order to meet the laboratory alpha spectroscopy sample preparation needs associated with the Np speciation project.

**Planned Activities**

- Develop methods and equipment for performing XANES/EXAFS experiments with spent fuel.
- Systematically analyze and characterize a wide range of oxides, hydroxides, carbonates, phosphates, silicates and environmental complexes to identify the atomic and structural contributions to the XANES/EXAFS and other solid phase analysis.
- Calculate the key structures of Np species.
- Analyze Np and alteration products.
- Determine the solubility and chemical behavior of Np species examined in earlier studies. Evaluate the effect of temperature and environmental ligands on Np speciation.
- Use project data to evaluate the behavior of Np in the repository.

# Experimental Investigation of Burn-up Credit for Safe Transport, Storage, and Disposal of Spent Nuclear Fuel

PI: Gary A. Harms, Sandia National Laboratories

Project Start Date: August 1, 1999 Projected End Date: August 31, 2002

Project Number: 99-0200

## Research Objective

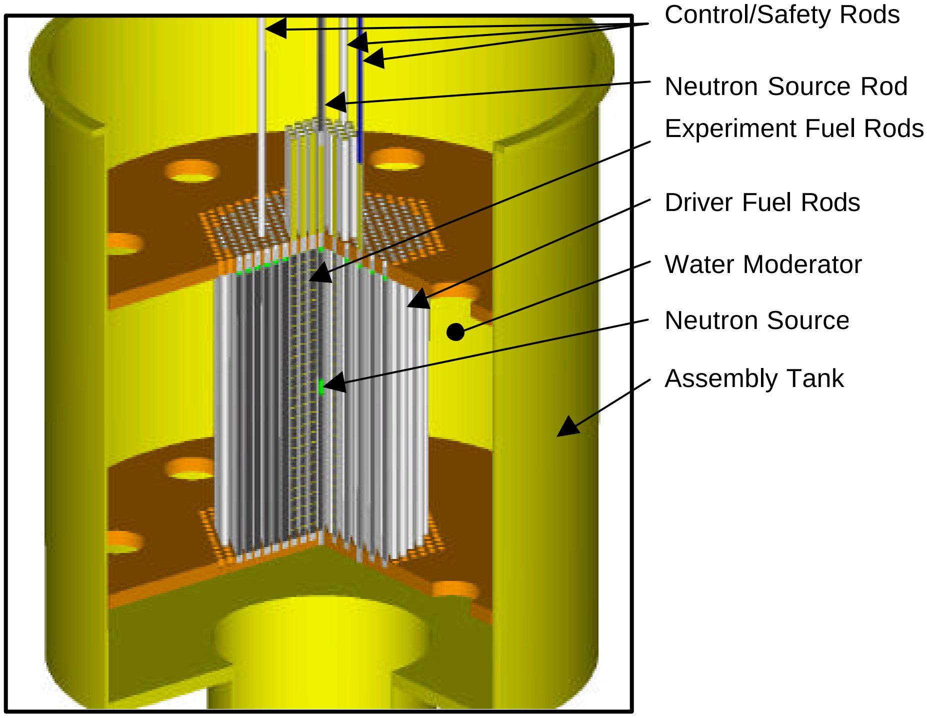
The Nuclear Energy Research Initiative has funded a critical experiment focused on burnup credit issues at Sandia National Laboratories. The experiment, when complete, will provide benchmark data that can be used to test the methods and data used in the criticality safety analyses of shipping, storage, and disposal of spent nuclear fuel.

Burnup credit is the process of accounting for the decrease in the reactivity of spent nuclear fuel produced by the changes in the fuel actinide concentrations and the buildup of fission product absorbers caused by the burning of the fuel. To apply burnup credit safely, the methods used in its application must be validated: the fuel isotopic composition in the burned state must be accurately predicted, and the neutron multiplication of spent fuel configurations must be accurately predicted. The current experiment addresses the second part of the validation issue.

A critical assembly with low-enriched $UO_2$ fuel will be built at Sandia. The assembly concept is shown in the figure below. It consists of a water-moderated array of driver fuel rods surrounding a smaller number of experiment fuel rods. The experiment fuel rods will allow for the insertion of test materials between the fuel pellets in these special fuel rods. The assembly also includes three fuel-followed control/safety rods and a fueled source rod. Critical experiments will be performed in the unperturbed assembly and with a test material, a fission product simulant, present in the assembly. The benchmark data from the experiment will be the difference in the critical array size between the two configurations.

The critical experiment is structured as a three-year project. The first two years will be used to obtain the necessary approvals for a new nuclear experiment and to design and procure the experiment hardware. The benchmark experiments will be performed in the third year. Five broad tasks were outlined in the project proposal:

- Task 1 - Obtain the necessary National Environmental Policy Act (NEPA) approvals.
- Task 2 - Prepare safety basis documentation for the experiment and obtain approvals.
- Task 3 - Design and procure the experiment hardware.
- Task 4 - Perform the benchmark experiments.
- Task 5 - Decommission and decontaminate the experiment.




**Layout of the critical assembly**

## Research Progress

In the first year of the project, work was performed on Tasks 1 through 3. The NEPA approvals for the experiment were obtained. Sandia filed an Environmental Checklist/Action Description Memorandum with the Department of Energy requesting that the experiment be categorically excluded from further NEPA documentation. The exclusion was granted.

The preparation of the safety basis for the experiment was started and will continue into the second year of the project. An Unreviewed Safety Question Determination (USQD) for the experiment was prepared against the safety bases of the Sandia Pulsed Reactor facility. Since the experiment differs significantly from the bare metal reactors normally operated in the facility, it was felt that the Technical Safety Requirements did not adequately bound the operation of the experiment. As a result, the USQD was positive. An addendum to the facility Safety Analysis Report is being prepared. A draft of the addendum is complete and under internal project review. Review by the Sandia Internal Review and Appraisal System and by the Department of Energy is yet to be accomplished.

The design and procurement of the experiment hardware was started and will continue into the second year of the project. The design of the critical assembly (the hardware in which the experiment is performed) is based on an earlier critical assembly that was built and operated at Sandia. Fuel for the current experiment was built for another Sandia burnup credit critical experiment that was never conducted. The hardware and fuel from the earlier experiments were archived temporarily at Los Alamos National Laboratory. This past year, both the hardware and the fuel were returned to Sandia. The design of additional hardware specific to the current assembly was started and continues.

Conceptual designs for the critical experiments were started. As part of the design process, an *ad hoc* panel of burnup credit experts was formed and asked to provide programmatic input to the design of the critical experiments. With this input, a conceptual design of the first experiment was completed. Experiment design will continue throughout the project.

**Planned Activities**

Final approval of the safety bases for the experiment will be sought in the second year of the project.

The design and procurement of the assembly hardware will continue into and be completed in the second year of the project. The assembly is expected to commence operation at the beginning of the third year of the project.

The benchmark critical experiments will be run in the third year of the project. Design activities for the experiments will continue in the second year and be complete when the experiments are finished. The experiments will be documented upon completion.

After the experiments are complete, and if no further experiments are planned, the assembly will be decontaminated and decommissioned in the third year of the project.

## Deterministic Prediction of Corrosion Damage in High Level Nuclear Waste


| | | |
|---|---|---|
| PI: | George Engelhardt, SRI International | |
| Collaborators: | Pennsylvania State University | |
| Project Start Date: | August 1, 1999 | Projected End Date: August 31, 2002 |
| Project Number: | 99-0217 | |


### Research Objective

This research involves developing deterministic models and associated computer codes for predicting the evolution of corrosion damage to high level nuclear waste (HLNW) containers. Safe disposal of our nation's HLNW represents one of the greatest technical challenges of the twentieth and twenty-first centuries. The principal challenge is to ensure isolation of the waste from the biosphere for periods up to 10,000 years under conditions that can only now be estimated. The lack of existing databases for the corrosion of candidate alloys over times that represent even a small fraction of the intended service life means that we cannot rely on empirical methods to provide the design, materials selection, and reliability assessment information that is required to assure the public that the technology chosen for the disposal of HLNW is effective and safe. Instead, only strategies based on the employment of deterministic models can be used, because the natural laws (laws of conservation) that are the foundation of these models constrain the solutions to physical reality and are invariant with time.

Existing deterministic models of general and localized corrosion allow us to predict the accumulation of corrosion damage in many systems. However, these models must be customized for predicting damage in HLNW canisters in a tuff repository. Thus, the influence of radiolysis on the corrosion potential and hence on the corrosion rate, for example, must be included in the models. Particular attention must be given to repassivation phenomena, because they eventually determine the extent of damage. Attempts to quantitatively describe localized corrosion damage without proper consideration of repassivation phenomena greatly underestimate the service lives of containers. It is also important to customize the models to the conditions to which the containers are expected to be exposed over their design lives.

The principal objectives of this project are to:

- Develop deterministic models and associated computer codes for predicting the evolution of corrosion damage (i.e., 'integrate' damage) to HLNW containers in the Yucca Mountain repository. Corrosion processes that will be considered include

general corrosion (oxidation), pitting corrosion, crevice corrosion, and stress corrosion cracking.
- Develop deterministic methods for extrapolating corrosion rate data obtained under "accelerated" laboratory conditions, to the field.
- Use the models to predict the fates of containers after exposure in the repository under various conditions (e.g., humid air, contact with dripping water, repository inundation).

It is evident that the first objective is the basis of the project, and that other objectives can be achieved only if deterministic models for predicting corrosion damage to HLNW containers are developed.

**Research Progress**

The following accomplishments have been achieved during the first year of research:

- The differential equation for calculating the damage function (DF) for localized corrosion has been derived. By analytical or numerical solution of this equation, it is possible to calculate DF under arbitrary conditions if the rate of nucleation and propagation and the probability of survival of corrosion events are known.
- A general computer code for calculating potential and concentration distributions in corrosion cavities has been developed.
- Simple, approximate analytical (but rather accurate) expressions for calculating potential and concentration distributions along with the cavity propagation rates for Alloy C-22 have been developed. This development is very important to the ultimate success of this program, because accurate numerical simulation of corrosion damage for a long period (up to 10,000 years) may require excessive amounts of computer time.
- Detailed radiochemical simulations of the effects of ionizing gamma and neutron radiation on the properties and chemical composition of electrolyte solutions under repository conditions indicate that the impact on pH should be minimal. However, the long exposure ties in actual repository systems preclude excluding radiolytic effects completely. Resolution of this issue will require accurate experimental data for the influence of pH on the kinetics of oxygen reduction on Alloy C-22.
- It has been shown that, in principle, the possibility that corrosion initiates and propagates on HLNW containers in the Yucca Mountain repository at short times (hundreds of years) when the temperature is significantly above the boiling temperature of water cannot be ignored. This is because surfaces are covered by highly hydrophilic oxides that will hydrate to form corresponding hydroxides, which are proton conductors and hence may act as electrolytes.
- A comparative experimental study of the electrochemical behaviors of Alloy C-22 and carbon steel has been carried out. The results show that Alloy C-22 has a unique resistance to pitting in NaCl solutions (concentration range to 1 mol/L, temperature range to 95 $^{o}$C). Results thus far indicate that the corrosion rate of this alloy is characterized by a very low current density of alloy passive dissolution, which lies

within the range of $10^{-7}$ to $10^{-8}$ A/cm. In neutral NaCl solutions, the reduction of dissolved oxygen is the most probable cathodic process. Basic kinetic parameters for anodic and cathodic processes have been determined.

**Planned Activities**

The experimental measurements of parameters embodied in the point defect model (PDM) for Alloy C-22 and carbon steels will be performed during the second and third years of this project. The PDM postulates that passivity breakdown occurs as a result of cation vacancy condensation at the metal/oxide interface at sites in the passive film that are characterized by high cation vacancy fluxes. These sites correspond to regions of structural discontinuity.

Calculations on the velocities of pit and crack propagation as a function of the depth of penetration and environmental parameters will continue, along with the efforts on developing general damage function analysis theory.

## A Single Material Approach to Reducing Nuclear Waste Volume

PI: James V. Beitz, Argonne National Laboratory

Project Start Date: August 1, 1999 Projected End Date: August 31, 2002

Project Number: 99-0219

### Research Objective

This project is developing an innovative single material, minimum volume approach for the selective sorption of metal ion radionuclides from aqueous waste solutions and creation of a final nuclear waste form that is suitable for long term storage or geological burial. The project is based on a chemically functionalized porous silica that is termed Diphosil. Diphosil was created as an ion exchange medium that selectively and nearly irreversibly sorbs highly charged metal ions, such as actinides, from appreciably acidic aqueous solutions. The chelating power of Diphosil is due to diphosphonic acid groups that are anchored to its silica surface via organic spacer groups. Approximately 90 percent of the weight of dry Diphosil is silica ($SiO_2$).

Underlying this project is the hypothesis that heating metal ion-loaded Diphosil in air will oxidize its organic content to water vapor and carbon dioxide and its phosphonic acid groups to phosphoric acid that would react with the sorbed metal ions to give metal phosphates. Based on literature reports of the properties of porous silica, it was further hypothesized that additional heating would either volatilize any excess phosphoric acid or cause it to react with the silica to form silicon phosphates. At still higher temperature, pore collapse should occur thereby microencapsulating and chemically fixing the sorbed metal ions in phosphate-rich metal phases in vitreous silica. Vitreous silica is one of the most radiation resistant glasses known.

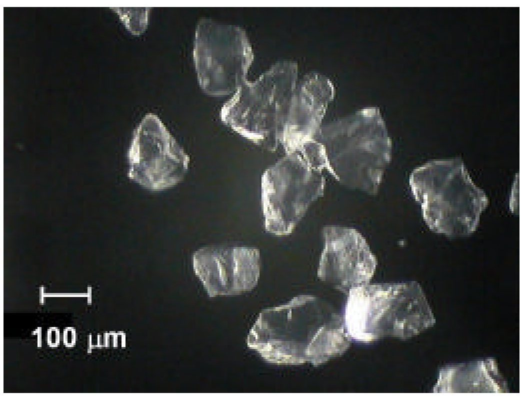
### Research Progress

Project activities to date confirm the hypotheses as to the events that might occur when metal ion-loaded Diphosil is heated in air. The process of converting porous silica to fully dense silica is referred to as thermal densification in the literature because it occurs at temperatures far below the melting point of bulk silica and, in consequence, does not involve a phase change such as melting. The term thermal densification has been adopted to refer to the entire set of processes that occur when metal-ion-loaded Diphosil is heated in air to the point of pore collapse. Specific research conducted during the first year includes:

<u>Solution Composition Effect on Metal Ion Sorption</u>: This work has investigated the influence of solution composition variables on sorption of heavy metal ions into a chemically functionalized porous silica (Diphosil). Diphosil has been shown to extract

metal ions from aqueous solutions that contain significant concentrations of ethylenediaminetetracetic acid (EDTA) at near-neutral pH. Aqueous solutions of EDTA are frequently used in decontaminating surfaces owing to its powerful chelating action for many metal ions. Using laser-induced fluorescence methods, evidence was obtained that Diphosil sorbs trivalent metal ions from concentrated phosphoric acid that contains a small concentration of nitric acid. This mixed acid media corresponds to the expected composition of the spent working medium of a nitric-phosphoric acid oxidation process for treating organic waste with significant plutonium contamination.

Maximum Metal Ion Loading: To determine the maximum heavy metal ion loading using Diphosil, optical spectroscopy was used to measure metal ion concentration during the sorption process. For example, the maximum uptake of trivalent neodymium ions ($Nd^{3+}$) from dilute nitric acid was determined by monitoring a characteristic near-infrared optical adsorption band of $Nd^{3+}$.




**Photomicrograph of thermally densified, heavy metal ion-loaded Diphosil**

Densification Optimization: On-line, real time infrared analysis of the gases evolved during thermal densification of Diphosil in purified air as a function of heating rate and metal ion loading has been carried out. By varying heating and gas flow rates, optimal thermal densification conditions have been identified. The resulting material (see figure ) contains the selectively sorbed heavy metal ions in fully encapsulated nanophases that are embedded in nearly colorless, nonporous vitreous silica that is highly resistant to radiation damage.

**Planned Activities**

Diphosil possesses the unusual ability to selectively and strongly sorb high valent metal ions, such as actinides, from aqueous solutions. Assessments of the full range of aqueous waste solutions that are amenable to processing via Diphosil are being pursued. During the second year, research will be completed on the influence of monovalent (1+) and divalent (2+) metal ions on the uptake of more highly charged metal ions by Diphosil in aqueous solutions. This work will emphasize common alkali and alkaline earth ions, such as $Na^{+}$ and $Ca^{2+}$, over a range of pH values that extend from significantly acidic to nearly neutral.

Densification studies will be completed by determining the temperature and time at temperature required to achieve complete densification. Samples containing high specific activity, short-lived radionuclides will be prepared as the starting point for radiation damage studies on thermally densified, metal ion-loaded Diphosil. As these short-lived radionuclides decay, it is anticipated that laser-based high resolution linear and nonlinear optical studies will quantify the effect of the resulting radiation damage on the local environment of the encapsulated heavy metal ions. To better understand the observed complex luminescence decays from the encapsulated metal ions, a theoretical modeling effort will begin on the basis of dipole-dipole energy transfer. Conventional leach rate studies will quantify retention of metal ions within thermally densified Diphosil prior to and following damage due to ionizing radiation.

## 7. FUNDAMENTAL NUCLEAR SCIENCE

This element addresses the long-term R&D goal of developing new technologies for nuclear energy applications; educating young scientist and engineers, training a technical workforce; and, contributing to the broader science and technology enterprise.

Today's U.S. reactors, which are based largely on 1970's technology, operate under close supervision in a conservative regulatory environment. Although the knowledge base is adequate for these purposes, improvements in our knowledge and reduction of the inherent uncertainties could bring costs savings in current reactor operations and reduce the costs of future reactors. Furthermore, they could enable innovative designs that reduce the need for excessively conservative and costly factors of safety and reliability and significant extension in safe operating lifetimes. Future reactor technologies are likely to involve higher operating temperatures, advanced fuels, higher fuel burnup, longer plant lifetimes, better materials for cladding and containment vessels, and alternative coolants. To implement such features, substantial research in fundamental science and engineering must be carried out to supplement applied research to 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 far reaching impact elsewhere in engineering and technology.

The five broad topics identified in the Long-Term R&D Plan include:

- The environmental effects on materials, in particular the effects of the radiation, chemical, 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; and,
- reactor physics.

Projects currently selected under this element includes 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.

# NUCLEAR ENERGY RESEARCH INITIATIVE

# Effects of Water Radiolysis in Water Cooled Nuclear Reactors


| | |
|---|---|
| PI: | Simon M. Pimblott, University of Notre Dame |
| Collaborators: | Pacific Northwest National Laboratory, Atomic Energy Canada Ltd. |



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|---|---|---|
| Project Start Date: | August 1, 1999 | Projected End Date: August 31, 2002 |
| Project Number: | 99-0010 | |


## Research Objective

The goal of this research program is to develop a model that describes the chemical effects of radiation on aqueous systems and on aqueous/solid interfaces at temperatures associated with nuclear power plants and the Advanced Light Water Reactors (ALWR). The program has four thrusts:

- Radiation Chemistry Modeling- An experiment-and-calculation based model will be developed to predict yields of the oxidizing and reducing radicals and the molecular species $H_2$ and $H_2O_2$ in aqueous systems like those associated with the ALWR chemistry.
- High Temperature and High Linear Energy Transfer (LET) Effects - Experiments will measure the effect of dose on yields of $O_2$ and $H_2O_2$ produced in radiolysis with $\gamma$-rays, electrons and with $H^+$, $He^{2+}$ and $O^{8+}$ ($C^{6+}$) ions.
- Interfacial Effects of Radiation - Experiments will gather information about radiation effects at aqueous/oxide interfaces of importance in fields such as reactor pipe corrosion and in storage of spent nuclear fuel.
- Low Energy Electrons at Zirconia and Iron Oxide Surfaces and Interfaces - ultra high voltage (UHV) experiments performed at Pacific Northwest National Laboratory with low energy electrons and photons will be used to simulate the damage at interfaces caused by the cascade of reactive secondary electrons produced by high-energy radiation.

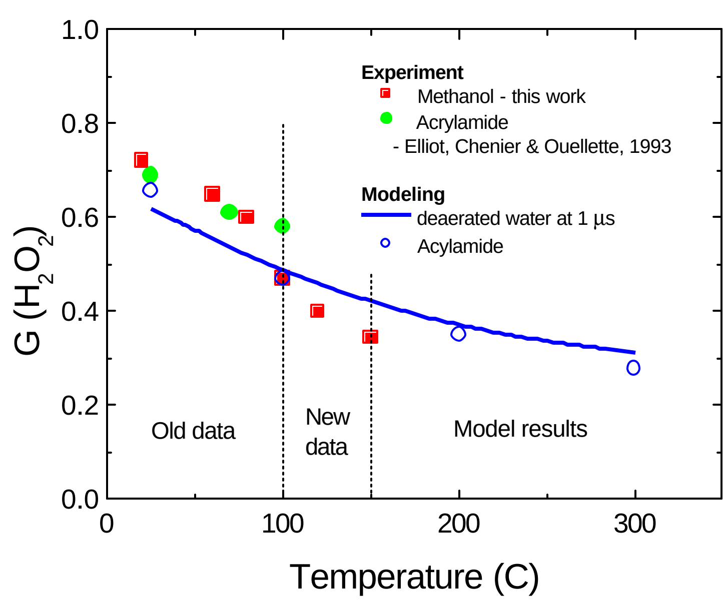
## Research Progress

An extensive review of the scientific literature on $\gamma$-radiolysis of water and aqueous solutions at room and at elevated temperatures has been performed. There is a large amount of data on the nonhomogeneous track chemistry at room temperature, and the track structure and diffusion-limited kinetics are well parameterized. This wealth of knowledge contrasts with the limited information about the effects of radiation on aqueous solutions (and on aqueous solution/metal oxide interfaces) at elevated temperatures.

The Notre Dame Radiation Laboratory (NDRL) suite of computer codes, TRACKKIN, for the simulation of low-LET track chemistry in water was extended to include the effects of temperature. These codes address two aspect of the radiolysis; the structure of the radiation track and the chemistry of the resulting spatially nonhomogeneous distribution of radiation-induced reactants.

Stochastic radiation chemical kinetic simulations have been made for water over the temperature range 25 $^{o}$C to 300 $^{o}$C. The predictions of these calculations were compared with available experimental data for γ-radiolysis. Good agreement is found for all of the radiation-induced species and for the combined yield of H and $H_2$.

Hydrogen peroxide is a source of corrosion for many structural materials in nuclear reactors and its yield is usually kept to minimum levels with the use of different additives. One common technique is to add various amounts of molecular hydrogen. The yield of hydrogen peroxide in the radiolysis of water has been examined with the goal of understanding the mechanism of its production and how various scavengers can influence its yield. The graph below shows the effect of temperature on the yield of hydrogen peroxide. The range over which experimental data is available has been increased by 50 percent. Modeling has been performed up to the normal operating temperatures of light water reactors.




A literature search of the radiation chemistry of iron-oxide and zirconium-oxide water interfaces was conducted. It showed that charge transfer from aqueous species to solid iron-oxide particles has been studied extensively and that a kinetic model has been developed for that system. There is little data for zirconium-oxide particles.

Pulse radiolysis experiments were conducted on zirconia suspensions at high particle concentrations. The yield of the hydrated electron was measured following a pulse of high-energy electrons in the presence of acceptor molecules.

Experiments measuring escape yield of electrons from zirconia into water employing several different scavengers (zwitterion-viologen and methyl-viologen) were used to determine effect of scavenger charge and its interaction with the surface potential on yield. It was found that adsorption of the electron acceptor onto the surface, due to electrostatic interaction with the surface, enhances yield of electron capture at the surface. This, therefore, leads to the conclusion that: a) escape of electrons from the solid particles can be intercepted by the addition of acceptors, and b) the same acceptors also compete with charge recombination within the particles.

Cubic and monoclinic single crystal zirconia films were grown on yttrium stabilized zirconia (YSZ) substrates by the oxygen plasma-assisted molecular beam epitaxy method. Nominal pure $ZrO_2$ films were grown by isothermal oxidation of pure (99.94 percent) zirconium metal foils. These unique and well-characterized $ZrO_2$ materials will be utilized in our future experiments on mechanistic understanding and modeling of radiolysis and radiation-induced corrosion of nuclear reactor fuel surfaces. Current work is focusing on understanding the adsorption and thermal desorption behavior of water at these interfaces and the development of techniques for growing $Fe_3O_4$ are underway.

**Planned Activities**

- Development and validation of a stochastic methodology for simulating high-LET, heavy ion track structure, and for modeling kinetics of heavy ion radiolysis. Subsequent calculations will involve the simulation of the energy loss characteristics of heavy ions, and the investigation of heavy ion track structure, including the role of daughter electrons.
- Perform high dose experiments on the effects of added molecular hydrogen on $O_2$ yields with $\gamma$-rays and with high LET heavy ions.
- Measure the temperature dependence of the effects of added molecular hydrogen on $H_2O_2$ yields with $\gamma$-rays.
- Determine effects of particle size and surface charge on the yields of escape for smaller band-gap materials (hematite and magnetite). For these materials, absorption of light may force the use of conductivity or EPR.
- Perform steady-state radiolysis of oxide suspensions to determine hydrogen and hydrogen peroxide yields, as well as dissolution rates if possible in order to obtain long term consequences of irradiation. Because of the Fenton reaction and the Haber–Weiss cycle it may be impossible to obtain both yields of molecular products and dissolution rates. The experimental results, in particular for $H_2$ and $H_2O_2$, will be tested against the computational predictions in Year 3.

- Investigate electronic structure of doped $ZrO_2$ using time-resolved luminescence and electron energy loss measurements.
- Begin controlled irradiation studies of water-covered iron-oxide.
- Perform radiation assisted redox dissolution studies.

# Measurements of the Physics Characteristics of Lead Cooled Fast Reactors and Accelerator Driven Systems

PI: P.J. Finck, Argonne National Laboratory (ANL)

Collaborators: Commissariat a l'Energie Atomique (French Atomic Energy Commission)

Project Start Date: August 1, 1999 Projected End Date: September 2002

Project Number: 99-0039

## Research Objective

Several recent studies in the U.S. and worldwide have indicated a strong interest in the potential development of lead-cooled critical and sub-critical systems. In order to permit the eventual industrial deployment of these systems, several key technical areas need to be carefully investigated, and solutions for potential technical problems need to be found and implemented.

The neutronic behavior of a lead-cooled fast spectrum system is believed to be relatively poorly known: difficulties arise both from nuclear data uncertainties and from methods related deficiencies. The French Atomic Energy Commission (CEA) has recognized this situation and has launched an ambitious experimental program aimed at measuring the physics characteristics of lead-cooled critical and sub-critical systems in an experimental facility located at the Cadarache Research Center. A complete analytical program is associated with the experimental program and aims at understanding and resolving potential discrepancies between calculated and measured values. The final objective of the two programs is to reduce the uncertainties in predictive capabilities to a level acceptable for industrial applications.

ANL teams are now participating in the experimental design, measurements, and analytical tasks. In exchange for our participation, all experimental data are available to us.

This program will have three critical outcomes: high quality experimental data representative of the physics of lead-cooled cores will be available to the U.S. programs; U.S. neutronics codes will be validated for calculating lead-cooled systems; and potential deficiencies in U.S. nuclear data and codes will be identified.

## Research Progress

Efforts this past year were concentrated in two areas: analysis of existing data from the MUSE 3 experiment, and preparation of the MUSE 4 experimental campaign.

- The MUSE 3 experimental program was carried out from 1997 to 1999. The experimental layout consists of a central neutron source with a well characterized spectrum and intensity, surrounded by a buffer zone made out of either sodium or lead, to simulate different design options and to provide the neutronic impact of these different materials. The remainder of the core is built out of MOX fuel with sodium coolant. Several configurations, both critical and sub-critical, have been measured. The complete set of experimental results for this phase has been provided to ANL.

  Very detailed models of the experimental configurations were set up, using both the European code system with European nuclear data (JEF 2.2) and deterministic or stochastic U.S. code systems with U.S. nuclear data.

  In general, reaction rate traverses are calculated with good accuracy, and no difficulties have been observed in the source region. This indicates that the source multiplication and propagation are well estimated at all sub critical levels. Significant difficulties appear close to the core-reflector interface: these discrepancies are attributed to uncertainties in nuclear data for structural materials and are typical in these types of cores. Large discrepancies have been observed in terms of predicted sub-criticality levels. Compared to experimental data, JEF 2.2 provides significantly better results, even though it tends to overestimate reactivity by about half a percent. In general, ENDF/B-VI overestimates reactivity by about one percent. Root causes for this over prediction are still being investigated.

  Kinetic measurements will be an important element of future experiments; the analysis of these measurements is particularly difficult, as it is necessary to employ explicit three dimensional time dependent transport calculations. ANL is hosting a French Ph.D. student to develop the adequate methodology, which will be made available to the French program.

  Significant analytical support has been provided to the French CEA in preparing the MUSE 4 experimental campaign.

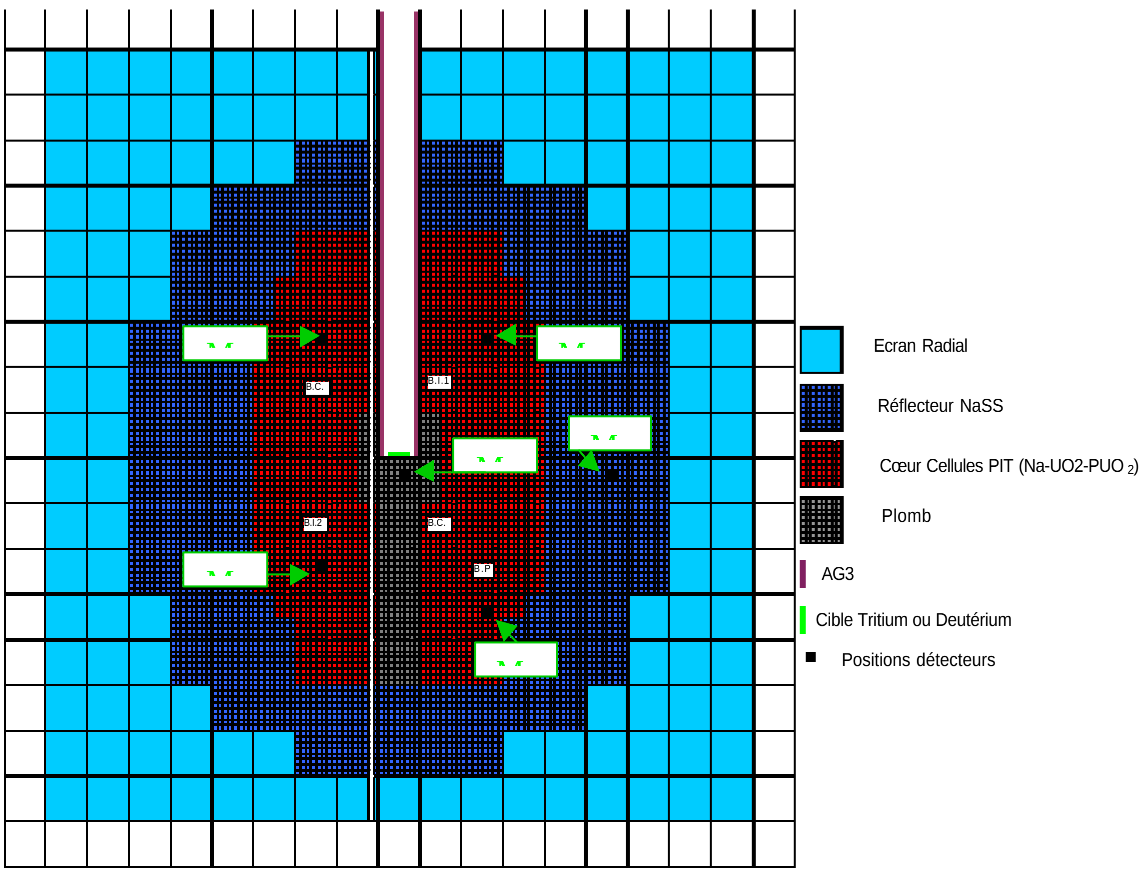
- ANL had a major impact on the preparation of the MUSE 4 experimental campaign. A project researcher has been on attachment in France for several months and has led the effort for developing the experimental techniques for dynamic measurements and for defining the required data acquisition system.

  The dynamic measures to be performed are Feynman/Rossi alpha, single pulse alpha, frequency modulation, and transfer function/noise techniques. Although these are all fundamentally related, different techniques of data acquisition and analysis will be used to yield different kinetic parameters. In addition, analysis over different time scales will lead to different information.

A set of data acquisition equipment and a series of measurements were defined in the Experimental Plan that will yield the most useful information for subsequent analysis.

The full Experimental Plan was developed to provide multiple measures of the parameters that are key to safety ($\beta$, l, source importance), as well as measures important to the feasibility of an accelerator driven system (spectrum, reaction rates). It is expected that these measurements will help to significantly reduce the uncertainty in calculated parameters.

The French Safety Authorities have given approval for the MUSE 4 experiments as of November 8, 2000. A series of critical reference measurements are planned until February 2001, at which time the new GENEPI accelerator will be installed and tested. Three sub-critical configurations will be implemented (successive sub-critical levels are: -1.5$, -10$, -17$) and the measurements will last until October 2001. The figure below describes the MUSE 4 configuration.



**Planned Activities**

Three major tasks are planned for FY 2001:

- Experimental activities: an ANL project researcher will lead the experimental team at Cadarache and realize all measurements described in the Experimental Plan.
- Analytical task: the analysis of MUSE 3 results will be completed by January 2001, and the first MUSE 4 results will be analyzed. Further measurements, in particular those for kinetic parameters, will be analyzed as they become available.
- Support task: the preparations for the following campaign, MUSE 5, will become a top priority, and the choice of options (fuel type and configuration) will be supported by ANL analysts.

# Mapping Flow Localization Processes in Deformation of Irradiated Reactor Structural Alloys

PI: K. Farrell, Oak Ridge National Laboratory

Project Start Date: August 1, 1999 Projected End Date: August 31, 2002

Project Number: 99-0072

## Research Objective

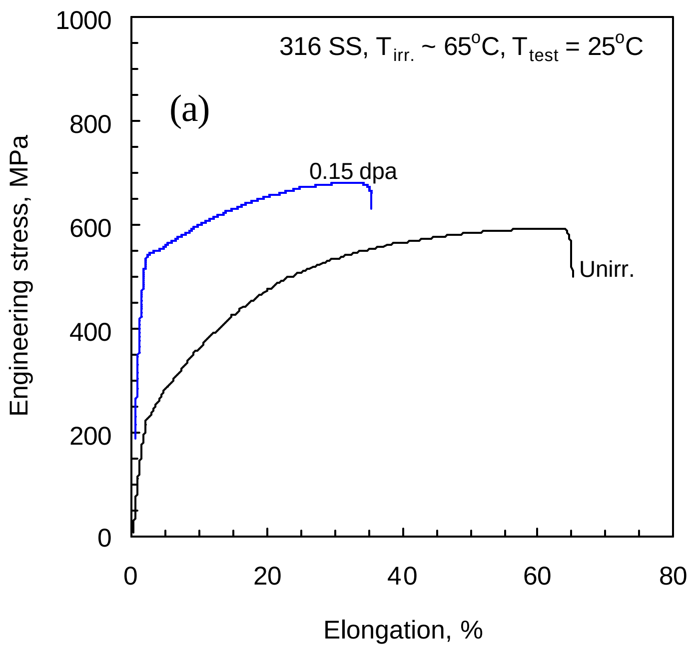
The materials from which nuclear power reactors are constructed, namely ferritic steels for pressure vessels, austenitic stainless steel for core internals and piping, and zirconium alloys for fuel cladding and tubing, are normally quite ductile and workable. They are ductile because they undergo plastic flow, or deformation, by the generation and movement of dislocations on slip planes within the atomic lattice of the metal. Many intersecting slip planes are operative. The dislocations can move from one slip plane to another and they become entangled into a three-dimensional network of dislocation cells. This ability to develop a network of dislocation cells ensures that the material work hardens and deforms in a homogenous manner. That ability is lost when the materials are exposed to the action of penetrating neutrons in the reactor. The neutrons create disturbed regions in the regular arrangement of atoms in the atomic lattice. These disturbed regions, or radiation damage clusters, impede the slip dislocations and inhibit the formation of dislocation cells. Instead, the deformation becomes localized in narrow bands or channels, and sometimes in twin bands. This intensification of strain and stress by dislocation channel deformation (DCD) changes the mechanical properties of the material and causes embrittlement. The degree of embrittlement is related to the nature and the details of the dominant deformation mode, which are functions of the radiation exposure and of the mechanical test conditions.

Most mechanical property data for use in design data banks is derived from tensile tests. Radiation damage raises the tensile yield strength and ultimate tensile strength (UTS), induces yield point drops in materials that do not normally show sharp yield points, reduces the work hardening rate and the elongation, and causes premature plastic instability and failure. All of these changes are now known or suspected to involve DCD but only a few quantitative correlations have been made. If such correlations are made in detail they can allow preparation of deformation mode maps in which the regions and boundaries of the deformation modes are plotted in terms of plastic strain and neutron fluence. Mechanical properties representing the different deformation modes can be overlaid on the maps, and the maps become pictorial repositories of knowledge relevant to the irradiation behavior of the materials. These maps will not only simplify, condense, verify and specify essential properties and applications limits for crucial reactor components, but they will add immeasurably to our understanding of the interplay between radiation damage microstructures, deformation modes and mechanical properties responses. They should bring cohesion and assurance into the processes of selection, assessment, and application of reactor materials. Presently, deformation mode maps for irradiated materials exist only for nickel and gold. The goal of this project is to determine deformation mode maps for A533B ferritic steel, 316 stainless steel, and Zircaloy-4 alloy.

**Research Progress**

Literature surveys have been made and dossiers on deformation behaviors of the three test materials have been compiled. These files proved to be very appropriate for the principal investigator to present an invited paper on strain localization at the Workshop on Dislocation-Defect Interactions in Irradiated Materials in Toledo, Spain, April 3-5, 2000. The workshop was the first of its kind devoted to flow localization in irradiated materials, and its timing was perfect for assessing and influencing the direction of the present NERI project. Mapping of deformation modes for irradiated materials entails irradiating suitable tensile specimens to prescribed neutron fluences, straining the specimens to predetermined strain levels and recording the tensile properties, cutting small pieces from the gauge sections of the specimens, electrothinning the pieces to make transmission electron microscopy (TEM) samples, and conducting a detailed study of the samples to obtain quantitative measurements of the radiation damage microstructures and the deformation mode microstructures. Each sample involves a great deal of work, and since the project is limited to three years, it was necessary to expedite the process. All of the above steps had to be minimized and honed to save time, cost, and effort, and to reduce radiation exposure to the operators. To those ends, a special, miniature, flat tensile specimen was developed that occupies minimum space in the irradiation capsule, permits excision of tiny TEM pieces without the need for sanding operations, and has reduced radioactivity. To allow remote handling of these small specimens in and out of the tensile machine without inadvertent damage, a sliding cradle that supports and protects the specimen during the test procedure was designed. The tiny TEM pieces are only 1.5 mm square, much smaller than standard 3mm diameter disks, and they required development of refined electrothinning and TEM clamping procedures. These refinements were achieved in parallel with specimen procurement, heat treatment, and encapsulation and documentation for irradiation in the High Flux Isotope Reactor (HFIR).

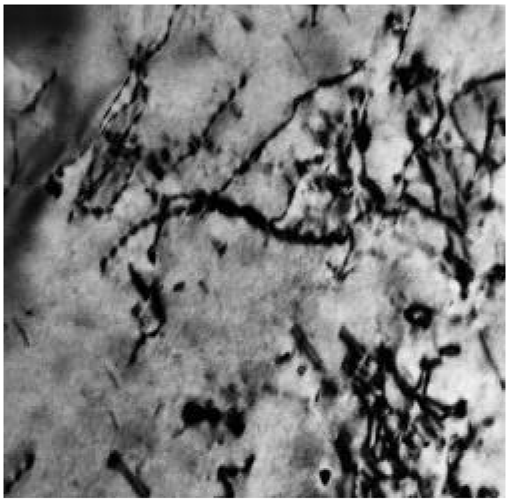
Five capsules for irradiations at 65$^{o}$C to neutron fluences in the range 6 x $10^{20}$ n•m$^{-2}$ to 6 x $10^{24}$ n•m$^{-2}$ at decade intervals were ready for irradiation by February 2000. These irradiations would normally have been treated as routine irradiations and should have been conducted in about four weeks. Unfortunately, several incidents occurred at the HFIR, unconnected with these experiments that provoked a revision of the rules for materials irradiation experiments in the HFIR. Coping with the revised regulations, and difficulties with an overcrowded schedule at the HFIR, delayed execution of our irradiations until August/September. This unexpected long delay threw project plans off schedule and, as a result, the investigators requested and were granted a six month, no-cost extension of the Year 1 phase of the program. To make up lost time and expenses, much of the planned specimen testing and TEM preparation phases has been rerouted from costly and slow hot cells operations to speedier and more cost-effective C zone operations. These moves allowed Year 2 TEM studies to begin on the original schedule. Presently, the specimens have been recovered from the capsules and are undergoing tensile testing, TEM preparation, and TEM examination. The first TEM results show that the deformation mode for irradiated 316 stainless steel is very narrow bands of microtwins. The graph below illustrates the irradiation effects for a dose of 0.15 dpa (9 x $10^{23}$ n. $m^{-2}$, E>1MeV). The tensile yield strength is raised from 230 Mpa to 540 Mpa and the elongation is reduced from 60 percent to 30 percent. Correspondingly, the deformation mode changes from random dislocation tangles (left picture below) to narrow twin bands (right picture below).

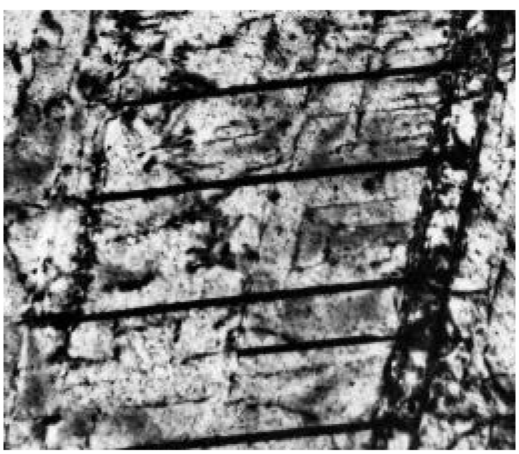



Some setbacks have been encountered in obtaining satisfactory electrothinned samples from the irradiated A533B steel and the Zr-4, however, the problems are surmountable.

**Planned Activities**

Before the end of Year 2 of the project, the irradiated tensile specimens and the unirradiated control specimens will be tested to five different strain levels and preliminary TEM examinations will be conducted to identify the deformation modes. These observations will be used to construct the deformation maps. Concurrently, selected specimens will be subjected to detailed TEM studies to measure and quantify the microstructural features involved in the deformation processes. This will involve measuring the sizes and wall thicknesses of dislocation cells, and characterization of the dislocation channels in terms of crystallographic planes, channel widths, channel frequency, degree of cross-channeling, amount of strain in the channels, and the effects created when channels impact grain boundaries and other barriers. These data will be analyzed and correlated with the corresponding tensile properties data.





**Changes in tensile properties and deformation microstructures of 316 stainless steel after irradiation to 0.15 dpa. The deformation microstructures represent 6% elongation in the picture above, the unirradiated steel and the picture to the left, the irradiated steel.**

In Year 3 more irradiations will be carried out on a reduced scale to look briefly at the effects of a higher irradiation temperature and a higher strain rate. An irradiation temperature of 300$^o$C will be used which seems to induce enhanced radiation embrittlement in all three materials.

With regard to higher strain rate, a higher rate is expected to give narrower dislocation channels. Correspondingly, the channel strains and the resultant stress intensification will be increased, and embrittlement and plastic instability will be worsened. The specimens will be irradiated to two fluences, 6 x $10^{23}$ n•m$^{-2}$ and 6 x $10^{24}$ n•m$^{-2}$. Specimens of the A533B steel will be irradiated to a fluence of 6 x $10^{23}$ n•m$^{-2}$. These specimens will be tested at two strain rates, $10^{-3}$•s$^{-1}$ as in the Year 1 tests, and $10^{-1}$•s$^{-1}$. Several specimens for each condition will be strained to failure. Other tests will be truncated at two strain levels, 5 percent and at the UTS, if sufficient ductility is maintained. Otherwise, the tests will be terminated at whatever minimum strain is achievable. TEM will be performed on each specimen to identify the deformation mode(s). Selected specimens will receive intense TEM scrutiny and extraction of quantitative data. A report of the findings will be published.

# A Novel Approach to Materials Development for Advanced Reactor Systems


| | |
|---|---|
| PI: | Gary S. Was, University of Michigan |
| Collaborators: | Pacific Northwest National Laboratory, Oak Ridge National Laboratory |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|---|---|---|
| Project Start Date: | September, 1999 | Projected End Date: August 31, 2002 |
| Project Number: | 99-0101 | |

**Research Objective**

Component degradation by irradiation is a primary concern in current reactor systems as well as advanced designs and concepts where the demand for higher efficiency and performance will be considerably greater. In advanced reactor systems, core components will be expected to operate under increasingly hostile (temperature, pressure, radiation flux, dose, etc.) conditions. The current strategy for assessing radiation effects for the development of new materials is impractical in that the costs and time required to conduct reactor irradiations are becoming increasingly prohibitive, and the facilities for conducting these irradiations are becoming increasingly scarce. The next generation reactor designs will require more extreme conditions (temperature, flux, fluence), yet the capability for conducting irradiations for materials development and assessment in the next 20 years is significantly weaker than over the past 20 years. Short of building new test reactors, what is needed now are advanced tools and capabilities for studying radiation damage in materials that can keep pace with design development requirements.

The most successful of these irradiation tools has been high-energy (several MeV) proton irradiation. Proton irradiation to several tens of displacements per atom (dpa) can be conducted in a short amount of time (weeks), with relatively inexpensive accelerators, and result in negligible residual radioactivity. All of these factors combine to provide a radiation damage assessment tool that reduces the time and cost to develop and assess reactor materials by factors of 10 to 100. What remains to be accomplished is the application of this tool to specific materials problems and the extension of the technique to a wider range of problems in preparation for advanced reactor materials development and assessment.

The objective of this project is to identify the material changes due to irradiation that affect stress corrosion cracking (IASCC) of stainless steels, embrittlement of pressure vessel steels and corrosion and mechanical properties of Zircaloy fuel cladding. Until such changes are identified, no further progress can be made on identifying the mechanisms and solving the problems. An understanding of the mechanisms will allow for the development of mitigation strategies for existing core components and also the development of radiation-resistant alloys or microstructures that are essential for the success of advanced reactor designs.

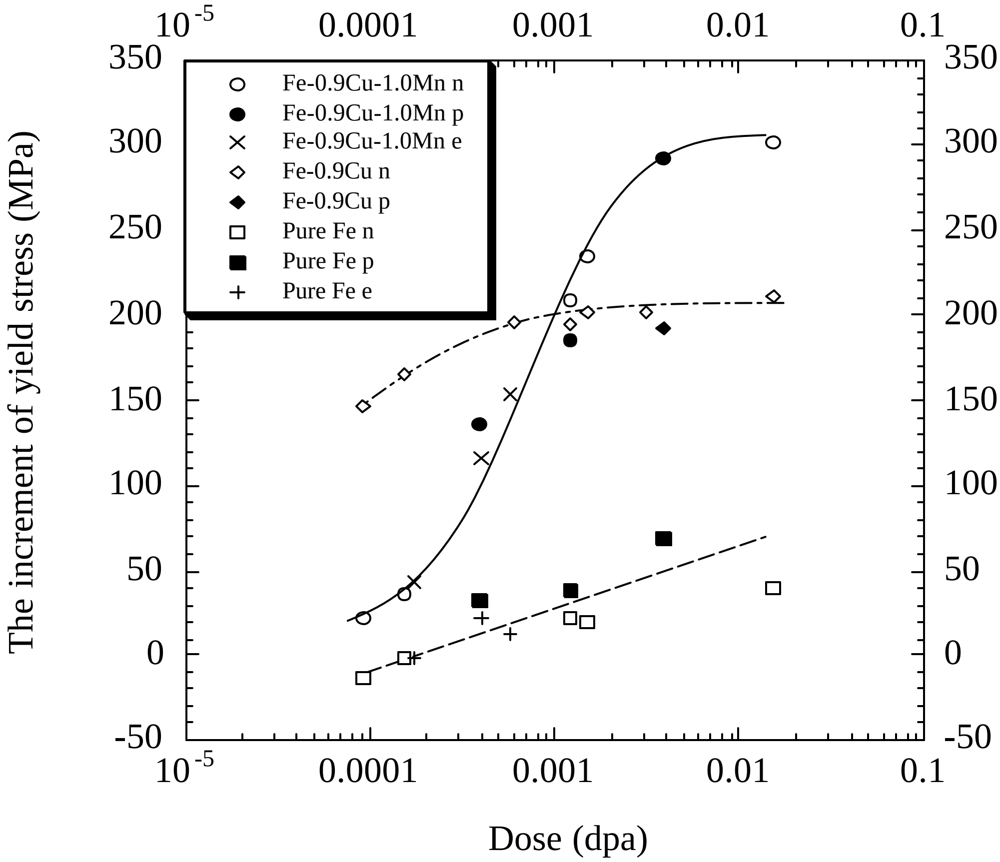
**Research Progress**

The objective of the first year of research was to understand the microstructure evolution in model alloys of reactor pressure vessel (RPV) steels and also in stainless steels under light water reactor irradiation conditions. The work focused on investigating the irradiated microstructure by using proton irradiation in comparison with neutron irradiation. The following points summarize the results:

- Proton-irradiation of model RPV alloys results in a comparable level of hardening as does neutron irradiation of the same alloys at the same temperature and dose. Annealing of the irradiated microstructure produces a recovery of hardening that also matches that from neutron irradiation.
- Small angle x-ray scattering data and preliminary results from transmission electron microscopy reveal that the precipitate size/density combination is similar to that from neutron irradiation. The agreement in hardening between proton and neutron irradiation is supported by the similarity in the character of the defect clusters. The results also support those from electron irradiation that imply that the character of the damage cascade does not strongly affect the resulting microstructure.
- The irradiation-induced microstructure in proton-irradiated austenitic stainless steels consists mainly of dislocation loops up to 5.0 dpa.
- The dose dependence of the dislocation loop density and size in proton-irradiated Fe-Cr-Ni alloys follows the same trend as in neutron-irradiated alloys. The higher loop density in commercial alloys is probably due to enhanced nucleation of loops by minor constituent elements (phosphorus, silicon).
- Yield strength in proton-irradiated austenitic alloys as a function of dose and temperature are consistent with neutron data. Across a wide dose range, the hardening estimated from micro-hardness measurements agrees with calculations from the dispersed barrier-hardening model.
- The difference in the effect of the character of the displacement cascade on loop nucleation between neutron irradiation (275$^{o}$C, 7x10$^{-8}$ dpa/s) and proton irradiation (360$^{o}$C, 7x10$^{-6}$ dpa/s) has little effect on the final irradiated microstructure. The reduced level of loop nucleation by in-cascade interstitial clustering in proton irradiation appears to be balanced by the higher cascade efficiency and higher vacancy supersaturation caused by the higher dose-rate and the lower sink strength at the higher irradiation temperature.

**Planned Activities**

The research plan for years 2 and 3 will focus on three areas. We will be studying the tradeoff in hardening between cold work and irradiation on the IASCC susceptibility of austenitic stainless steels. We will also be experimenting with pre-segregation at grain boundaries to neutralize the effect of radiation induced stress (RIS) on IASCC. The




**Yield strength increment as a function of dose for neutron, electron and proton irradiation of alloys VA (Fe), VH (Fe-0.9Cu) and VD (Fe-0.9Cu-1.0Mn). The trend lines ---, -· and ––– represent VA, VH and VD hardening trend with dose respectively. Hardening with proton irradiation is in good agreement with that from neutrons and electrons.**

activity on RPV model alloys will focus on the composition effects of proton irradiation, the development of hardness with dose, and the comparison with neutron irradiation results. The effort is aimed at understanding the role of alloying additions on the hardening behavior of these steels. The last task will focus on the irradiation of Zircaloy–2 and –4 to assess the capability of proton irradiation to emulate neutron irradiation in terms of the dislocation microstructure, precipitate structure and morphology, and corrosion behavior.

# Complete Numerical Simulation of Subcooled Flow Boiling in the Presence of Thermal and Chemical Interactions



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| PI: | Vijay K. Dhir, University of California, Los Angeles | |
| Project Start Date: | August 1, 1999 | Projected End Date: August 31, 2002 |
| Project Number: | 99-0134 | |

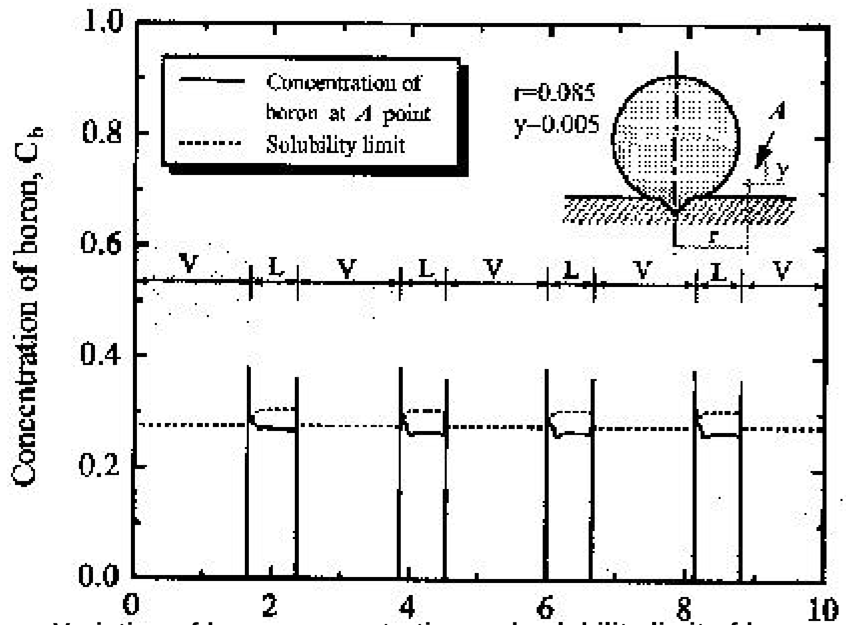


## Research Objective

The key objective of the proposed research is to develop a mechanistic basis for the thermal and chemical interactions that occur during subcooled boiling in the reactor core. The axial offset anomalies (AOA) are influenced by local heat flux for subcooled nucleate boiling, the nucleation site density on the fuel cladding, and the concentration of boron and lithium in the primary coolant. The approach proposed in this work is very different than what has been employed in the past in that complete numerical simulations of the boiling process along with thermal, hydraulic and concentration fields in the vicinity of the cladding surface will be carried out. This approach is considered to be the only viable one that can provide, simultaneously, a mechanistic basis for the portioning of the wall heat flux among vapor and liquid and the concentration of boron and lithium, at, and adjacent to, the heated surface. The model will be validated with data from detailed experiments. A building block type of approach will be used where, starting with a bubble at a single nucleation site, the complexity of the numerical model and experiments will be increased to include merger of bubbles at the wall as well as interaction of the detached bubbles with the bubbles present on the heated surface. The concentration of boron and lithium in water, pH value of water, and system pressure will be important variables of the problem.

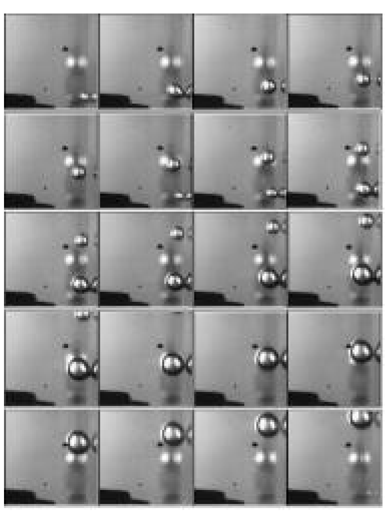
## Research Progress

During the past year, an axi-symmetric numerical simulation model of a single bubble formed on a horizontal surface containing a chemical species has been developed. In carrying out the analysis, the conservation equations of mass, momentum, and energy for the two phases along with the conservation of species equations for chemicals present in water have been solved simultaneously. The level set method is used in the numerical simulation. As such, a single momentum equation is solved for both liquid and vapor regions. A function representing distance from the interface is derived and the distance function is advanced at each time step by solving the advection equation. The results of numerical simulation using orthoboric acid as the chemical species present in water reveal that during growth and departure phases of bubble the concentration of orthoboric acid varies both spatially and temporally. As shown in graph below, the local concentration especially in the regions very close to the heater surface can exceed the solubility limit at a given temperature. However, experimental validation of the predicted




**Variation of boron concentration and solubility limit of boron in solution with time at point *A*.**

behavior is pending. The numerical simulation tool has also been extended to three dimensions with flow along the heater surface. It is found that consistent with experimental observations the bubbles slide along the surface before departure. An experimental apparatus for flow-boiling studies has been developed and experiments using silicon strips made from polished silicon wafer with a microfabricated cavity have been performed. The experiments show consistent with the model predictions that bubble lift off diameter is larger than the bubble departure diameter. Both bubble lift off and departure diameters decrease with flow velocity. Below are photographs of bubbles before and after departure, but prior to lift off on a vertical surface with imposed flow velocity.



**Growth Cycle for Vertical Surface, Upflow, (*near field view*); *V* = 0.025 m/s, $\Delta T_{wall}$= 5.9°C, $\Delta T_{sub}$= 0.3°C.**

**Planned Activities**

During the next two years, the three-dimensional code will be augmented to include the species conservation equation. The code will be exercised more thoroughly to study the effect of liquid subcooling, wall superheat, flow velocity and surface wettability on bubble dynamics and precipitation of the solute in water. The experiments will be continued to obtain data on bubble dynamics and heat transfer with and without the presence of chemical species in the liquid. If possible, bubble-bubble interaction as may occur at high wall superheats will also be investigated. The results of the research will be disseminated to the technical community by presenting papers at conferences and publication in peer reviewed journals.

# NUCLEAR ENERGY RESEARCH INITIATIVE

## Developing Improved Reactor Structural Materials Using Proton Irradiation as a Rapid Analysis Tool


PI: T.R. Allen, Argonne National Laboratory-West

Collaborators: University of Michigan



Project Start Date: August 1, 1999 Projected End Date: August 31, 2002

Project Number: 99-0155


### Research Objective

The purpose of this program is to design advanced reactor materials with improved resistance to void swelling and irradiation assisted stress corrosion cracking (IASCC) using three principal methods: bulk composition engineering, grain boundary composition engineering, and grain boundary structural engineering. The focus of the first year was bulk compositional engineering in which five different alloying additions were made to a base Fe-18Cr-8Ni-1.25Mn alloy whose bulk composition corresponds to 304 stainless steel. This alloy was chosen as the reference alloy for the program because 304 stainless steel is known to be susceptible to both swelling and IASCC. In addition to the studies on bulk composition engineering, work commenced on the grain boundary structural engineering. Thermomechanical treatments were developed for the Fe-18Cr-8Ni-1.25Mn alloy that increased the fraction of coincidence site lattice (CSL) boundaries.

Each of the bulk composition alloying additions was chosen for a specific purpose. Fe-18Cr-40Ni-1.25Mn was chosen because higher bulk nickel concentration is known to reduce swelling, but its affect on IASCC is unknown. Fe-18Cr-8Ni-1.25Mn+Zr was chosen because Zr is an oversized element that might trap point defects and prevent swelling and grain boundary segregation. Fe-16Cr-13Ni-1.25Mn, Fe-16Cr-13Ni-1.25Mn+Mo, and Fe-16Cr-13Ni-1.25Mn+Mo+P were chosen to determine why 316 stainless steel is more resistant to swelling and IASCC than 304 stainless steel.

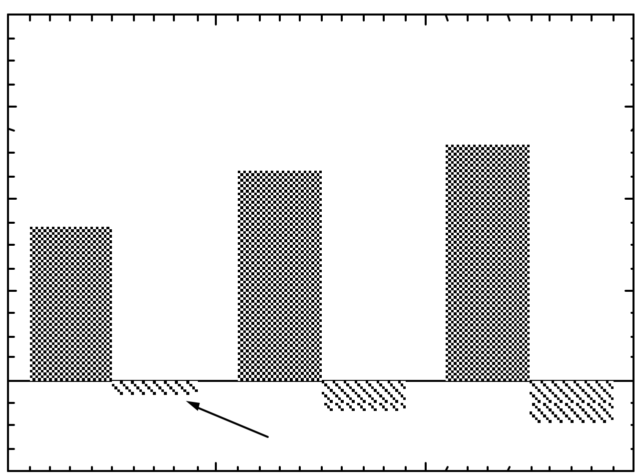
### Research Progress

In the first year of the project, Fe-18Cr-8Ni-1.25Mn, Fe-18Cr-40Ni-1.25Mn, Fe-18Cr-8Ni-1.25Mn+Zr, and Fe-16Cr-13Ni-1.25Mn were studied. Samples were irradiated using 3.2 MeV protons at 400°C to 1 displacement per atom (dpa). Swelling was characterized by measuring the void size distribution using a transmission electron microscope (TEM). Radiation-induced grain boundary segregation was measured using a field emission gun scanning transmission electron microscope (FEG-STEM). Microhardness measurements were performed on irradiated and non-irradiated alloys to estimate the effect of irradiation on strength.

New insight on the relationship between IASCC, grain boundary composition, and irradiation hardening was reached in the first year of the program by studying the Fe-18Cr-8Ni, Fe-18Cr-40Ni, and Fe-16Cr-13Ni alloys. Increasing the bulk nickel concentration decreases void swelling, increases matrix hardening, and increases grain boundary chromium depletion and nickel enrichment. Two effects of radiation on microstructure have been hypothesized to contribute to IASCC: Cr depletion leading to decreased grain boundary corrosion resistance and matrix hardening leading to a grain boundary mechanically weakened relative to the matrix. Comparing the Fe-18Cr-8Ni and Fe-16Cr-13Ni alloys, moving toward the 316 composition (and in general to alloys with greater bulk nickel concentrations) causes greater hardening and greater Cr depletion (figure below). Greater hardening (yield strength) and greater Cr segregation should make 316 more susceptible to IASCC. Yet 316 is typically less susceptible than 304 to IASCC.

Alloys with greater bulk nickel concentration have greater radiation induced segregation (RIS), causing a decrease in grain boundary volume. They also have increased hardening and Cr depletion, theoretically making the alloy more susceptible to IASCC. But Cookson et. al. found that increasing Ni content decreased IASCC susceptibility. Decreased IASCC susceptibility may be related to boundary strengthening associated with the grain boundary volume decrease. The lattice parameter and shear moduli decrease with decreasing Cr concentration and with increasing Ni concentration. Cr depletes and Ni enriches at the boundary during irradiation. The smaller modulus and smaller solute atoms caused by RIS may strengthen the boundary, mitigating grain boundary deformation and cracking. While typical studies of IASCC assumed RIS was a contributing factor to cracking, it may be that properly controlled RIS can be used as a mitigating factor.

- IASCC Causes (Traditional thinking)
  - Cr depletion weakens grain boundary corrosion resistance
  - Matrix hardening weakens grain boundary relative to matrix
- 316 (and in general alloys with greater bulk Ni) more resistant to IASCC than 304
- This study:
  - 316 surrogate (and in general alloys with greater bulk Ni) has greater grain boundary Cr depletion and greater matrix hardening (should be more cracking susceptible)
  - Increasing bulk Ni changes RIS such that grain boundary volume decreases (decreased lattice parameter, decreased shear modulus)
  - Properly controlled RIS may reduce susceptibility to IASCC



**Effect of Bulk Composition on Grain Boundary Cr Depletion and on Irradiation Hardening**

**Planned Activities**

For year two of the project, the research will focus on all three research areas; bulk composition engineering, grain boundary composition engineering, and grain boundary structural engineering. Bulk composition engineering and grain boundary compositional engineering will be studied on the 316 series of alloys, Fe-16Cr-13Ni-1.25Mn, Fe-16Cr-13Ni-1.25Mn+Mo, and Fe-16Cr-13Ni-1.25Mn+Mo+P. These alloys will be irradiated in the solution-annealed condition and following special treatments to set the grain boundary composition prior to irradiation. The greater resistance of IASCC in 316 stainless steel may also be related to the addition of Mo, which is not present in 304 stainless steel. The study of Fe-16Cr-13Ni-1.25Mn-2.5Mo is planned to address the effect of Mo. Bulk composition engineering and grain boundary structural engineering will be focussed on zirconium containing alloys. These alloys will be irradiated in the solution-annealed state and following special processing to alter the grain boundary structures. The microhardness, void swelling, radiation-induced grain boundary segregation, and the radiation-induced microstructural changes will be determined for each irradiation condition.

# An Investigation of the Mechanism of IGA/SCC of Alloy 600 in Corrosion Accelerating Heated Crevice Environments

PI: Jesse Lumsden, III, Rockwell Science Center

Project Start Date: August 1999 Projected End Date: September 2002

Project Number: 99-0202

## Research Objective

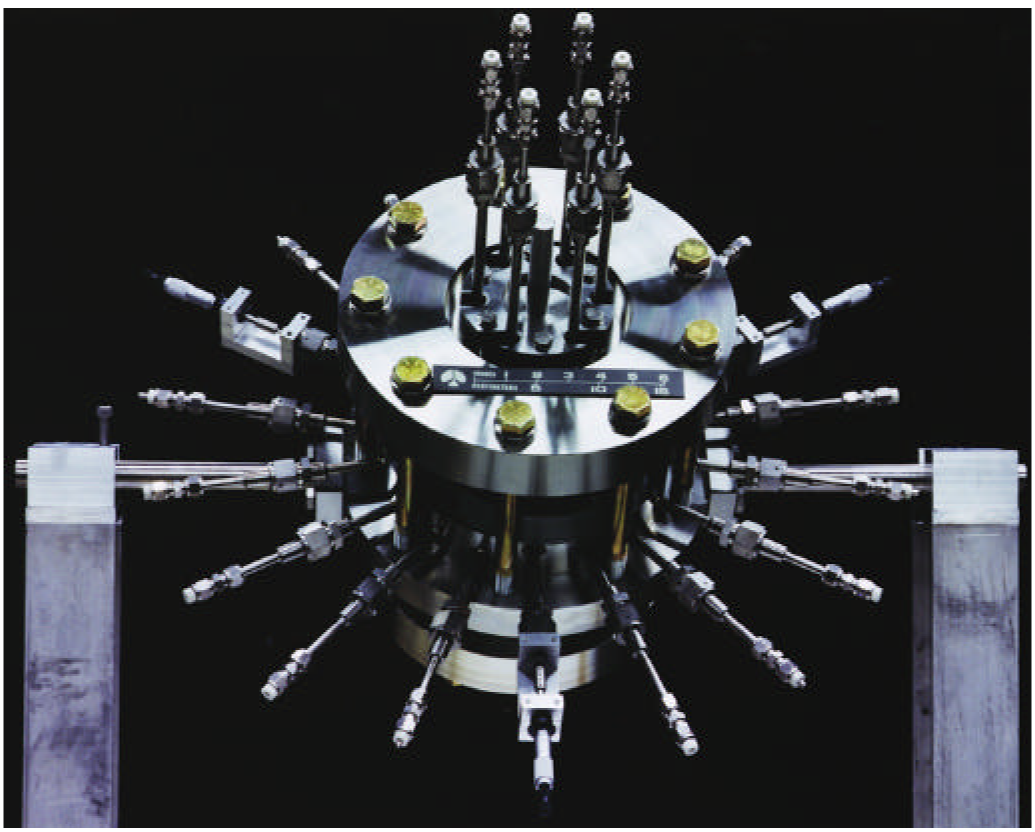
The concentrated solutions and deposits in tube/tube support plate crevices of nuclear steam generators have been correlated with several forms of corrosion on the outer secondary side of Alloy 600 steam generator tubes including intergranular attack/stress corrosion cracking (IGA/SCC), pitting, and wastage. Crevice chemistries in an operating steam generator cannot be measured directly because of their inaccessibility. In practice, computer codes, which are based upon hypothesized chemical reactions and thermal hydraulic mechanisms, are used to predict crevice chemistry. The objective of the Rockwell program is to provide an experimental base to benchmark crevice chemistry models, to benchmark crevice chemistry control measures designed to mitigate IGA/SCC, and to model IGA/SCC crack propagation processes. The important variables will be identified, including the relationship between bulk water chemistry and corrosion accelerating chemistries in a crevice. One important result will be the identification of water chemistry control measures needed to mitigate secondary side IGA/SCC in steam generator tubes. A second result will be a system, operating as a side-arm boiler, which can be used to monitor nuclear steam generator crevice chemistries and crevice chemistry conditions causing IGA/SCC.

## Research Progress

The research approach uses an instrumented heated crevice, which is a replica of a PWR steam generator tube/tube support plate crevice (T/TSP). During the first contract year, the construction of this apparatus was completed.

The heated crevice consists of an Alloy 600 steam generator tube inserted through a drilled hole in a 1-inch thick Alloy 600 ring. The gap between the outer diameter (OD) of the tube and the drilled hole is 15 mils. The heated crevice operates at simulated steam generator thermal conditions and pressure. The entire assembly is contained in a 2 liter, Alloy 718 autoclave. The tube, the ring, and the autoclave are structurally independent and electrically isolated from each other. A cartridge heater is inside the Alloy 600 tube, which heats the tube to simulated primary water temperatures. The autoclave is heated by strip heaters and can be maintained at 280°C independent of the tube heater, simulating the bulk water temperature in a steam generator. In addition to thermocouples for temperature control in the bulk water in the autoclave and inside the tube, eight thermocouples are brazed onto the inner diameter (ID) of the Alloy 600 tube. These thermocouples are in a helical pattern at different depths in the crevice, and monitor the temperature profile in the crevice. Capillary tubes are located in the bulk water and extend into the crevice for extracting solution. A silver/silver chloride reference electrode is located in the bulk water for measuring the electrochemical potential (ECP) of the freespan of the Alloy 600 tube. A second silver/silver chloride reference electrode extends through the ring into the crevice for monitoring the electrochemical potential (ECP) of the crevice. Additional electrodes extend through the ring to the crevice for monitoring IGA/SCC of the tube.

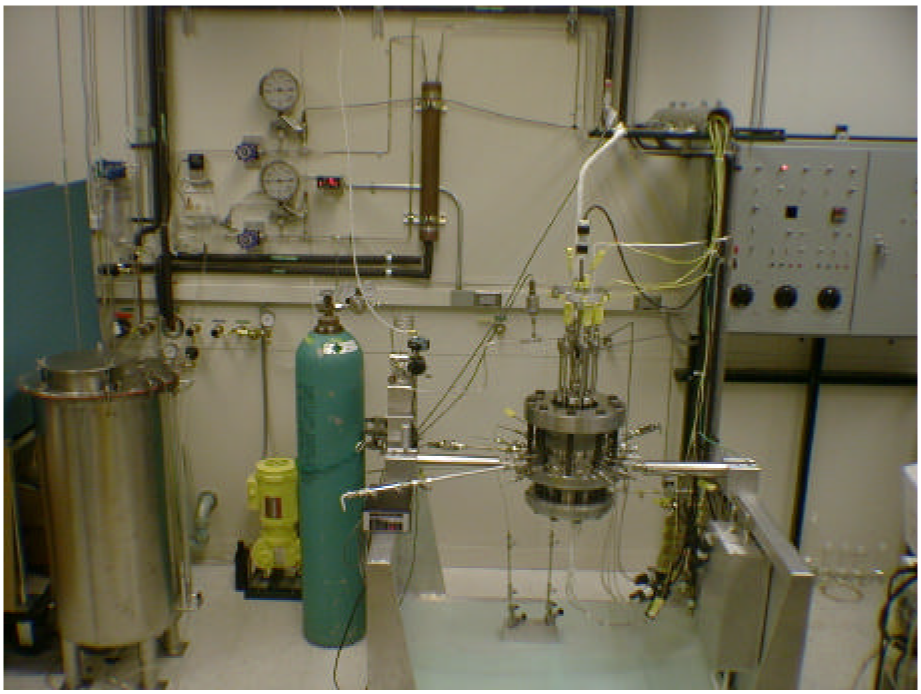
Illustrated below is a photograph of the assembled heated crevice. The radial array of ports for sensors surrounds the center section of the autoclave. An Alloy 600 tube, which does not have the heater assembly attached, is clearly visible in the center of the top section of the autoclave. There are six feedthroughs located in the top of the autoclave. These are for the water system and for inserting probes and thermocouples into the bulk water. Stainless steel rods, inserted into the center clamping ring, support the heated crevice on a stand so that it is suspended above the floor.



**Assembled heated crevice before installing the tube heater**

A continuously flowing water system is used. A high-pressure pump delivers water from the 500-liter makeup tank through the autoclave. A backpressure regulator allows the pressure in the autoclave to be adjusted to the 280°C boiling point. A system qualification run has been successfully completed, and experiments are now underway.

The photograph below shows the complete layout. The heated crevice assembly is in the center of the photograph. The pressurized Alloy 600 tube containing a cartridge heater extends trough the top. The connectors, surrounding the tube extension, are for thermocouples located at various locations in the tube and in the crevice. Compressed He, in the cylinder to the left of the autoclave, is used to pressurize the tube. A high pressure pump pumps deoxygenated water from the feed tank (located at the far left in the photograph) through the remainder of the water circuit Water exits the system after passing through a condenser. The panel on the wall at the far right contains the circuits and controls for the band heaters on the autoclave and the tube heater.



**Complete set-up showing the heated crevice, the water circuit, and the control panel**

An electrochemical noise (EN) system was set up for corrosion monitoring. This technique is based on the electrochemical nature of corrosion processes and the distinctive nature of EN signatures for all corrosion processes. The EN signature from SCC of Alloy 600 results from the creation of new surface area when a crack is initiated or advances. When a crack initiates or propagates, there is a transient surge in current associated with the oxidation processes of dissolution and film formation on the new surface exposed to the aqueous solution. Most of the current surge is from dissolution, which decreases rapidly as new oxide film is formed on the newly created surface.

EN was measured from stressed samples (C-rings) in a static autoclave containing a caustic solution at 320°C. These conditions simulate the chemistry and temperature in the heated T/TSP crevice when feedwater is used with a high concentration of NaOH. The length of SCC cracks in the specimens depended upon the magnitude of the applied stress and the time of exposure. A comparison of SCC crack lengths with the EN, indicated that crack propagation was discontinuous and that the cracks remained dormant for long intervals of time between propagation periods. The amplitude of current transients from stressed samples was over an order of magnitude greater than the amplitude from identical samples with no stress.

The EN results obtained using static autoclaves provide a baseline for measurements from the heated crevice. A heated crevice run is underway using deaerated feedwater with 40 ppm NaOH, simulated primary water of 320°C, and a bulk water temperature of 280°C. The heated crevice is packed with diamond powder to simulate the deposits found in steam generator crevices. Stress is applied by pressurizing the tube to 2800 psi. An analysis of solutions extracted from the crevice indicate that the crevice chemistry is 30 percent NaOH at a pH of 10.1. Early results show current transients suggesting the occurrence of SCC. This run will be continued until the tube is depressurized by a through-wall crack. After the run a metallographic evaluation will be performed to identify the SCC and other corrosion damage in the tube.

**Planned Activities**

The present strategy for mitigating IGA/SCC is based on the assumption that the crack initiation and propagation rate in Alloy 600 steam generator tubes in T/TSP crevices depend only on pH and the electrochemical potential. Planned work will examine the pH and electrochemical potential dependence of IGA/SCC in Alloy 600. The plan is to adjust the pH in the heated crevices from the caustic condition now used to lower pHs. This will be accomplished by replacing the presently used 40 ppm NaOH feedwater with feedwaters having progressively lower $Na^+/Cl^-$ ion ratios. Computer codes indicate that the pH of the concentrated crevice solutions decrease as the $Na^+/Cl^-$ ion ratio in the feedwater decreases. Crevice chemistries will be determined by chemical analysis of solutions extracted from the crevice. The crevice chemistry results will be used to benchmark the EPRI computer codes used by utilities to calculate crevice chemistry and crevice pH.

Planned work will also examine the effectiveness of the present practice of adding hydrazine to the feedwater to inhibit the initiation and propagation of IGA/SCC. The hypothesized rationale for adding hydrazine is that it lowers the ECP of the crevice chemistry to a regime where IGA/SCC does not occur. Measurements will be made of IGA/SCC and ECP at various pH with air saturated feedwater and with hydrazine added to deaerated feedwater.

Signal analysis and other data analysis procedures will be developed for the EN technique. The analysis will model the transition from microcracks to macrocracks and crack propagation processes. This will enable steam generator crevice monitoring for the initiation and severity of IGA/SCC.

# Interfacial Transport Phenomena and Stability in Molten Metal-Water Systems

PI: M. Corradini, University of Wisconsin-Madison (UW)

Collaborators: Argonne National Laboratory (ANL)

Project Start Date: August 1, 1999 Projected End Date: August 31, 2002

Project Number: 99-0233

## Research Objectives

One concept being considered for steam generation in innovative nuclear reactor applications involves water coming into direct contact with a circulating molten metal. The vigorous agitation of the two fluids, the direct liquid-liquid contact, and the consequent large interfacial area give rise to very high heat transfer coefficients and rapid steam generation. For an optimum design of such direct contact heat exchange and vaporization systems, more detailed knowledge is necessary of the various flow regimes, interfacial transport heat transfer coefficients, and operational stability under reactor relevant operating conditions. This research projects studies these transport phenomena involved with the injection of water into molten metals (e.g., lead alloys) with the following objectives:

- Design, fabricate and operate experimental apparatuses which investigate molten metal-water interactions under prototypic thermal-hydraulic conditions;
- Measure the integral behavior of such interactions to determine the flow regime behavior for a range of conditions and stability of these flow regimes;
- Measure the local interfacial mass and heat transfer behavior to ascertain the interfacial area concentration and heat transport length and time scales; and
- Analyze test results to determine an envelope of operating conditions, which yield optimum energy transfer between molten metal and water and maximizes stability.

## Research Progress

In its first task of the project, the research team has done a comprehensive review of past experimental investigations, fabricated experimental apparatuses, and developed an experimental plan. Some of the highlights of this work are detailed here. Over the years, experimental studies have been conducted to provide measurements on direct contact heat transfer and vaporization of cold, volatile liquid drops dispersed in a continuous phase of hot liquid. A key measurement of these experimental studies is the evaporation zone height, *L*, which is the approximate height of the continuous phase of the hot liquid needed for complete evaporation of the injected dispersed liquid. This overall height, *L*, is related to the overall volumetric heat transfer coefficient for the evaporation zone, $U_v$, by an energy balance:

$$L\Delta T = (\dot{m}\Delta h)/U_v \qquad (1)$$

where $\dot{m}$ is the mass flux of the dispersed phase, $\Delta h$ is the change in enthalpy of the dispersed liquid to vapor (primarily the latent heat of vaporization of the cold liquid), and $\Delta T$ is the average temperature difference between the injected volatile liquid and the liquid metal pool. This temperature difference between the two fluids is rigorously the log-mean temperature difference (in these initial estimates we use the arithmetic difference). Basically, equation (1) represents a method to determine $U_v$ by measuring the overall height empirically for volatile liquid vaporization and superheat. These past data indicate that the $L\Delta T$ product is constant for a low flow of injected volatile liquids (bubbly flow regime). In the direct contact heat transfer application for innovative liquid metal reactors, the flow regime is expected to be higher flow and churn-turbulent. Thus, the challenge is to measure this overall heat transfer coefficient in this flow regime and use X-ray diagnostics to measure the local area concentration to determine the local heat transfer coefficient.

Two experimental apparatuses were designed and constructed during the first year of the research contract as illustrated below. The ANL and UW facilities, while sharing this common goal, are designed to provide mutually complementary information. The ANL experiments focus on the heat transfer and flow stability behavior of water injected into molten metal and provide measurements on the evaporation zone length and associated volumetric heat transfer coefficients. The UW experiments focus on two-dimensional mixing behavior and provide real-time X-ray imaging of the multiphase structure of vaporizing water in the molten metal. The ANL 1-D and UW 2-D test sections are also expected to generate complementary aerosol data on the geometry effect of the molten metal pool.

**Argonne One-Dimensional Test Apparatus**

**UW Two-Dimensional Test Apparatus and X-ray Imaging System**

**Planned Activities**

Current analysis using a drift-flux model has verified the review of the past investigations and has supported the conclusion for experiments in the churn flow regime. Experimental work is clearly required to determine whether the predicted transition from bubbly to churn flow is correct or not. Moreover, tests would determine whether past data indicate any churn flow behavior are in the transition zone, as well as any potential differences in the observed heat transfer coefficients. The following test matrix is proposed to study such parameters and investigate them more deeply.

| | |
|---|---|
| Water mass flow rate (g/s): 0.5 to 5.0 | Water Subcooling ($^{o}$C): 0 to 70 |
| Melt Superheat ($^{o}$C): 50 to 400 | System Pressure (MPA): 0.1 to 1.0 |

Near term experimental activities also include test preparatory experiments and calibration of the X-ray imaging system for local area and heat transfer measurements:

- Assemble test section, support structure, water suppression tank, metal reservoir.
- Conduct imaging tests with X-ray system to calibrate void detection system.
- Setup power control and data acquisition systems for the first experimental test series.

The initial experimental test series is to begin this calendar year and will be compared to past liquid metal experiments from Japanese investigators.

# Fundamental Thermal Fluid Physics of High Temperature Flows in Advanced Reactor Systems

PI: Donald M. McEligot, Idaho National Engineering and Environmental Laboratory (INEEL)

Collaborators: Iowa State University, University of Maryland, General Atomics, University of Manchester (UK), University of Podgorica (Montenegro), Kyoto University (Japan), Toyama University (Japan)

Project Start Date: August 1, 1999 Projected End Date: September 5, 2002

Project Number: 99-0254

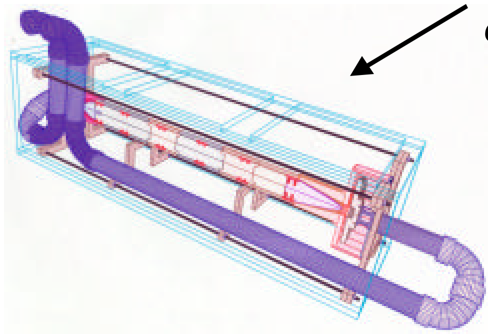
## Research Objective

This laboratory/university/industry collaboration of coupled computational and experimental studies addresses fundamental science and engineering in an effort to develop supporting knowledge required for reliable approaches to new and advanced reactor designs for improved performance, efficiency, reliability, enhanced safety and reduced costs and waste. For small reactors, it addresses remote power and hydrogen generation. This research will provide basic thermal fluid science knowledge to develop increased understanding for the behavior of fluid systems at high temperatures, application and improvement of modern computation and modeling methods, and incorporation of enhanced safety features. The project promotes, maintains and extends the nuclear science and engineering base to meet future technical challenges in design and operation of high efficiency reactors, low output reactors, and nuclear plant safety.

The unique INEEL Matched-Index-of-Refraction (MIR) flow system, the world's largest such facility, is being applied to obtain fundamental data on flows through complex geometries important in the design and safety analyses for advanced reactors for the first time. A graphical representation of the MIR system is shown below. Successful completion of the study will provide the following new fundamental and engineering knowledge, which is not presently available in the literature:

- Time-resolved basic measurements of turbulence quantities (e.g., turbulence kinetic energy and Reynolds stresses) in internal gas flows with large property variation.
- Time-resolved data plus flow visualization of turbulent and laminarizing phenomena in accelerated flow around obstructions (spacer ribs) in annuli.
- Separation of effects of phenomena – buoyancy, property variation, and acceleration – occurring in strongly-heated gas flow to evaluate their individual importance and consequent flow behavior (by application of Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS)).

***World's Largest Matched-Index-of-Refraction Flow System***



*Ribbed annulus*

*Ribbed annulus mixing and impingement*

- Application of DNS and LES for the first time to complex turbulent flows occurring in advanced reactors.
- Fundamental data of internal turbulence distributions for assessment and guidance of Computational Thermal Fluid Dynamic codes proposed for advanced gas cooled reactor (AGCR) applications.

## Research Progress

- Heat transfer and fluid flow in advanced reactors: Six areas of thermal hydraulic phenomena in which the application of Computational Fluid Dynamic techniques can improve the safety of advanced gas cooled reactors have been identified.
- Complex flow measurements: Conceptual experimental models were developed for laser Doppler velocimeter measurements in the MIR flow system to examine flow in complex core geometries (ribbed annular cooling channels and control rod configurations) and in the transition from cooling channels to formation of jets issuing into a plenum. The initial experimental model is a ribbed annulus forming an annular jet exhausting into the MIR flow system. This model was designed, fabricated, and tested with the MIR system. The second experiment addresses two-

stage jet transition from generic coolant channels to a plenum; preliminary design of experiment and auxiliary flow control system has been completed.

- DNS development: DNS of laminarizing gas flow has been completed; subturbulent case initiated.
- LES development: Preliminary LES results have been obtained for vertical upward flow of air in a channel heated on one side and cooled on another; such a channel flow corresponds closely to the flow in an annular passage with a large radius ratio. This work is the first known LES study of a vertical flow accounting for buoyancy and variations in fluid properties.
- Multi-sensor probe development: Completed the design and construction of a four-sensor miniaturized probe. A calibration and testing facility has been designed and constructed for testing these probes.
- Mixed convection: Circular tube test facility in operation with a vertical, heated section providing either specified distributions of heat flux or temperature along the tube with air flow in either the upward or downward direction. Measurements of mean velocity and temperature profiles in the radial direction have been obtained near the exit for the upward flow case under buoyancy-influenced conditions at Reynolds numbers from 6,000 to 20,000.

**Planned Activities**

- DNS and LES development: Work will continue.
- Complex Flow Measurements: laser doppler velocimeter (LDV) measurements of velocities and turbulence will be conducted with the initial model. The second experiment will be fabricated.
- Mixed Convection and Multi-sensor Probes: Three experiments emphasizing buoyancy effects are planned. The first obtains data on velocity in strongly heated air flow through a heated pipe under conditions of mixed convection to determine the effects of buoyancy forces combined with property variation on local mean velocity and turbulent fluctuations. A second experiment would measure the influences of the temperature dependence of fluid properties and buoyancy for air flowing in an annulus. The third will measure local mean velocities and turbulent fluctuations.

# An Innovative Reactor Analysis Methodology Based On a Quasidiffusion Nodal Core Model

PI: Dmitriy Y. Anistratov, Texas A&M University

Collaborators: Oregon State University, Studsvik Scanpower, Inc.

Project Start Date: August 1999 Projected End Date: September 2002

Project Number: 99-0269

## Research Objectives

The present generation of reactor analysis methods uses few-group nodal diffusion approximations to calculate full-core eigenvalues and power distributions. The cross sections, diffusion coefficients, and discontinuity factors (collectively called “group constants”) in the nodal diffusion equations are parameterized as functions of many variables, ranging from the obvious (temperature, boron concentration, etc.) to the more obscure (spectral index, moderator temperature history, etc.). These group constants, and their variations as functions of the many variables, are calculated by assembly-level transport codes. The current methodology has two main weaknesses that this project will address. The first weakness is the diffusion approximation in the full-core calculation; this can be significantly inaccurate at interfaces between different assemblies. This project will use the nodal diffusion framework to implement nodal quasidiffusion equations, which can capture transport effects to an arbitrary degree of accuracy. The second weakness is in the parameterization of the group constants; current models do not always perform well, especially at interfaces between unlike assemblies. The project will develop a theoretical foundation for current models and use that theory to devise improved models. The new models will be extended to tabulate information that the nodal quasidiffusion equations can use to capture transport effects in full-core calculations.

## Research Progress

Homogenization and Group Constants Functionalization: During the first year, part of the research efforts were concentrated on studies of the problem in one-dimensional geometry in order to develop basic ideas of functionalization and homogenization procedures. To model reactor physics phenomena of interest, first a code was developed for solving one dimensional (1D) one-group eigenvalue neutron transport problems based on the quasidiffusion (QD) method. Then a code was developed for solving 1D multigroup transport problems by means of the QD method.

Certain approaches have been formulated for spatial assembly homogenization that are based on consistent discretization spatially averaged QD low-order equations and their fine-mesh discretization. The homogenization procedure must preserve the averaged reaction rates, surface-averaged group currents, and eigenvalue. The homogenization fits naturally into the framework of the QD method that is based on the idea of successive averaging of the transport equation over angular and energy variables. The averaging over spatial variables is the next logical step. An approach has been developed for exact spatial averaging of the discretized QD low-order equations and generating a coarse-mesh discretization that is exactly consistent with the given fine-mesh discretization. The developed technique can be applied to any number of spatial zones. This is a rigorous mathematical result. The proposed method uses the quantities that are similar by their definitions to discontinuity factors, however, the resulting solution preserves continuity of both the scalar flux and the current on interfaces. The procedure of spatial decomposition based on albedo boundary conditions was formulated. The proposed methodology creates a theoretical background for homogenization of spatial regions. The presented approach of consistent coarse-mesh discretization can be extended to multigroup and multidimensional problems, as well as to different kinds of discretization methods. These results were presented at the Winter ANS Meeting 2000 in Washington D.C. and published in its transactions.

Numerical Method for Solving Two Dimensional (2D) QD Low-Order Equations: During the first year of this project, effort has been focused on developing nodal solution techniques for the quasidiffusion low-order equations (QDLO) in x - y geometry. There are several important differences between these equations and the standard neutron diffusion equation. First, the neutron current is equal to the gradient of the QD tensor times the scalar flux, rather than using a standard diffusion Fick's law representation and, second, this QD tensor is a complex function of space, in that it is computed directly from the solution of the transport equation. The partial differential equation (PDE) associated with the QD low-order equations is much more challenging to work with than standard diffusion, especially in the context of advanced nodal discretizations.

Initially, the focus was on using standard polynomial based nodal techniques (namely the QPANDA method) with the QDLO equations. In the QPANDA approach, the diffusion equations within a node are transverse-integrated to generate coupled one-dimensional diffusion equations. These transverse-integrated fluxes are then approximated by a fourth-order polynomial expansion, and the resulting systems of equations are then solved iteratively. Project researchers attempted to apply the QPANDA technique to the QDLO equations in two ways. First, all the leakage terms were treated implicitly; i.e., leaving the equations in coupled x - y form and second, by treating the leakage terms semi-implicitly, causing each direction to be decoupled, but with an extra level of iteration on the transverse leakage terms. Then the nodal discretization techniques were fundamentally changed by adopting instead the combination polynomial-analytic nodal method that was shown to provide the accuracy needed in the simulation of mixed oxide-uranium oxide fueled reactor cores.

The non-linear marching method was also evaluated—a solution technique designed for use with the QDLO equations with a finite volume discretization, as a potential solution strategy for the nodal QDLO equations. It was discovered that the added complexity of the nodal discretization made the non-linear marching method less desirable than standard iterative techniques.

**Planned Activities**

Research activities will focus upon two areas—the full-core few-group diffusion-like calculation and the assembly-level many-group transport calculation—and upon the interface between them. Work will proceed on developing homogenization procedures as well as methodologies for functionalization of data based on single-assembly calculations. The effects of an unlike neighboring assembly upon a given assembly's group constants must be accurately estimated without knowledge of the neighbor. Capturing such "interface effects" is one of the major issues studied on this project. The developed methodologies will be applied to multidimensional geometries. Research will proceed on advanced discretization schemes for the multidimensional quasidiffusion low-order equations that will enable researchers to efficiently solve reactor physics problems of core designs with MOX fuel.

# Radiation-Induced Chemistry in High Temperature and Pressure Water and Its Role in Corrosion

PI: David M. Bartels, Argonne National Laboratory

Collaborators: Atomic Energy of Canada LTD - Chalk River Laboratories

Project Start Date: August 1999 Projected End Date: August 2002

Project Number: 99-0276

## Research Objective

Commercial nuclear reactors essentially provide a source of heat, used to drive a "heat engine" (turbine) to create electricity. A fundamental result of thermodynamics shows that the higher the temperature at which any heat engine is operated, the greater its efficiency. Consequently, one obvious way to increase the operating efficiency and profitability for future nuclear power plants is to heat the water of the primary cooling loop to higher temperatures. Current pressurized water reactors run at roughly 300$^oC$ and 100 atmospheres pressure. Designs under consideration would operate at 450$^oC$ and 250 atmospheres, i.e., well beyond the critical point of water. This would improve the thermodynamic efficiency by about 30 percent. A major unanswered question, however, 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 direct measurement of the chemistry in reactor cores is extremely difficult, if not impossible. The extreme conditions of high temperature, pressure, and radiation fields are not compatible with normal chemical instrumentation. There are also problems of access to fuel channels in the reactor core. For these reasons, theoretical calculations and chemical models have been used extensively by all reactor vendors and many operators, to model the detailed radiation chemistry of the water in the core and the consequences for materials. The results of these model calculations can be no more accurate than the fundamental information fed into them, and serious discrepancies exist between current models and reactor experiments. The object of this research program is to generate the necessary radiation chemistry data (yields and reaction rates) needed to accurately model chemistry in both existing water-cooled reactors, and the higher temperature reactors proposed for the future. This will allow engineers to define the optimum chemical conditions conducive to long life of the primary heat transport system.

## Research Progress

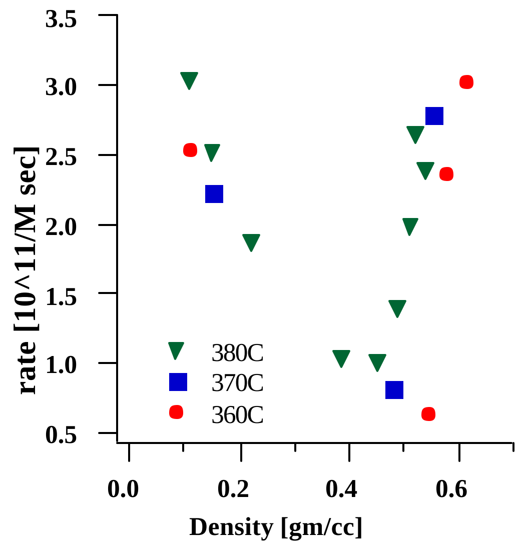
Irradiation of water produces mostly $H_3O^+$, OH radicals, and solvated electrons—$(e-)_{aq}$ . Using the Argonne Chemistry Division's 20MeV electron linac, a short pulse can be used to create a high concentration of these species for kinetic studies. The solvated electron absorbs intensely in the visible and near-IR, making it easy to detect even on subnanosecond time scales. Reaction rates are measured by monitoring how fast the absorption disappears in the presence of a scavenger. In the first year of the project, researchers have focussed on measuring the spectra and some reactions of this important species.

Cell Design: As the necessary first step, a flow system was constructed for the experiment in order to allow signal averaging of solutions, and also to allow fast analysis of products after the irradiation. The intention is to analyze products with liquid chromatography methods, using the pulse radiolysis as the “injector.” Typically two HPLC pumps provide flow of pure water and a scavenger solution, which is mixed in a "T" before the cell. The flow rate of 2-10 ml/minute is sufficient to flush the cell quickly and also maintain the pressure drop in a back pressure regulator or capillary after the cell. The most difficult aspect of the experiment is to maintain stable flow conditions inside the cell. If the temperature of water entering the cell is not the same as water already inside, schlieren effects scatter the analyzing light very severely. Details of the entire apparatus have been published as the first "deliverable" of the project.

Solvated Electron Spectrum: The strongest absorption induced by irradiation of supercritical water is that of solvated electrons, and it is natural that efforts begin with a study of its spectrum. Extinction coefficients of this species will be needed to determine second order recombination reaction rates in a later study. A great deal can already be learned about the electron solvation environment and energetics just from the shape of the spectrum.

Solvated electron spectra were recorded in heavy water at various temperatures from 300 to 450 degrees. The temperature shift of the maximum absorption, roughly –.0028eV/ deg K, is similar to that found by other workers. Above $300^oC$, the spectrum becomes sensitive to the pressure (i.e., density) as well as the temperature. Data from a series of spectra recorded at different densities at $380^oC$ (just above the critical temperature) showed the spectrum shifting to the red as density (pressure) is decreased, just as observed for solvated electron spectra in other liquids.

Reactions with $O_2$: The figure below shows the first measurements of reaction rate for electrons with the oxygen molecule in supercritical water. At temperatures below $300^oC$ in liquid water this reaction obeys a "normal" Arrhenius law, but close to and above the critical temperature the rate is a strong function of density. A qualitative explanation of this behavior might be found in the hydrophobic nature of the $O_2$ molecule. At low density it is expected that the negatively charged $(e-)_{aq}$ will be clustered with water molecules, but the hydrophobic $O_2$ molecule will be found in the voids between clusters. As density is increased the clusters around $(e-)_{aq}$ should become larger. The clustered water molecules may simply prevent the hydrophobic $O_2$ from approaching the electrons, presenting a “potential of mean force” barrier, so the reaction rate goes down as clusters get larger. At some point the density becomes large enough that transient clusters merge into a more continuous medium. Then the reaction rate increases again to approach the high-density liquid limit as extrapolated from lower temperature Arrhenius plots. Based just on this initial study, it is clear that simple extrapolation of lower-temperature reaction rate data for the purpose of making model predictions in reactor cores will not be possible.




**Rate constant for reaction of solvated electrons with $O_2$ at several temperatures as a function of water density.**

**Planned Activities**

Additional experiments in progress include final precise measurements of the electron spectra at selected temperatures and pressures, some further $O_2$ reaction rates, and a similar investigation of $SF_6$ reaction rates with the solvated electron. (Similar density effects appear to apply to this reaction.) Publications on the spectra and oxygen reactions are in preparation. A survey of reactions of the hydrated electron with numerous solutes including $NO_3^-$, $NO_2^-$, $N_2O$, $Fe_3^+$, and $Ni_2^+$ can now be carried out in a routine fashion. A very important reaction to measure is the solvated electron with hydronium ion (acid), which cannot be introduced into the normal high pressure cell for fear of corrosion. The project team has built a second cell with special acid-resistant coating for the purpose of measuring this reaction.

A reaction of critical importance to understanding the kinetics at elevated temperatures is the bimolecular recombination of hydrated electrons:

$(e-)_{aq} + (e-)_{aq}$ ? $H_2 + 2\,OH^-$

Project researchers will be building equipment to allow high-pressure hydrogen-saturated water to be pumped into the cell in order to measure this reaction, and also the reaction of OH radicals with $H_2$. The latter reaction is the key to suppression of corrosion effects in the primary heat transport system of a nuclear reactor.

# Novel Concepts for Damage-Resistant Alloys in Next Generation Nuclear Power Systems

PI: S.M. Bruemmer, Pacific Northwest National Laboratory

Collaborators: General Electric Corporate Research & Development, University of Michigan

Project Start Date: August 1, 1999 Projected End Date: August 31, 2002

Project Number: 99-0280

## Research Objective

The objective of the research is to develop the scientific basis for a new class of radiation-resistant materials to meet the needs for higher performance and extended life in next generation power reactors. New structural materials are being designed to delay or eliminate the detrimental radiation-induced changes that occur in austenitic alloys, i.e., a significant increase in strength and loss in ductility (<10 displacements per atom (dpa)), environment-induced cracking (<10 dpa), swelling (<50 dpa), and embrittlement (<100 dpa). Non-traditional approaches are employed to ameliorate the root causes of materials degradation in current light water reactor (LWR) systems. Changes in materials design are based on mechanistic understanding of radiation damage processes and environmental degradation and the extensive experience of the principal investigators with core component response.

## Research Progress

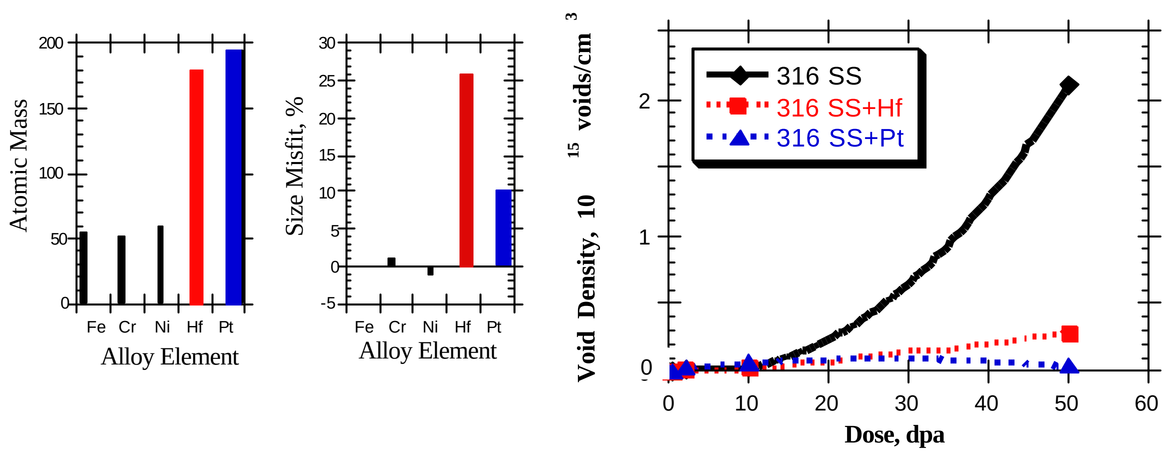
Phase 1 research has focused on the lattice perturbation mechanism for damage resistance. Alloy fabrication for heavy-ion, proton and neutron irradiations, and for stress corrosion cracking (SCC) testing, was completed. Three sets of Ni-ion irradiations (to various dose levels) were conducted and microstructures characterized by transmission electron microscopy. These experiments are being used to establish direction for further studies using protons and neutrons. The proton irradiation source was upgraded for this high-dose study and the first series of samples were irradiated. Stress corrosion crack growth rates have been established in high-temperature water environments for strengthened, non-irradiated stainless steels. The tests on the intermediate strength stainless steel were completed.

### Materials Processing

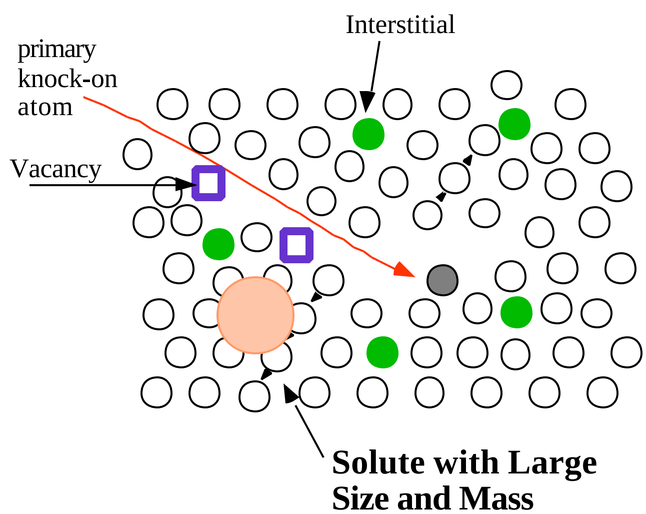
- Alloys were successfully fabricated having the optimum small grain structure with grain interiors of low network dislocation density. Research alloys were fabricated from button melts of pure metals. Alloy samples were processed to achieve the desired sheet form and grain microstructure for subsequent irradiations.

Irradiations

- Charged particle irradiation techniques were enhanced to enable the high-dose conditions needed for the project. In particular, the $Ni^{++}$ ion irradiation technique was improved to produce uniform temperatures and beam flux over a large sample area and reach very high radiation doses. Stainless steel samples were irradiated to a series of irradiation doses from 0.5 to 50 dpa. The proton accelerator system was upgraded to increase the maximum beam current by more than 3 times. Initial irradiations were completed at 5 dpa.




**Solute additions of large mass and size misfit have been shown to suppress radiation damage in stainless steels. Similar behavior between Pt and Hf alloys suggests that atomic mass (cascade production) is more important than atomic misfit (point defect trapping) for nucleation of voids.**




**Minor additions of massive oversized solute are being explored to delay or eliminate detrimental radiation-induced material changes. Next generation water reactors will require damage resistance to very high irradiation doses.**

Materials Characterization

- Techniques for reliable examination of near surface regions were optimized for the $Ni^{++}$ ion samples and defect microstructures were characterized. Transmission electron microscopy revealed distinctly different microstructural evolution paths for the base stainless steel alloy compared to the alloys with small platinum or hafnium additions. Dislocation loop development and void development were affected indicating that large misfit solute atoms can alter the formation of detrimental microstructures by modifying defect recombination, migration, and aggregation.

Mechanical Behavior and Stress Corrosion Cracking

- Reliable stress corrosion crack growth rate measurements on stainless steels in high-temperature water (290 to 340$^oC$) were established at low growth rates. Unexpectedly, an increase in matrix strength alone was demonstrated to promote intergranular stress corrosion cracking in both oxidizing and non-oxidizing environments. Detrimental changes in grain boundary composition were not required for cracking. This result is the first step toward isolating radiation strength effects on stress corrosion cracking from other radiation-induced material changes.

**Planned Activities**

In Phase 2, property evaluation of lattice-perturbation alloys studied in Phase 1 will be continued with an emphasis on the proton-irradiated materials. The ability of the large misfit solutes to alter the evolution of detrimental microstructures and effects on irradiation-assisted stress corrosion cracking will be evaluated. Additional charged particle irradiations will be performed as needed to establish radiation resistance to very high dose levels. Strength effects on stress corrosion crack growth will be quantified in the non-irradiated alloys and compared to cracking for irradiated stainless steels. Research will begin on the metastable precipitate alloys that are tailored to alter radiation-induced material changes and improve properties. New alloys will be fabricated and heavy-ion irradiations will be conducted.

# Advanced Ceramic Composites for High-Temperature Fission Reactors

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|---|---|---|
| PI: | Russell H. Jones, Pacific Northwest National Laboratory | |
| Project Start Date: | August 1, 1999 | Projected End Date: August 31, 2002 |
| Project Number: | 99-0281 | |

## Research Objective

This research seeks to develop the understanding needed to produce radiation-resistant SiC/SiC composites for advanced fission reactor applications. Structural and thermal performance of SiC/SiC composites in a neutron radiation field depends primarily on the radiation-induced defects and internal stresses resulting from this displacement damage. The researchers are working to develop comprehensive models of the thermal conductivity, fiber/matrix interface stress and mechanical properties of SiC/SiC composites as a function of neutron fluence, temperature, and composite microstructure. This model will be used to identify optimized composite structures that result in the maximum thermal conductivity and mechanical properties in a fission neutron field.

## Research Progress

Task 1 (Develop a Model of Radiation Effects on the Dimensional Stability of Monolithic SiC) accomplishments are as follows:

- Development of a method for calculating spectral-averaged displacement cross sections for SiC using the SPECOMP code to integrate the numerically determined displacement functions in SiC over the spectrum of recoil atom energies for a given neutron energy. The spectral averaged displacement cross section for a specific neutron field is then obtained by integrating over the spectrum of neutron energies.

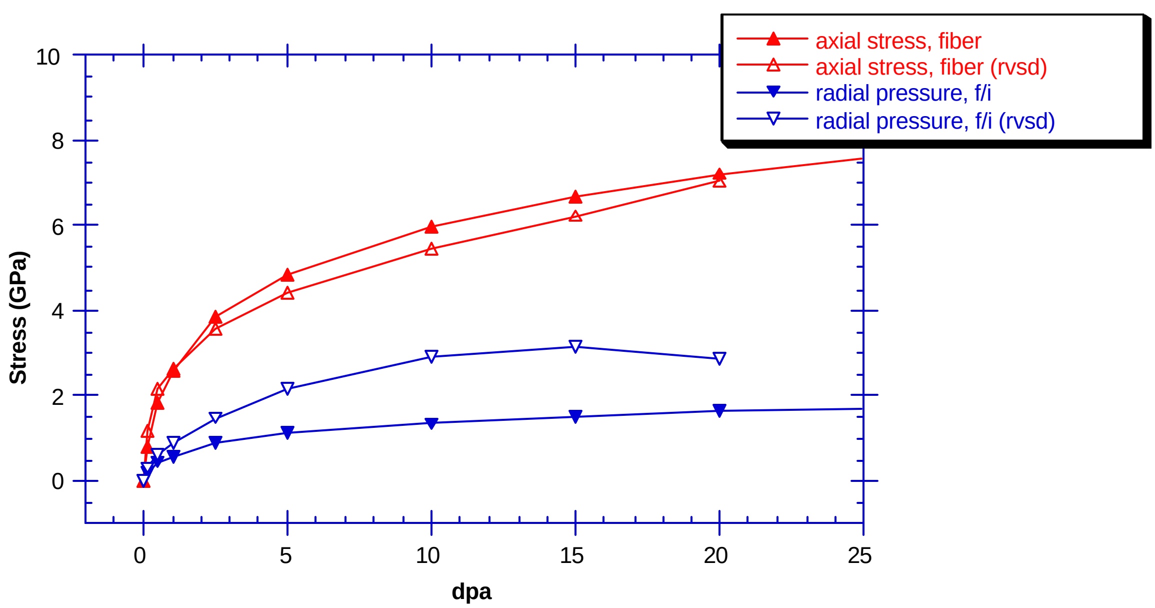
- The transmutation of atoms under neutron irradiation can significantly affect material properties. Transmutation can lead to production of gaseous impurities, especially He and H through (n, $\alpha$) and (n,p) reactions, respectively. Helium may play an important role in the dimensional stability of SiC. Transmutation also leads to production of substitutional and interstitial impurity atoms, and the burnout of the original material. Transmutation calculations were performed for pure SiC irradiated in the neutron spectra of the fast reactor EBR-II and the mixed spectrum reactor HFIR using the REAC-3 code with FENDL-2.0 nuclear cross sections.

Task 2 (Develop a Model of Radiation Effects on the Dimensional Stability, Internal Stress and Thermal Conductivity of SiC/SiC Composites) accomplishments include:

- SiC fibers are either prepared from polymer precursors or SiC powders so their dimensional stability is not identical to that of monolithic SiC. All existing data on the dimensional change due to neutron irradiation for all available SiC fibers has been collected and reviewed. A mathematical description of the dimensional change of these fibers has been derived as a function of neutron fluence, temperature, and fiber type.

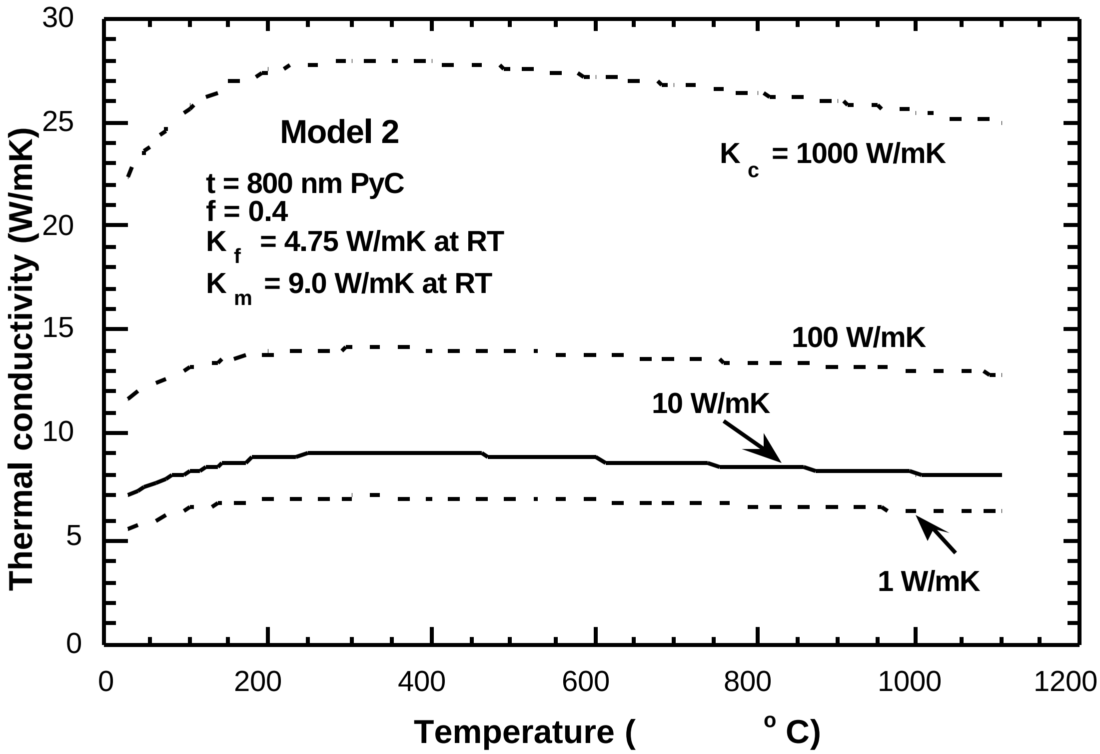
- Interphases between the fiber and matrix are critical to the dimensional, thermal, and mechanical performance of SiC/SiC composites. Evaluation of the response of various phases of carbon to neutron irradiation was carried out. Carbon interphases exist as amorphous, turbostratic or graphitic forms. The data for the irradiation effects on dimensional changes for all forms of C have been reviewed with consideration of anisotropic effects. It is known that the graphitic form of C exhibits considerable anisotropic swelling from the formation of defect clusters on the basal plane. Concepts for beneficial use of this anisotropy to minimize the stress between fibers that shrink and a matrix that swells were evaluated.

- Preliminary formulation of a 3-cylinder dimensional change/interfacial stress model was developed to examine the dissimilar dimensional changes between the fiber, interphase and matrix resulting from neutron irradiation that leads to internal stress between these composite components. The preliminary results for the stress between the fiber and matrix that develops during irradiation are demonstrated below.




**A comparison of stresses predicted for Hi-Nicalon fibers in a silicon carbide matrix composite with a carbon interphase.**

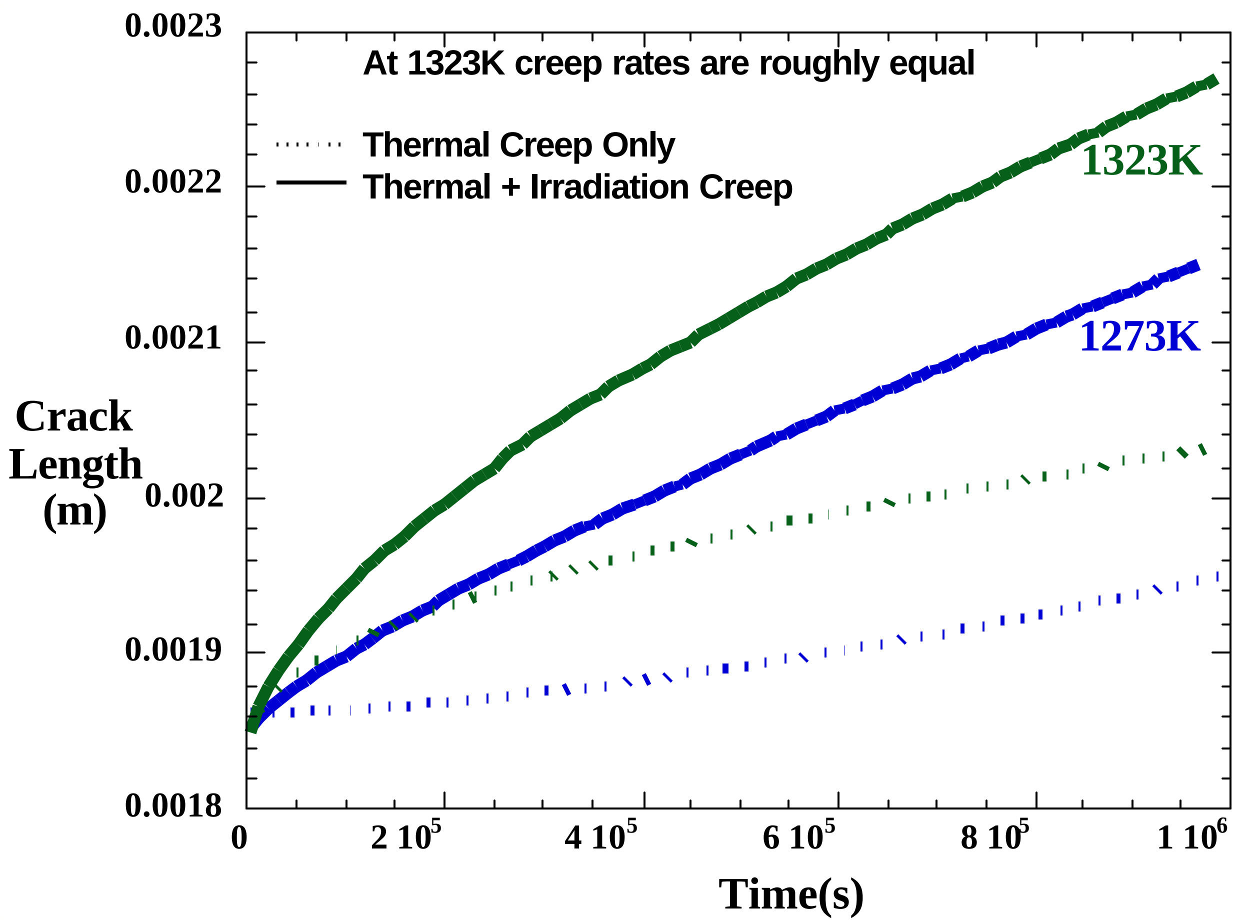
- Models for predicting the effective-transverse, thermal conductivity of SiC/SiC composites were evaluated and compared to experimental data. The modeling effort demonstrated the strong dependence of the composite thermal conductivity on the interphase conductance, $K_c$, which are in turn dependent on the interphase thermal conductivity, bonding to the matrix and phonon coupling between the matrix/interphase and interphase/fiber. An example of the model calculations is shown in the graph below.




**Model predictions of $K_{eff}$ for a 2D-Hi-Nicalon/PyC/SiC composite when the PyC fiber coating has a 800 nm thickness.**

Task 3: (Model the Mechanical Properties of Irradiated SiC/SiC Composites ) accomplishments include:

- A dynamic crack-growth model has been developed to predict crack growth in ceramic composites containing creeping fibers in an elastic matrix. Mechanics for frictional bridging and both linear and nonlinear fiber-creep equations are used to compute crack extension dynamically. Thermal creep of polymer derived ceramic fibers is often nonlinear, or viscous-like, in time and stress, but irradiation creep of these same fibers appears to be linear in both time (dose) and applied stress. Accordingly, we used a standard thermal creep equation and a simple irradiation creep equation suitable for SiC-based fibers and generated some model results for two test temperatures, 1273 and 1373K (1000 and 1100 Centigrade). The thermal creep equation has an activation energy of about 600 kJ/mol. The irradiation creep equation assumes a temperature independent regime below 1173K (900 C) and an activation energy of 50 kJ/mol for temperatures greater than 1173K. The creep rate is linear in dose rate and stress. We obtain the following results from the model.




**Model result in terms of crack length as a function of time for the indicated test temperatures. We observe that irradiation creep of the fibers dominates the fiber deformation process for temperatures below 1273K (1000 C) but thermal creep dominates at higher test temperatures. This implies that we will need to further understand and model irradiation creep processes in SiC-based fibers since apparently that process is important in applications, such as fission reactors, that operate at or below 1000 C.**

## Planned Activities

The relationship between radiation damage, displacements per atom, chemical transmutations, and fluence will be established for an HTGR neutron spectrum. The thermal conductivity model will be used to identify composite microstructures with optimized thermal conductivity. A concentric cylinders model was used to determine the stresses in a three constituent system: fiber, interphase, and matrix but the preliminary model needs further development to include dimensional change with various C interphase microstructures. The concentric cylinders model and data on the irradiation creep of fibers will be utilized with PNNL's creep crack growth model to predict the creep behavior of SiC/SiC composites in a neutron field with the combination of thermal, irradiation and oxidation enhanced creep crack growth.

## 8. FY 2000 NERI RESEARCH AWARDS

The following abstracts summarize the NERI research awards for FY2000.

## 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: 00-0014

The thorium-U-233 fuel cycle promises a number of benefits relative to the conventional U-Pu cycle for commercial reactors, including reduced plutonium generation/enhanced proliferation resistance, reduced waste generation per unit energy production and reduced toxicity characteristics of the spent fuel. Heterogeneous assembly and/or core design options allow the flexibility needed to maximally realize the potential benefits of this cycle; this work is therefore complementary to a study of homogeneous approaches currently underway by a team headed by Idaho National Engineering Laboratory (INEEL). The assessments concentrate on key measures of performance, including: proliferation characteristics of the spent fuel focusing on quantity and quality of weapons usable material produced, fraction of power generated in U-233, safety, cost, and the characteristics of the waste stream. Key to this evaluation is the identification of any feasibility "go-no-go" issues, as well as areas requiring further study. The focus of the investigations will be on current and advanced pressurized-water reactor (PWR) designs (e.g., AP600 with its 19x19 fuel assembly), with the ability to retrofit into the envelope of a standard 17x17 fuel assembly, and utilize available control and burnable designs viewed as a positive attribute; some limited examination of “clean-slate” concepts will be performed as time and resources permit.

## Study of Cost Effective Large Advanced Pressurized Water Reactor that Employs Passive Safety Features

PI: J. W. Winters, Westinghouse Electric Company LLC

Project Number: 00-0023

Market analysis of the U.S. market indicates that a new electric generating facility must have an overnight capital cost of approximately $1000/kw. More importantly, the generating cost must be less than $0.03/kw-hr, when such factors as an attractive return on investment and payback period are considered. Industry executives indicate that any new nuclear plant must be able to compete in the deregulated generation wholesale marketplace and provide a return to the shareholders.

Against this standard, the costs of Generation III nuclear power plants (ABWR, AP600, System 80+) are too high. For example, Westinghouse Electric Company has designed an advanced 600 MWe Generation III nuclear power plant called the AP600. The AP600 has recently received Design Certification by the Nuclear Regulatory Commission when it formally approved the final rule amending 10 CFR Part 52 to certify the AP600 standard plant design. The overnight capital cost for the first AP600 plant is estimated to be between $1300-1500/kw depending on the site selection. This places the AP600 as the most cost effective nuclear power option (Generation III or other) available for deployment in the world today. It is, however, too expensive to compete in the U.S.

Implementation of aggressive cost reductions combined with conventional, state-of-the-art power upratings could potentially realize a 10% decrease in the $/kw for a Generation III plant. This still will not place its cost within the competitive range. Therefore if nuclear power is to be commercially attractive in the U.S. in the next 5-7 years, a dramatic decrease in the capital cost of a Generation III plant is necessary. This program is to complete a feasibility study and perform design activities to increase the power output of an AP600 to at least 1000 MWe while preserving the design and licensing basis of the plant. This will require innovative engineering solutions to design issues associated with increasing the power output of the AP600. By increasing the generating capacity of the AP600 to this level while incurring not more than an additional $50 million in capital cost, the overnight capital cost of this Generation III+ plant will be dramatically reduced and be competitive to approximately $1000/kw.

The DOE and the nuclear industry have invested heavily in the design and licensing of the so-called Generation III reactors including the AP600, ABWR and System 80+. These plants are ready for the U.S. market today. However, even though the AP600 is the most cost competitive nuclear option available today and is cost-competitive with coal plants, it is still not competitive with combined-cycle natural gas plants in the United

States. Successful implementation of this program would provide the impetus for the industry to realize the rewards of the investment in the Generation III reactors. It will permit competitive, near term deployment of a Generation III+ nuclear power plant. It will be based upon the safest, simplest, most advanced and most cost competitive nuclear plant available today with a Design Certification. It will also be cost competitive in the U.S. market with any available electric energy choice today including combined-cycle natural gas plants.

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

PI: Fred R. Mynatt, The University of Tennessee

Project Number: 00-0047

Development and deployment of a new generation of nuclear electric power plants is urgently needed both within the United States and worldwide. The need for new electric power plants is very evident both to replace old power plants and to expand the power supply. While global warming is widely debated, there is a growing consensus that it is a potential worldwide problem and that generation of greenhouse gases should be avoided in new and replacement electric power plants. It is also clear that new nuclear power plants will not be readily accepted by the public until sufficient changes are evident to resolve economic, safety, waste and proliferation concerns. The public generally accepts nuclear power plants already deployed, but this same public will demand resolution of long-standing problems prior to deployment of new nuclear power plants.

Generation IV nuclear power plant concepts developed in the U.S. Department of Energy (DOE) Nuclear Energy Research Initiative offer the potential for resolving the problems that prevent the deployment of new nuclear power plants. Concepts for compact, modular, power plants have been developed with inherent design features to mitigate proliferation and safety concerns (1,2,3,4,5,6). The biggest concern for these compact plant concepts is economics. Can they be produced at an acceptable cost, and will they facilitate innovative financing and ownership arrangements to make deployment economically feasible?

The purpose of this research project is to develop compact Generation IV nuclear power plant design and layout concepts that maximize the benefits of factory-based fabrication and optimal packaging, transportation and siting. The potentially small footprint of Generation IV systems offers the opportunity for maximum factory fabrication and optimal packaging for transportation and siting. Barge mounting is an option to be considered and will offer flexibility for siting including floating installation, on-shore fixed siting, and transportation to nearby inland sites. Railroad and truck transportation of system modules will also be considered in this work.

## Integrated Nuclear and Hydrogen-Based Energy Supply/Carrier System

PI: David C. Wade, Argonne National Laboratory

Project Number: 00-0060

This proposed three year program of R&D aims to develop an economical, proliferation resistant, sustainable nuclear-based energy supply system suitable for deployment in both industrialized and developing economics in the decades following 2020.

It is based on a modular-sized fast reactor, passively safe, and cooled with heavy liquid metal which supplies high temperature heat to an integrated gas turbine power/process heat chemical plant to generate dual energy carriers - electricity and hydrogen (with optional capability for potable water production from brackish or salt water desalinization).

Innovations and benefits include:

- Flexible mix of energy products - The integrated system is to be compatible with state of the art energy conversion systems (gas turbines, fuel cells, etc.) producing a flexible mix of "billable" product including electricity, high level and low level process heat, hydrogen, oxygen, and fresh water supply (via desalinization). The energy carrier can be stored to meet energy peaking needs, and may be used to power fuel cells for emission-free vehicle propulsion.
- Flexible system capacity - The use of standardized modules for the heat source, hydrogen production, and energy conversion functions enables the system capacity to be sized for small service areas using a single set of modules (300 MWt) or for larger and growing service areas using multiple, coupled sets of modules.
- Economic competitiveness - The nuclear and hydrogen-based energy system is aimed at low capital and operating cost through:
  - Compactness and radical simplification.
  - Modularization and standardization for factory "mass production" and fast site assembly.
  - Long-life core with cartridge refueling (15-30 year interval) and near 100% capacity factor.
  - High fuel energy utilization.
  - High-energy conversion efficiency (~50 percent for hydrogen production, >50 percent for fuel cells).
  - Base load operation and storable energy products (synthetic fuel and potable water).
  - Semi-autonomous operation.

- Sustainability - The system is designed for sustainability:
  - The nuclear fuel source utilization in a fast reactor is sustainable and lessens competition in the electric power, process heat, and vehicle propulsion sectors for other scarce, irreplaceable energy sources.
  - The integrated, nuclear and hydrogen-based energy supply/carrier system essentially eliminates greenhouse emissions in the electric power, process heat, and fuel cell based transportation sectors which it serves.
  - The integrated system reduces waste streams to low level heat and used nuclear fuel, and enables use of "waste" from one process to be a beneficial input to another process.
  - Integration of desalinization into the process system for recovery of "waste" heat and for sustainable production of fresh water for public works, industrial, and agricultural purposes.
  - The nuclear heat source achieves maximum utilization of the nuclear energy resource whether based on the once-through fuel cycle or, where permitted, fuel recycle.
- Proliferation resistance - The defense-in-depth approaches addressing proliferation concerns include:
  - Long-life core with cartridge refueling (15-30 year interval) and no on-site
  - fuel handling equipment.
  - Fuel ownership and (15-30 year interval) cartridge refueling by internationally monitored regional consortium.
  - Fuel facility and material transportation under international, guarded conditions.
  - Fuel protected by a high-level radiation "shield" at all stages.
- Inherent/Passive reactor safety - The liquid-metal-cooled fast reactor incorporates and extends proven inherent and passive safety features based on decades of development of sodium-cooled systems, which are heightened using Pb or Sn heavy liquid metal coolant. The nuclear heat source features:
  - Low power density core.
  - 100 percent natural circulation heat transport (eliminating the loss of coolant flow class of accident initiators).
  - Reactivity coefficients are such to inherently shut the reactor down in case of power-to-flow mismatch.
  - Passive decay heat rejection together with passive system shutdown eliminates concern from "loss-of-heat sink" accident initiators.
  - High boiling temperature of Pb and Sn together with system passive response eliminates core melt accidents.
  - Large fuel rod diameter and very large lattice spacing (eliminates core blockages).
  - Worth of burnup reactivity control system < $1 (eliminates possibility of prompt excursion).
  - Low atmospheric pressure system and use of guard vessel eliminate loss of coolant accident initiators.

- Core compaction is eliminated by integral core design (without subassemblies) and use of spacer grids and recriticality potential is eliminated by fuel, which floats in coolant.
- Seismic isolation is provided in the basic design.
- The reactor and heat transport modules are compact, enveloped by a close-fitting containment, and are located in a silo which can be "hardened" to the extent necessary to protect against external threats.
- The inexhaustible heat sink is site-specific, including atmospheric air, ground, or ground water.
- The coolant and working fluids are separate systems, eliminating possibility of radiological transport to the hydrogen production or energy conversion parts of the plant even in the event of heat exchanger tube rupture (insofar as the working fluid pressure is higher than the reactor system pressure).

This proposal is responsive to the Generation IV/Alternative Power Conversion Cycles element of the NERI call for proposals.

## Development of Design Criteria for Fluid-Induced Structural Vibration to Steam Generators and Heat Exchangers

PI: Ivan Catton, University of California, Los Angeles

Project Number: 00-0062

Present designs of heat exchangers and steam generators in pressurized water reactors (PWR) are based on past designs that worked, over design or difficult to obtain one-of-a-kind expensive empirical data. Although present guidelines provide an ad-hoc solution to the problem of fluid induced vibration, at present a unified approach based on simultaneous modeling of thermal-hydraulics and structural behavior does not exist. As a result designs are overly constrained with a resulting economic penalty. If, on the other hand, less constrained designs are developed, the possibility of occurrence of damaging component vibration exists. The objective of the proposed work is to develop complete models that will delineate stability boundaries for fluid-structural interactions that are supported by laboratory experiments and can be used for steam generator and heat exchanger design avoiding economic penalties resulting from overdesign and conservatisms needed to accommodate safety issues.

A basic study of single and two-phase flow across tube bundles is proposed. The study has both experimental and theoretical components to it. Single-phase studies will involve velocity and pressure measurements in tube arrays. Laser Doppler Anemometry will be used to determine the velocity field. In two-phase flow studies, void profiles in the passages between tubes and pressure distribution around tubes will be measured. Most of the experiments will be conducted on arrays of flexible tubes. The tube arrangement and tube pitch to diameter ratio will be varied parametrically. In the experiments, data for transient fluid force acting on the tube, average void fraction around the tubes, damping factors in two-phase flow, and displacement of the tubes from their initial position will be obtained. Instability maps for the onset of fluid-elastic instability in tube arrays will be developed. To study the effect of stiffness of the flow system, experiments will be conducted with air-water and steam-water mixtures. In the experiments with steam-water mixtures, tubes will be heated to initiate boiling on the tubes.

Theoretical work will include development of constitutive relations and the solution of governing fluid-structure equations with appropriate boundary conditions. Vorticity transport formulation will be used to solve the governing equations numerically. A combination of experimental data and modeling will be used to develop design guidelines that include the functional relationship of stability and the design parameters like tube material, wall thickness, distance between supports and type of support.

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

PI: Donald Miller, Ohio State University

Project Number: 00-0069

The three Generation IV reactor designs currently supported by the DOE have the common characteristic that they are expected to operate up to 15 years with a sealed core. These reactors will be built, operated and disposed of without access to the core, minimizing opportunities for proliferation and for servicing. Monitoring the power distribution and coolant conditions of such a reactor poses a challenge. Serviceable ex-core sensors can only monitor neutron flux on the periphery of the core. Existing in-core sensors do not have sufficiently long lifetimes, with the possible exception of low-sensitivity platinum SPNDs. This research effort proposes to develop a new sensor that is particularly well suited for use in a sealed reactor core, and to apply this sensor to produce a robust in-core monitoring system that is suitable to all three reactor designs

The sensor is fabricated from a small kernel of actual reactor fuel sealed in a metal tube that provides a thermal conduction path to the coolant. A small electric heating element surrounds this fuel/tube assembly. The total heat flux from the fuel kernel and electric heater is measured by differential thermocouples placed on the conduction path. The heater is then controlled by feedback from the thermocouples, such that a constant heat flux is maintained regardless of the nuclear energy generation in the fuel kernel. The input electrical power provided to the heater is thus inversely related to the actual nuclear energy generation. Because the temperature of the sensor remains nearly constant, the sensor will have a better time response than that of a similar uncontrolled sensor.

This controlled calorimeter concept, denoted the constant-heat flux power sensor (CHFPS), is well suited for use in a sealed core. It will give a measure of the local nuclear power generation, including decay heat, so it can be used to monitor thermal limits during operation, post-shutdown, and in permanent storage. The sensor will be fixed to, and will deplete with, the local fuel, so no compensation for depletion will be required. The sensor will simply act like the surrounding fuel over the entire core lifetime. Unlike any other sensor, this sensor is in a feedback control loop. This means that the sensor dynamic response can be monitored, allowing measurement of the heat transfer characteristics of the coolant while simultaneously measuring the generated power. In addition, feedback control combined with modern signal processing techniques offer a means of evaluating the sensor calibration and performance *in-situ.* It is expected that the sensors could operate with substantial degradation given this capability, an important feature in a sealed-core reactor. The basic performance characteristics of this type of sensor, very high sensitivity combined with good bandwidth, have already been proven through testing of an earlier design of controlled calorimetric sensor.

The project team thus proposes to design, fabricate, and test CHFPS sensors, along with the supporting digital control and signal processing capabilities, using fuel materials specific to the DOE-supported Generation IV reactor designs. The sensor design will include a high degree of internal redundancy. This sensor will then be incorporated, with other complementary neutron flux or temperature sensors if advantageous, into an integrated in-core monitoring system with a high degree of external redundancy and *in-situ* diagnostic capability. This final monitoring system is expected to provide a high degree of reliability, safety, operating efficiency, and flexibility for each of the three DOE-supported Generation IV reactors.

## 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: 00-0100

The Modular Pebble Bed high temperature Reactor (MPBR) has been proposed as a candidate to meet future needs of the nuclear industry, due to its safety, high-efficiency, and proliferation resistance. This type of reactor requires a unique on-line fuel burnup monitoring and handling system. This project will conceptually design and experimentally test an advanced on-line fuel burnup monitoring system for the MPBR. Compared with previous designs, this work proposes a novel approach to analyzing pebble bed fuel in real time using combinations of gamma spectroscopy and passive neutron counting of spontaneous fission neutrons in order to provide the speed, accuracy, and burnup range required for the MPBR. The real time results will be used to provide on-line automated go/no-go decision on fuel disposition on a pebble-by-pebble basis. Advanced design concepts included here are not limited to just the counting methods—also included are innovative concepts for handling pebble bed fuel in order to provide the throughput and reliability which this system will require.

## Design and Analysis of Turbo-Machinery and Heat Exchangers for the Gas-Cooled Reactor Systems

PI: Ronald G. Ballinger, Massachusetts Institute of Technology

Project Number: 00-0105

The purpose of this project will be to develop systems analysis tools for the evaluation of turbo-machinery and BOP power conversion in high temperature gas cooled reactor systems. These tools will then be used to develop optimized power conversion systems for 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 which must be addressed in order for such systems to be adequately evaluated 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?

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

PI: L. M. Hively, Oak Ridge National Laboratory

Project Number: 00-0109

A deviation from normal operating conditions may indicate performance degradation or the onset of imminent failure in critical equipment. Real-time monitoring can detect a deviation in process-indicative data. Prompt response is needed to avoid failures, maintain optimal performance, and improve performance savings. Oak Ridge National Laboratory has patented technology for assessment of condition change in complex nonlinear systems. The method is data-driven and makes no assumptions about the underlying process dynamics. One- or multichannel time-serial data is converted to geometric (phase space) representation, which in turn is transformed to a distribution function (DF). The dissimilarity between a nominal base case DF and a test case DF is quantified by robust nonlinear metrics. A significant trend in the dissimilarity measures over time indicates a change in the system's condition and provides forewarning for appropriate response. Next-generation nuclear power plants will have many imbedded sensors in critical equipment, such as turbines, pumps, and valves. These sensors will acquire data, such as vibration (acceleration), motor current, electrical power, and acoustic data for both continuous and transient operations. If successful, this technology will reliably detect condition change and/or forewarn of failure in critical next-generation machinery, allowing just-in-time maintenance to improve plant efficiency, to avoid plant down time, and to eliminate safety faults. This project will be conducted jointly with Duke Engineering & Services, which, will provide operational data and expertise.

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

PI: John A. Becker, Lawrence Livermore National Laboratory

Project Number: 00-0123

The 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. There would be enormous payoffs to the Department of Energy and the country as a whole if such energy sources could be identified and applied to a range of civilian applications.

Despite the potential payoff, efforts in applied isomer research have been rather limited and sporadic. There has been basic research on nuclear isomers since their discovery in 1935 with an occasional hint to tantalize interest in HEDM. In most cases, these hints were refuted by careful examination by other groups.

The project team believes it is time for the Department of Energy to re-examine its strategy in this area. The potential payoffs are large enough to warrant inclusion of applied nuclear isomer research in the U.S. portfolio of high-risk, high-payoff activities. This research proposal details a strategy for such a program. It is in direct response to a call for the fundamental science studying nuclear isomers that could be beneficial for civilian application by DOE/NE (LAB-NE-2000-1). There are several key elements of this strategy, which we propose for the Department's consideration.

- Every effort should be made to leverage the strengths in nuclear physics that exist at the DOE National Laboratories. Appropriate collaborations with university groups should be encouraged.

- A solid base of knowledge about and experimental capabilities in nuclear isomers must be established and maintained. In the current environment, there is a tendency to spend limited resources to refute spurious experimental results. A coordinated program of basic experiments and theory is needed to establish the knowledge base required for civilian applications.

- While the long-term goal includes amassing significant quantities of any new energy source, the Department should not proceed with such production activities until and unless there is compelling, proven scientific evidence that such a source exists.

- The Department needs an independent, expert isomer evaluation capability so that claims of discovery can be checked quickly with the highest precision warranted and policy decision makers are fully and accurately informed.

The project team believes that the needs of the country can be best met by collaboration among the National Laboratories specializing in nuclear physics research. That collaboration would initially involve Lawrence Livermore National Laboratory (LLNL) and Los Alamos National Laboratory (LANL) to form the equivalent of a Virtual National Laboratory on applied nuclear isomer research. The LLNL and LANL co-Principal Investigators will control the scientific direction of this program while LLNL will serve as the administrative lead laboratory for this effort. The collaboration includes nuclear physicists, radiochemists, and atomic physicists with access to unique resources, and it would hopefully become a major element in the Department's arsenal as it attempts to understand the place of applied nuclear isomer research in its overall R&D portfolio. It is expected also to serve as the advocate for appropriate collaborative research among the university community, other national laboratories, and industry.

The isomer research area is rich with possibilities and several areas have been prioritized that are likely to be the most rewarding and fruitful for initial experimental and theoretical investigation because these areas directly bear on important issues: Can the energy stored in nuclear isomers be released on demand? Is the size of the atomic-nuclear mixing matrix element large enough to be useful? Can we initiate quantal collective release of isomeric energy from a crystal? What is the precise energy of the 3.5 eV level in $^{229m}$Th?

The specific target experiments are:

- X-ray induced decay of $^{178m2}$Hf with a sensitivity $10^5$ times recent work.
- Nuclear Excitation by Electronic Transition (NEET): A measurement of the atomic-nuclear mixing matrix element in $^{189}$Os.
- Superradiance in $^{93m}$Nb.
- TEEN (defined as the opposite of NEET): Nuclear isomer energy release in $^{178m2}$Hf.
- Energy and lifetime of the $^{229m}$Th isomeric level at 3.5 eV.